

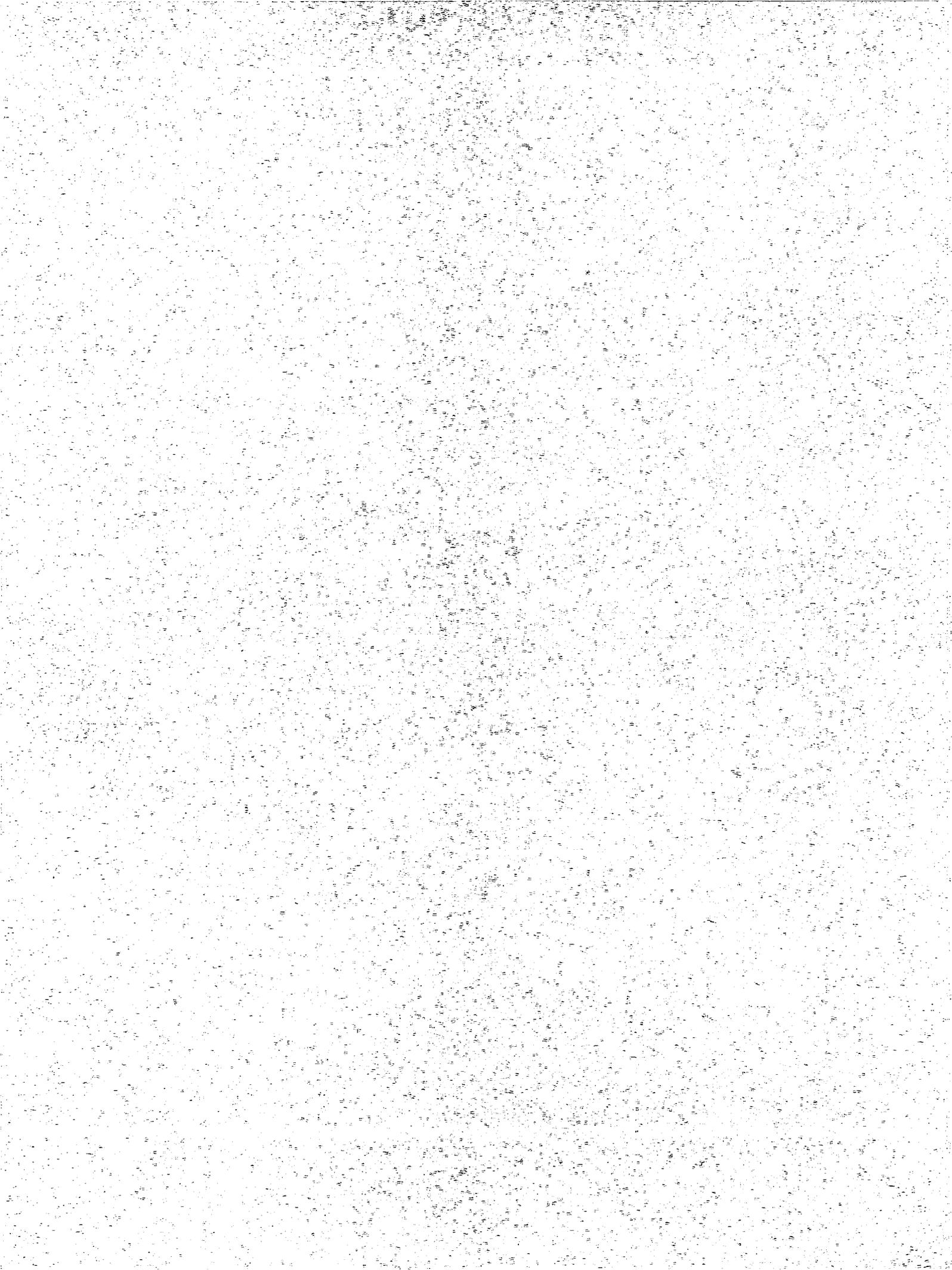
RESEARCH  
DEVELOPMENT  
AND  
DEMONSTRATION  
NEEDS OF THE  
OIL AND GAS  
INDUSTRY

VOLUME

III

**Laboratory  
Capabilities Appendix**

A REPORT OF THE NATIONAL PETROLEUM COUNCIL • AUGUST 1995



RESEARCH  
DEVELOPMENT  
AND  
DEMONSTRATION  
NEEDS OF THE  
OIL AND GAS  
INDUSTRY

V O L U M E

III

**Laboratory  
Capabilities Appendix**

**A REPORT OF THE NATIONAL PETROLEUM COUNCIL • AUGUST 1995**  
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**U.S. DEPARTMENT OF ENERGY**

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**APPENDIX E**  
**LABORATORY CAPABILITIES DATA**



**PART I**  

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**PROJECT SUMMARIES**



# Project Index By Primary NPC Technology Needs Category

May 1, 1995

Page 1

Index	Project Title	Sub-Topics	Funding (\$K)
<b>EXPLORATION</b>			
72	Design of a Robust Numerical Model for Multiphase Flow		150
84	Locating and Numerically Modeling Geopressed Hydrocarbon Reservoirs and Associated Pressure Seals in Soft, Clastic Sediments		440
88	Large Downhole Seismic Sensor Array	3, 14	1200
104	Vertical Seismic Profiling While Drilling	3, 4	300
115	Subsalt Imaging with Marine Magnetotellurics	14, 1	350
134	Integrated Isotopic Studies of Fluid Flow Processes and Time Scales in Sedimentary Basins	1, 7	500
148	Petroleum Geochemistry and Basin Modeling Project	1, 7	1800
166	Synthetic Seismic Data (SSD) Calculations - part of the GONII project	14, 3, 4	500
175	Velocity Analysis, Parameter Estimation, and Constraints on Lithology for Transversely Isotropic Sediments	4, 6, 10, 12	600
181	Massively Parallel Computing	1	1000
192	Facility for Information Management, Spatial Analysis, and Visualization	15, 2	10000
208	Testing Advanced Computational Tools for 3D Seismic Analysis Using the SEG/EAEG Model Dataset	4, 3	775
213	Modeling Ocean Currents and Eddies for Offshore Operations	2	150
216	Gulf of Mexico Sub-Salt Seismic Imaging Project	3, 4	1625
221	New Methods for Modeling and Processing Seismic Data	4, 3	900
226	Society of Exploration Geophysicists Synthetic Seismic Database	4, 3	1500
243	Risk-Based Decision Management		321
275	Exploration Keys Used to Reduce Risk in Exploration Prospect Generation in Selected U.S. Basins		1500
280	Joint High-Performance, High-Resolution Ocean Circulation Modeling for Enhancing Offshore Oil and Gas Exploration and Production	15	350
285	Airborne Geophysical Surveying	8, 15	2405
291	Airborne Remote Sensing of Natural Gas Leaks	8, 10	1065
296	Advance Computational Tools for 3-D Seismic Analysis using the SEG/EAEG Model Dataset	3, 4, 6, 10, 13	2550
311	Experimental and Analytical Geochemistry	7	1890
368	3-D Seismic Imaging of Complex Geologies: Remote and Rapid Processing of Terabyte Data Sets (ACTI)	4, 3, 10, 13	1650
380	Gas and Oil National Information Infrastructure (GONII)	4	4500

Index	Project Title	Sub-Topics	Funding (\$K)
<b>DEVELOPMENT</b>			
64	Microparticle Analysis by Laser Spectroscopy	4, 21	1080
71	Application of Multitracer Technology to Petroleum Reservoir Studies	4, 21	1080
82	Measurement of Fluid Flow and Fluid-Rock Interactions Using Synchrotron Computed Microtomography	5, 18, 22	380
86	Interactive Computer Visualization of TETRAD Results	2	100
107	LBL/Industry Fractured Reservoir Performance Definition Project	10, 14, 29, 30	1300
108	Influence of Clay and Clay Fluid Interaction on Seismic Wave Attenuation in Reservoir Rocks	9, 3, 8, 10	400
110	Effects of Heterogeneity on the Mechanical Properties of Rock	9, 5, 6, 13	300
112	Laboratory and Theoretical Analysis of Transport Paths in Single Natural Fractures	9, 13	300
113	Energy Partitioning of Seismic Waves in Fractured Rock	3, 9, 10, 12, 14	300
114	Application of Guided Waves to the Detection and Characterization of Continuous Flow Units and Bounding Surfaces	3	500
116	Surface-to-Borehole Electromagnetic Surveying (Vertical Electromagnetic Profiling)	10, 14, 17	120
117	Geophysical Measurements Facility	10, 14, 29, 30	400
120	Characterization of Fractured Reservoirs	1, 6, 9, 10, 11, 12	3000
121	Analysis and Reduction of Well Failures in Diatomite Reservoirs	9	350
132	Multifrequency Electromagnetic (EM) Imaging for Reservoir Characterization	10	785
135	Advanced Flux Visualization and Virtual Reality for Reservoir Engineering	25, 30, 31, 33	200
136	Electromagnetic (EM) Imaging through Steel-Well Casing	10, 15	200
137	High-frequency Seismic-Acoustic Imaging	10, 14, 29, 30	1000
138	Subsurface Imaging for Characterizing the Effects of Natural Heterogeneity on Transport Properties	10, 14, 29, 30	1420
141	Definition of Reservoir Heterogeneities	1, 6, 10, 14, 12	799
142	Geothermal Reservoir Engineering	25, 30, 31	2000
152	EQ3/6, Software for Modeling Rock/Water Interactions	23	1500
154	Analysis of Wellbore Stability, Seal Integrity, and Rock Fracture in the Subsurface Using Statistical Models.	8, 9	600
158	Electromagnetic methods for reservoir characterization and process monitoring	10	5500
163	Atomic Scale Electrochemical Modeling	8, 19, 23	800
169	Evaluation of Geologic Specimens with CT	22, 5	7000
172	Oil and Gas Well Log Imaging		2000
174	Laboratory Analysis of Rock Core Using Electrical Resistance Tomography	18	50
176	Optimization Methods for Reservoir Management	33	1500
184	Electrical Resistance Tomography for Subsurface Imaging and Leak Detection	10	1120
187	Computer Simulation of Nuclear Well Logging Devices	15, 14, 20	800

Index	Project Title	Sub-Topics	Funding (\$K)
188	Oil and Gas Data Infrastructure		2500
191	Development of a Uniform Resource Characteristics Service	33	300
196	Mapping Conductive Fractures Using a Through-Tubing Geophone Receiver Array (Slimline Through-Tubing Geophone Receiver Array)	16, 3, 8, 10	780
199	Advanced Sensor Technology for Microholes and Other Seismic Applications	16, 3, 8, 10	225
200	Advanced Instrumentation for Fracture Mapping/Microseismic (Downhole Microprocessor for Mono-cable Telemetry Systems)	16, 3, 8, 10	265
204	National Information Infrastructure Technologies Applied to Database Synthesis and Remote Problem-Solving for the Carpinteria Reservoir Re-Development Project	25,2,6	100
212	Binary Liquid Explosive and Initiator System for Wellbore Applications	10	1000
214	Innovative Gridding and Solution Techniques for High-Performance Reservoir Simulation	25, 1, 27	2100
217	Prepare Information for the Los Alamos/Petroleum Recovery Research Center Electronic Information System as a Means for Communications and Data Transfer to Independent Gas and Oil Producers	33, 25	500
219	Microseismic Fracture Mapping and Determination of Fluid Flow Paths in a Producing Reservoir	16, 3, 8, 10	1500
223	Pore-Scale Flow and Examination of Effects of Scaling on Improved Oil Recovery Processes	25, 5, 8, 30	1400
224	Reservoir Studies and Information Delivery Tools for Independent Oil Producers	25, 33	1600
225	Scale-Up in Heterogeneous Reservoirs	27, 25, 33	175
227	Computer Simulation in Support of Nuclear Well-Logging	14, 16, 20	1200
229	Multicomponent Labeled Tracer Technology: Characterization of Coupled Transport and Chemical Interactions in Petroleum Reservoirs	4, 8, 21, 25, 30	650
231	Sunrise: A National Information Infrastructure Prototype	25,28	3500
232	Parallel Object Oriented Methods and Applications	25,2	1250
234	The Development of a General Reservoir Simulation for Massively Parallel Computers	25	875
235	Advanced Reservoir Management (ARM) for Independent Oil and Gas Producers	25, 28, 33	6500
236	Characterization of Fractured Rock to Produce Remaining Oil in Place.		300
237	Field Demonstrations in High Priority Reservoir Classes	2	17736
238	Integrated Geoscience/Engineering Methods of Optimal Reservoir Upscaling		3827
263	Relative Permeability - Development of Relative Permeability measurement Methodology and Correlations of Pore Characteristics with Multiphase Relative Permeability and Capillary Pressure Functions		1507
271	Imaging Techniques Applied to the Study of Fluids in Porous Media		2163
302	Tracer Technology	4, 21, 23, 24	8000
310	Borehole Geophysical Logging	5, 7, 8, 9, 17, 23	975
335	Fluid/Rock Interactions - Mineral Dissolution and Precipitation Kinetics, Sorption, and Surface Charge Speciation	8	1800
341	Three Component Borehole Seismic Source	10, 3	3160
346	Geomechanics of Petroleum Reservoirs	14, 2, 9, 25, 33	1400

<b>Index</b>	<b>Project Title</b>	<b>Sub-Topics</b>	<b>Funding (\$K)</b>
350	Rock Mechanics Investigations	9, 2, 5, 14, 18	2070
356	Natural Fractures	7, 17, 18	1800
357	Advanced Borehole Seismic Receiver	10, 3	3100
361	Single-well Imaging of Salt Dome Flanks (ACTI)	3, 10	1550
362	Electromagnetic Reservoir Characterization	10, 6, 14	3700
363	Computational Geomechanics for Geologic Structure and Reservoir Mechanics (ACTI)	2	1250
366	Flow Visualization Laboratory for Multiphase Flow Processes	8	5000
370	Seafloor Earthquake Measurement System (SEMS)	9, 3	700

## DRILLING & COMPLETION

29	Mechanical Properties of Materials	8	2000
32	Thin Diamond Films Deposited by Microwave-Enhanced Chemical Vapor Deposition	8	950
70	Geothermal Materials Development	4	1840
83	In Situ Containment and Stabilization of Buried Waste	4	870
160	Design, Testing, and Improved Manufacturing of Well Perforation Devices	5	200
207	Ultrasonic Reduction of Wellbore Deposits and Formation Damage	5, 1, 6	550
218	Coupled Rock/Fluid Mechanics Numerical Simulations Applied to Well Completions	5, 1, 3	1650
222	Perforator Design and Testing	5	150
228	Advanced Perforator Technology	5	1800
230	Multi-Phase Fluid Simulator for Underbalanced Drilling (Hydrodynamic Modeling of Multi-Phase Drilling Fluid Flow to Simulate Underbalanced Drilling)	10, 1, 2, 9, 12, 13	600
242	Drilling, Completion and Re-Completions (Underbalanced Drilling, Wellbore Stability, Coiled Tubing and Slimhole Drilling)		475
332	Advanced Synthetic-Diamond Drill Bit Technology for Hard-Rock Drilling	8	1500
333	Near Wellbore Mechanics (ACTI)	6, 1, 3, 5, 10	1700
340	Acoustic Telemetry	11	2700
343	Downhole Instruments for Slim, High-Temperature Wells	9,11	2000
348	Hydraulic Fracturing Diagnostics	3	3500
353	Slimhole Drilling for Geothermal Exploration and Reservoir Assessment	9	5000
354	Hydraulic Fracturing	3	600
359	Geothermal Drilling Organization	13	2000
367	Increased Effectiveness Of Hydraulic Fracturing Through Advanced Computational Technology (ACTI)	6, 1, 3	825
371	Shallow Directional Drilling Development for Environmental Use	13	1600
378	Lost Circulation Technology	4, 3, 13	3000

Index	Project Title	Sub-Topics	Funding (\$K)
<b>PRODUCTION</b>			
28	Development of Environmentally Acceptable Microbial Corrosion Control Methods	3, 4	525
31	Development of Environmentally Acceptable Microbial Corrosion Control Methods	3	1680
65	Combustion Kinetics & Reaction Pathways	24	3030
78	Mechanisms of Metal-Environment Interactions	3	1820
80	Economic Feasibility of Biochemical Processes for the Upgrading Of Crudes and the Removal of Sulfur, Nitrogen, and Trace Metals From Crude Oil - Benchmark Cost Establishment of Biochemical Processes on the Basis of Conventional Downstream Technologies	18	540
98	Microbial Enhanced Oil Recovery and Reservoir Fundamentals	21	4000
109	Feasibility of Steam Drive in Diatomite	23, 18	400
118	Mechanisms of Mobility Control with Foams	16	1500
123	Optimal Fluid Injection and Producibility in Fractured, Low-Permeability Reservoirs		250
133	Subsidence, Analysis, and Control		200
147	Chemistry of Diatomite Dissolution and Silica Precipitation during Steam Flooding	23, 24	100
155	Corrosion Sensors	3	200
167	Perforation Dynamics in Geological Media	27, 25	700
178	Battery-powered Portable Micro-machined DNA Detector	21	1600
247	Chemical Methods for Improved Oil Recovery		2000
250	Biotechnology for Improved Oil Recovery		2417
261	Gas Flooding Methods for Advanced Oil Recovery		2060
262	Thermal Methods for Advanced Oil Recovery		833
283	Pipeline Safety	3, 4, 6, 9, 12, 15	4500
304	Computational Simulation of Hydrofracturing	25, 26	155
306	Enhanced Recovery of Petroleum Using High-Power Microwaves	11, 16, 18, 23	2300
365	Applied Production Technology	10, 3, 5, 7, 8	1700
375	Macroscopic Transport in Geologic Media: A Lattice Gas Automata Study	17	500
<b>DEEPWATER OFFSHORE</b>			
62	Fluid Forces Acting on Tube Arrays in Crossflow	9, 16	220
144	Large-Eddy Simulation of Separating Turbulent Flow Using the Finite Element Method	9, 16	500
161	Integrity Testing of Offshore Structures	16	1000
177	Seismic Hazard Assessment for Santa Barbara Channel Offshore Platforms	16	250
201	Fatigue Failure of Top Drive Drilling Rigs to Jarring Operations	11	175
203	Damage Detection and Health Monitoring of Structures and Mechanical Systems	16, 9	1400
351	Advanced Computational Models for Deep Water Oil and Gas Production (ACTI)	9, 16	650

<b>Index</b>	<b>Project Title</b>	<b>Sub-Topics</b>	<b>Funding (\$K)</b>
<b>ARCTIC REGION ACTIVITIES</b>			
90	Alaska North Slope Oil and Gas Resource - Exploration, Development, Production, and Environmental Issues	3, 2, 1	1100
165	Site Characterization for Exploration and Production Systems	1, 2, 5, 7	120
<b>OIL PROCESSING &amp; REFINING</b>			
8	Micro Laser Desorption Time-Of-Flight Mass Spectrometer	20,19	900
9	Ab Initio Studies of Reactive and Non-Reactive Potential Surfaces	25, 4	1000
10	Synthesis and Characterization of Molecular Sieve Materials	1,7	300
12	Development of Ceramic Membranes for Partial Oxidation of Methane Into Syngas	2	1475
20	Fundamental Chemistry of Coals	21, 24	3690
22	High-Performance, Compact Evaporators and Condensers	16,17	1230
24	Molecular Sieve Materials Research	1,25	300
26	Magnetic Separation and Recovery of Solids	19, 4, 11	300
27	Computer Software for Fluid/Solids Systems Hydrodynamics and Erosion	25	2000
30	Process Chemistry of California Crudes	20, 21	400
33	Analytical Support Services/Methods Research and Development Provided by the Analytical Chemistry Laboratory	19	3500
34	Improved Resid Upgrading	21,1	1650
36	Fluid Catalysis Program	1,21	1340
37	On-Line Nuclear Magnetic Resonance Sensor System for Upgrading Residuum and Heavy Oil	21,20	1750
38	Fouling Mitigation in Processing of Residuum and Heavy Oil	21,3	1110
39	Organic-Fluid Fouling	3,12	2400
40	Generation of a Validated Computational Capability to Support Advanced Fluid Catalytic Cracker (FCC) Development	25,6	5565
41	Creep Testing of Structural Materials	3,5	300
43	Particle and Droplet Removal from Gas Streams	6,19	250
44	Conversion of Spent Catalysts into Marketable Products	4,7	160
45	Fluidized-Bed Upgrading of Heavy Oils and Resids	21,25	855
47	Analysis and Modeling of Multi-Dimensional, Multi-Phase, Multi-Species, Turbulent Reacting Flow Using ICOMFLO Computer Code	25, 21	450
56	Evaluation of FCC Feed Nozzles	6,25	1500
68	Biodegradation of Selected Organic Compounds and Complexing Agents of Radionuclides and Metals	11	1340
69	Advanced Biochemical Processes for Geothermal Brines	11	1020

<b>Index</b>	<b>Project Title</b>	<b>Sub-Topics</b>	<b>Funding (\$K)</b>
85	Use of an Environmental Risk Based Approach for Industrial Design	8	240
87	Improved Catalyst Development	1	1330
91	Plasma Upgrading of Heavy Oil and Residuum	4, 21	950
92	Industrial Plant Life Extension and Integrity Evaluations	12, 13, 3	200
102	Polyphosphazene Membranes for Chemical Separations	19	760
105	Human Centered Performance Systems	15	3600
122	Solid Superacid Catalysts for Isomerization and Alkylation	9	230
127	Development of Solid Acid Catalysts for Gasoline Alkylation	9, 11	840
128	Development of Poison Resistant, Low Deactivation Rate, Platinum-Based Bimetallic Catalysts	9, 11	300
129	Synthesis and Characterization of Heterogeneous Catalysts for the Petroleum Industry	7, 9, 23	475
130	Catalytic Membranes for Paraffin Activation and Hydrogen Transport	2, 1, 4	425
153	Production Of Hydrogen From Municipal Solid Waste	2	850
162	Computational Modeling of Hydrocarbon Chemical Kinetics	22, 23, 24, 25, 27	1000
168	Granular Flow	6	4900
170	Oil Shale Technology	4	5000
179	Compact Analytical Neutron Interrogation System	12	100
180	Biomimetic Catalysts for the Conversion of Methane to Methanol	23	3000
182	Heavy Crude Oil Processing	25, 21, 4	1550
185	Economic Analysis and Modeling	26	600
190	Quantifying Corrosion Damage	12	7800
195	Synthesis and Evaluation of New Mixed Metal Nitride Catalysts for Petroleum Refining and Specialty Chemical Manufacturing	1, 7	100
202	Microwave Driven Chemistry	1, 11	3000
209	Computer Simulation of Reactive Multiphase Flow	25,6	2100
211	Modeling and Simulation of Hydrocarbon Catalysis in Zeolites.	1, 19, 25	2300
220	Neural Networks for Chemical Process Control	26, 3	1300
245	Processing and Utilization Research - Thermodynamic and Thermophysical Property Measurements		500
246	Conduct Round Robin Tests on Heavy Crude and Bitumen		150
248	Processing and Utilization Research - Analysis and Remediation of Contaminated Soil and Groundwater		200
252	Processing and Utilization Research - Analysis of the Refining Industry		547
253	Development of Analytical Methodology for Analysis of Heavy Crudes: Catalytic Cracking Behavior of Compound Classes in Petroleum Resid		1500
255	Processing and Utilization Research - Nuclear Power Training Unit Diesel Fuel Testing		100
257	Processing and Utilization Research - Additives for Coke Reduction during Heavy Oil Processing		445
258	WFO - Petroleum Product Surveys		225

Index	Project Title	Sub-Topics	Funding (\$K)
259	Processing and Utilization Research - Upgrading and Environmental Concept		643
260	Processing and Utilization Research - OER and Thermodynamic Properties for Polycyclic Systems by Non-Calorimetric Methods		3000
264	Processing and Utilization Research - Naval Air Warfare Center - Jet Fuel Support		250
265	Processing and Utilization Research - Navy Petroleum Office - Fuel Reclaiming		100
267	Processing and Utilization Research - Process Engineering Property Measurements on Heavy Oils		10000
270	Strategic Petroleum Reserve Supporting Research		3750
273	Crude Oil Analysis Database		225
274	Processing and Utilization Research - Defense Fuel Supply Center Problem Fuel Chemistry		750
276	Renewable Hydrogen Production for Fossil Fuel Processing	2, 16, 18, 4	500
277	Separations Concepts	16, 18, 4	300
286	ANS Flow blockage Computational Fluid Analysis and Experimentation	15, 5	1300
287	ANS and HFIR Thermal and Hydraulic Analysis and Experimentation	3, 15, 19, 25	12000
290	Low Emmissions Diesel Fuels	24, 27, 28, 20, 21	1050
295	Advanced Bioreactor Concepts and Development	16, 18, 1, 2, 4, 6, 21	1400
299	Development of Materials for Black Liquor Recovery Boilers for Pulp and Paper Mills	16, 17, 6, 23	550
300	Biological Catalysts in Organic Media	(16, 18, 1, 6, 21, 23	1100
303	Fuel Models	15, 20, 27, 28	500
308	Advanced Mass Spectrometry for the Characterization and Quantitative Analysis of High Molecular Weight Materials	20, 24, 28	3500
309	Heavy-Section Steel Technology and Irradiation Programs	17, 5, 15	5000
318	Catalytic Hydrotreating of Biomass Pyrolysis Oils	11	160
319	Nanophase Catalyst Synthesis and Reaction Mechanisms	11	1585
322	Superacidic Solid Acid Catalysts	7	680
330	Molecular Modeling of Macromolecular Structure of Complex Hydrocarbons and Fuels	4, 20, 24, 25, 27	750
336	Organic Destruction/Re-Use and Recycling Methodologies	11,4	2300
338	The Origin and Fate of Toxic Combustion By-Products in Process Heaters	11	2140
339	Design and Development of Smart Membranes for Small Molecule Separations	1, 4, 19	2100
347	Catalyst Assessment and Reactor Hydrodynamics for Indirect Liquefaction	1, 6, 7, 12, 16, 22	2500
352	Conversion of Carbon Dioxide Using Biomimetic Catalysts	1, 4, 11, 25	1500
355	Study of Catalysts Using ab initio Codes on Massively Parallel Computers.	1, 25	1050
358	Replacement of Liquid H2SO4 and HF Acids with Solid Acid Catalysts in the Paraffin Alkylation Process	9, 1, 7, 16	765
369	Highly Dispersed Catalysts	1, 21, 22	1200
372	Advanced Thermally Stable Jet Fuels and Field Measurement of Oil Properties	12, 3, 6	2660
373	Catalyst Development for Direct Liquefaction and Dehydrogenation Processes	1,7,16,22	4350

<b>Index</b>	<b>Project Title</b>	<b>Sub-Topics</b>	<b>Funding (\$K)</b>
376	Catalysts for the Conversion of Light Hydrocarbons to Alcohols	22, 23, 25	1125
377	Advanced Direct Liquefaction Concepts for Improved Efficiency and Economics in the Refining of Coal-Derived Liquids	22, 4, 21, 16	715
381	Reduction of Nitrogen Oxide Emissions for Lean Burn Engine Technology	1, 16	2000
382	Simulation of Residual Oil Hydroprocessing Units on Massively Parallel Supercomputers	21, 25	800

## **GAS PROCESSING**

1	Trainable Electrocatalytic Cermet Gas Microsensors Program	6, 12	530
4	Gas Chromatography/Matrix-Isolation/Fourier Transform Infrared Spectroscopy	6	300
5	Reformers for Fuel Cells		350
6	Capturing Carbon Dioxide Emissions From Flue Gas Streams	2,8	500
7	Continuous Fiber Ceramic Composites: Testing and Evaluation	6	120
17	Recovery of Hydrogen from Hydrogen Sulfide	2, 7	3095
23	Hot-Gas Filters	6	200
67	Fischer-Tropsch Synthesis with Fine Particle Catalysts		320
139	Transition Metal-Catalyzed Conversion of CO, NO, H <sub>2</sub> , and Organic Molecules to Fuels and Petrochemicals		260
279	Heterogeneous Catalysts Related to Energy Systems	2, 3, 8	3520
284	Advanced Bioreactor Systems for Gaseous Substrates	2, 3, 8	300
294	Removal of Heteroatoms form Crude Oil	3	900
313	High Pressure Heat Exchange System - Advanced Materials for Steam-Methane Reforming	4	1600
379	Microengineered Polymer-Derived Adsorbents for Natural Gas	4, 8	300

## **GAS GATHERING**

18	Information/GIS System to Understand the Natural Gas Industry and Infrastructure		300
19	Using Geographic Information Systems to Site Gas Pipelines		750
93	Measurement of Component Ratio in Oil/Water/Gas Mixtures and Determination of Flow Regime	5	150
94	Complex Multi-Fluid Flow Analysis	5	1000
205	Thermoacoustic Natural Gas Liquefier	1	850
345	The Development of a Real-Time Video Imaging System for Natural Gas Leaks	2	800

## **GAS STORAGE**

75	Adsorbent/Natural Gas Vehicle Storage Systems		3250
106	Gas Storage in Aquifers	3	100

<b>Index</b>	<b>Project Title</b>	<b>Sub-Topics</b>	<b>Funding (\$K)</b>
151	Quantitative Gas Leak Detection / Pressure Safety Training	2	1100
383	U.S. Strategic Petroleum Reserve Geotechnical Support	7	16500

## **ENVIRONMENTAL & REGULATORY**

2	Restoring Wetlands After Pipeline Installation	12	400
3	Evaluation of Contaminated Sites Using Heavy Metal Speciation Techniques	12, 14	335
11	Integrated Spatial Analysis Techniques for the Gas Industry	12, 14	1300
13	Trace-Level Organic Analysis	4, 5	800
14	Nuclear Counting Technique	10, 14	1750
15	Application of Dynamic Stability to Liquid-Filled Tanks	14, 5	350
16	Computer Software for Seismic Response of Liquid-Filled Tanks	14, 5	450
21	Integrated Electrodialysis/Reverse Osmosis Process for Produced Water Treatment	2, 12	260
25	Recycling Waste Lubricating Oils	11	300
35	Designing a Remediation Plan to Restore Drinking Water From a Contaminated Site	12, 6	575
42	In-Situ Bioremediation by Electrokinetic Injection	12	100
46	Gas Sensors for Environmental Control Technologies	5, 7	490
48	Passive and Active Millimeter-Wave Spectrometry for Detection of Trace Gases From Remote Locations	5, 10	2250
49	Establishing "Banks" to Replace Wetlands Lost to Industrial Development	12	600
50	STRATEX for Treatment of Soils	12	325
51	Solvent Extraction Processes for Removal of Inorganic Components From Aqueous Streams	2, 12	2230
52	Magnetically Assisted Removal of Soluble Contaminants From Liquid Streams	2, 12	400
53	Implementing a Systems Approach to Remediate a Gasoline-Contaminated Site	12, 9	350
54	Development and Application of Novel TiO <sub>2</sub> Photocatalysts for Treating Combined Wastes	10, 2	300
55	Ultrasonic Soil and Groundwater Cleanup	12	330
57	Pipeline Leak and Rupture Assessment	5, 6	800
58	South Louisiana and Mississippi Delta Subsidence and Wetlands Losses	14, 6	700
59	Land Loss in the Deltaic Plain of Louisiana	14	1100
60	Pipeline Right-Of-Way Research Program	12, 14	2300
61	Bioremediation of Contaminated Soil by Enhanced Phytoremediation	12	400
63	Integrated Electrodialysis/Reverse Osmosis Process for Produced Water Treatment	2	260
66	EPA/DOE Interagency Project on Environmental Pathway Modeling	9, 14	550
73	Produced Water Risk Assessment and Programmatic Support	4, 14	440
74	Drinking Water Standards	10, 14	390
76	Conversion of Waste Sulfur from Petroleum and Natural Gas Production into Cost Effective, Beneficial, and Environmentally Safe Secondary Products		240

<b>Index</b>	<b>Project Title</b>	<b>Sub-Topics</b>	<b>Funding (\$K)</b>
77	Comprehensive Assessment	14	440
79	Materials Characterization & Innovative Technology Group (MCIT)		2000
81	Development and Testing of BLT-EC, a Coupled Finite-element Geochemical Transport Code		900
89	Above-Ground Storage Tank Leak Detection System Certification Facility	5, 14	110
95	Removal of Organic Contaminants from Solid Materials	10, 12	110
96	Development and implementation of enhanced bioremediation of hydrocarbons in the petroleum industry: production, refinery, distribution systems	12	300
97	Hydrothermal Oxidation of Toxic Materials	10	3000
99	Large-Scale Infiltration Study	9, 10	6000
100	US Air Force Installation Restoration Program	6, 9, 11, 14	10000
101	Development of Biofilters for the Treatment of Hazardous Gases and Vapors	10	590
103	Heavy Metals and Halocarbon Removal from Aqueous Waste Streams	10	500
111	Low Temperature Catalysts for the Oxidation of Methane	10	125
119	Airborne Emissions Monitoring and Analysis	10	200
124	Design, Construction, and Application of a Very-Early-Time Electromagnetic (VETEM) System for Detailed Mapping of the Shallow Subsurface	5, 6	305
125	Analog Site for Characterization of Fractured Rock	9, 2, 6, 9, 15	634
126	Site Remediation Analysis and Decision Support	4, 8, 9, 12, 14	800
131	Fractionation and Cycling of Selenium in the Biogeochemical System of Suisun and San Pablo Bays	10	800
140	Airborne Emissions and Air Quality	8, 14	500
143	Control and Measurement of Toxic and Hazardous Compounds	10, 12	1000
145	High-Performance Computing Strategies for Subsurface Flow and Chemical Migration	9	2100
146	Chemical Kinetics of Refinery Toxic Emissions and the Clean Air Act	7, 10, 8, 14	2000
149	Increased Efficiency and Pollution Reduction in Engine Systems	7	3000
150	Naturally Occurring Radioactive Materials (NORM) Analysis for Oil and Gas Operations	15	600
156	Portable Electrochemical Sensor for Environmental Monitoring and Process Control	2, 10	1000
157	In Situ Microbial Filters	12, 6, 9, 2	8280
159	Advanced Infrared Imaging Sensors	7	4180
164	Plasma Processing of Diesel Engine Exhaust	7	3000
171	Gas Phase Sensors	7	310
173	3-D Simulation of Multiphase Contaminant Transport and In Situ Remediation of Low Permeability Soils Using an Alternating Current Based Ohmic Heating Technique	9	385
183	Capacitive Deionization	2, 10, 11	1800
186	Dynamic Underground Stripping	12	10500
189	Portable Micro-machined Gas Chromatograph	10, 12	480
193	Advanced Lidar Systems for Pollution Monitoring	10, 7,14	5000

Index	Project Title	Sub-Topics	Funding (\$K)
194	A Simple New Monitor For Air Emissions	10, 5, 7	3100
197	Microcellular Foams for the Separation of Heavy Metal-Ions from Waste Streams	11	500
198	Atmospheric Transport and Fate of Pollutants Over Complex Terrain	8, 14	5250
206	An Intelligently Controlled Three-Phase Centrifuge for Petroleum Waste Separation	12, 2, 11	1830
210	Modeling Transport and Remediation of Soil and Groundwater Contaminants	9, 6, 12, 14	5000
215	Naturally Occurring Radioactive Materials (NORM) Analysis For Oil And Gas Operations	15, 4, 14	120
233	Lithology Characterization for Remediation of Underground Pollution	9,6	875
239	Natural Gas Technology Enhancements		3000
240	AMFA Fleet Fuel and Oil Analyses		278
241	Establishing California Air Resources Board Reactivity Rating for Ethanol		185
244	California Pipeline and Gathering Line Assessment		650
249	Area of Review Variance Program		650
251	Biodiesel, Commercialization of a Renewable Fuel		695
254	Impacts of Alternative Fuels on Air Quality		278
256	Safety and Environmental Management Program		240
266	Monitoring Tulsa Public Schools Alternative Fuel Fleet		315
268	Monitoring of Tinker Air Force Base Alternative Fuel Fleet		900
269	Safety and Environmental Management Demonstration Program		660
272	Regulatory Streamlining		1000
278	In Situ Vitrification	1, 2, 3, 4, 9	2000
281	Programmatic Environmental Assessment for the Oil Research Program	14	250
282	Mercury Air/Surface Exchange in the Environment	4, 10, 12, 14	1100
288	METER and AENEC Programs	7, 8, 10, 14	600
289	Prediction of Air Pollution Dispersion/Transformation/Fate	7, 8, 10, 14	3000
292	Seismic Reflection Acquisition, Processing and Source Comparison	3, 6, 9, 14	575
293	The Seasonal SOIL Compartment Model (SESOIL) and Computational Fluid Dynamics Modeling	3, 6, 9, 12, 14	135
297	Environmental Regulations and Compliance Requirements for Clean Air Act and Other Regulations	7, 8, 10	4500
298	In Situ Chemical Oxidation of Organic Contaminants in Soil and Groundwater	1, 2, 10, 12, 14	555
301	Remediation of DNAPL Compounds in Low Permeability Media	3, 6, 9, 12, 14	1000
305	Quantitative Assessment of Environmental Risks	3, 4, 7, 14	5000
307	Estimating the Externalities of Fuel Cycles Associated with Electric Power Production	7, 14	4000
312	Applied Analytical Mass Spectrometry (Emissions/Process Monitoring, Field Instrumentation, Residuum/Product Characterization)	5, 7, 8, 10, 14	3500
314	The Effects of the Exxon Valdez Oil Spill on Pacific Herring	5, 6	3500

<b>Index</b>	<b>Project Title</b>	<b>Sub-Topics</b>	<b>Funding (\$K)</b>
315	Effects of Petroleum Products on Bull Kelp; Perform Field Assessment of Possible Damages to Eelgrass in Faadalgo Bay, WA; Investiagte Effects of Oil on Kelp Nereocystis Leutkeana; Analyses Using Seimpermeable Membrane Devices	4, 5	201
316	Low-Temperature Catalytic Gasification of Wet Wastes	7, 8	1905
317	Investigation of Self-Help Oil-Spill Response Techniques and Equipment and Effects of Petroleum Contaminated Waterways on the Spawning Migration of Pacific Salmon		173
320	Conduct Literature Review on Polychlorinated Biphenyl (PCB) Sorption from Gas Line Condensates into Soils	9, 10	106
321	Predicting TPH Biodegradation & Leaching in Contam. Soils Using State-of-the-Art Hydrocarbon Charact. Evaluate Chem. & Phys.Properties in Solids, Water, & Oil Samples Great Lakes; Evaluate Environmental Monitoring Program for Legovan Amuay Oil Refinery	4, 5	117
323	U. S. Coast Guard Human Factors Engineering	5	3943
324	Petroleum Sludge Treatment; Spent Catalyst Processing	4, 6, 7, 12	1100
325	Toxicological Monitoring of Ballast-Water Effluent Discharge	5, 6	300
326	Perform Field Assess of Possible Damage to Eelgrass in Fidalgo Bay, WA During Oil Spill Cleanup, Investigate Effects of Oil on Kelp Nereocystis Luetkeana, Conduct Analyses Using SPMD to Estimate Bioconcentration Potential of Oil Additives in Aquatic Life	4, 5	152
327	Conduct Histopathological Evaluation and Body Burden Analysis of Alaska Salmon Potentially Affected by the Exxon Valdez Oil Spill	5, 6	100
328	Alyeska Sediment Studies	5, 6	250
329	Soil Washing for Removal of Heavy Metals and Radionuclides		1214
331	Photocatalytic Detoxification of Organic Contaminants	10, 11, 12	3200
334	Monitoring of Contaminants, In-Situ Remediation, Subsurface Barriers, and Landfill Covers Using Tracers	9, 5	970
337	Leak Detection Using Horizontal Logging and Electromagnetic Sensor Techniques	5	500
342	Laser-Spark Spectroscopy for Continuous Metal Emissions Monitoring	10	1800
344	Transport and Fate of Oil Spilled in a Marine Environment		600
349	In Situ Permeable Flow Sensor	6	1520
360	Numerical Modeling of Thermal Enhanced Vapor Extraction Remediation Technology	12, 9	2500
364	Natural Geochemical Attenuation and Chemical Manipulation to Stabilize Groundwater Contaminants	9, 5	580
374	Risk-Based Decision Analysis Tools for Remedial Alternatives Selection Based on Probabilistic Flow and Transport Simulators	4, 6, 9, 14	2200

Index	Project Title	Sub-Topics	Funding (\$K)
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## EXPLORATION

66	EPA/DOE Interagency Project on Environmental Pathway Modeling	2	550
142	Geothermal Reservoir Engineering	14, 16, 10	2000
204	National Information Infrastructure Technologies Applied to Database Synthesis and Remote Problem-Solving for the Carpinteria Reservoir Re-Development Project	15	100
231	Sunrise: A National Information Infrastructure Prototype	13	3500
234	The Development of a General Reservoir Simulation for Massively Parallel Computers	13	875
292	Seismic Reflection Acquisition, Processing and Source Comparison	4	575
335	Fluid/Rock Interactions - Mineral Dissolution and Precipitation Kinetics, Sorption, and Surface Charge Speciation	9	1800
341	Three Component Borehole Seismic Source	3, 10, 14, 16	3160
350	Rock Mechanics Investigations	1, 9	2070
357	Advanced Borehole Seismic Receiver	3, 10, 14, 16	3100
361	Single-well Imaging of Salt Dome Flanks (ACTI)	4, 14	1550
362	Electromagnetic Reservoir Characterization		3700
363	Computational Geomechanics for Geologic Structure and Reservoir Mechanics (ACTI)	5, 9, 11	1250

## DEVELOPMENT

88	Large Downhole Seismic Sensor Array	3, 16	1200
100	US Air Force Installation Restoration Program	4	10000
134	Integrated Isotopic Studies of Fluid Flow Processes and Time Scales in Sedimentary Basins	4, 8	500
145	High-Performance Computing Strategies for Subsurface Flow and Chemical Migration	25	2100
175	Velocity Analysis, Parameter Estimation, and Constraints on Lithology for Transversely Isotropic Sediments	3, 9, 11	600
181	Massively Parallel Computing	2	1000
213	Modeling Ocean Currents and Eddies for Offshore Operations	33	150
218	Coupled Rock/Fluid Mechanics Numerical Simulations Applied to Well Completions	9, 8	1650
226	Society of Exploration Geophysicists Synthetic Seismic Database	3	1500
296	Advance Computational Tools for 3-D Seismic Analysis using the SEG/EAGE Model Dataset	2, 12	2550
304	Computational Simulation of Hydrofracturing	26	155
308	Advanced Mass Spectrometry for the Characterization and Quantitative Analysis of High Molecular Weight Materials	5, 18, 30	3500
311	Experimental and Analytical Geochemistry	4, 5, 6, 14, 18, 21, 22, 23, 24, 28	1890

Index	Project Title	Sub-Topics	Funding (\$K)
334	Monitoring of Contaminants, In-Situ Remediation, Subsurface Barriers, and Landfill Covers Using Tracers	4	970
340	Acoustic Telemetry	31	2700
349	In Situ Permeable Flow Sensor	31	1520
367	Increased Effectiveness Of Hydraulic Fracturing Through Advanced Computational Technology (ACTI)	9, 26	825
380	Gas and Oil National Information Infrastructure (GONII)	33	4500

## DRILLING & COMPLETION

104	Vertical Seismic Profiling While Drilling	11	300
243	Risk-Based Decision Management		321
310	Borehole Geophysical Logging	3	975
334	Monitoring of Contaminants, In-Situ Remediation, Subsurface Barriers, and Landfill Covers Using Tracers	11	970
335	Fluid/Rock Interactions - Mineral Dissolution and Precipitation Kinetics, Sorption, and Surface Charge Speciation	2, 6	1800

## PRODUCTION

29	Mechanical Properties of Materials		2000
73	Produced Water Risk Assessment and Programmatic Support		440
93	Measurement of Component Ratio in Oil/Water/Gas Mixtures and Determination of Flow Regime	6	150
100	US Air Force Installation Restoration Program	2, 16, 17, 18, 19	10000
144	Large-Eddy Simulation of Separating Turbulent Flow Using the Finite Element Method	22	500
163	Atomic Scale Electrochemical Modeling	3, 4, 6, 17, 19	800
170	Oil Shale Technology	24	5000
188	Oil and Gas Data Infrastructure		2500
207	Ultrasonic Reduction of Wellbore Deposits and Formation Damage	5, 18, 25	550
212	Binary Liquid Explosive and Initiator System for Wellbore Applications	25	1000
218	Coupled Rock/Fluid Mechanics Numerical Simulations Applied to Well Completions	25, 13	1650
222	Perforator Design and Testing	25	150
228	Advanced Perforator Technology	25	1800
237	Field Demonstrations in High Priority Reservoir Classes	3, 2, 11	17736
287	ANS and HFIR Thermal and Hydraulic Analysis and Experimentation	3, 4	12000
300	Biological Catalysts in Organic Media	16, 18, 1, 6, 21, 23	1100
310	Borehole Geophysical Logging	25	975

<b>Index</b>	<b>Project Title</b>	<b>Sub-Topics</b>	<b>Funding (\$K)</b>
311	Experimental and Analytical Geochemistry	4, 5	1890
333	Near Wellbore Mechanics (ACTI)	11, 13, 25	1700
348	Hydraulic Fracturing Diagnostics	11, 25	3500
354	Hydraulic Fracturing	11, 13, 25	600
367	Increased Effectiveness Of Hydraulic Fracturing Through Advanced Computational Technology (ACTI)	11, 25	825
372	Advanced Thermally Stable Jet Fuels and Field Measurement of Oil Properties	5	2660

## DEEPWATER OFFSHORE

29	Mechanical Properties of Materials		2000
78	Mechanisms of Metal-Environment Interactions	8	1820
93	Measurement of Component Ratio in Oil/Water/Gas Mixtures and Determination of Flow Regime	6	150
283	Pipeline Safety	1, 2, 4, 5, 6, 8, 15	4500
286	ANS Flow blockage Computational Fluid Analysis and Experimentation	1, 4, 5, 6, 7	1300
309	Heavy-Section Steel Technology and Irradiation Programs	4, 5, 7, 8	5000
370	Seafloor Earthquake Measurement System (SEMS)	1, 16	700

## ARCTIC REGION ACTIVITIES

29	Mechanical Properties of Materials		2000
280	Joint High-Performance, High-Resolution Ocean Circulation Modeling for Enhancing Offshore Oil and Gas Exploration and Production	2, 3, 5, 7	350
283	Pipeline Safety	5, 7	4500
309	Heavy-Section Steel Technology and Irradiation Programs	4, 5, 6	5000

## OIL PROCESSING & REFINING

29	Mechanical Properties of Materials		2000
31	Development of Environmentally Acceptable Microbial Corrosion Control Methods	3,5	1680
62	Fluid Forces Acting on Tube Arrays in Crossflow		220
65	Combustion Kinetics & Reaction Pathways	27	3030
66	EPA/DOE Interagency Project on Environmental Pathway Modeling	8	550
82	Measurement of Fluid Flow and Fluid-Rock Interactions Using Synchrotron Computed Microtomography	1	380
94	Complex Multi-Fluid Flow Analysis	16, 17	1000
149	Increased Efficiency and Pollution Reduction in Engine Systems	1	3000
155	Corrosion Sensors	12	200
161	Integrity Testing of Offshore Structures	E-16	1000

Index	Project Title	Sub-Topics	Funding (\$K)
163	Atomic Scale Electrochemical Modeling	1, 7, 25	800
206	An Intelligently Controlled Three-Phase Centrifuge for Petroleum Waste Separation	11	1830
279	Heterogeneous Catalysts Related to Energy Systems	1, 4, 16	3520
283	Pipeline Safety	14, 15	4500
284	Advanced Bioreactor Systems for Gaseous Substrates	4, 6, 21	300
294	Removal of Heteroatoms from Crude Oil	16, 18, 4	900
307	Estimating the Externalities of Fuel Cycles Associated with Electric Power Production	8	4000
313	High Pressure Heat Exchange System - Advanced Materials for Steam-Methane Reforming	16, 17, 2, 6, 23	1600
324	Petroleum Sludge Treatment; Spent Catalyst Processing		1100

## GAS PROCESSING

22	High-Performance, Compact Evaporators and Condensers		1230
29	Mechanical Properties of Materials		2000
33	Analytical Support Services/Methods Research and Development Provided by the Analytical Chemistry Laboratory	6	3500
36	Fluid Catalysis Program		1340
41	Creep Testing of Structural Materials		300
43	Particle and Droplet Removal from Gas Streams		250
282	Mercury Air/Surface Exchange in the Environment	6	1100
339	Design and Development of Smart Membranes for Small Molecule Separations	4, 5, 6	2100
342	Laser-Spark Spectroscopy for Continuous Metal Emissions Monitoring	6	1800

## GAS GATHERING

64	Microparticle Analysis by Laser Spectroscopy	2	1080
71	Application of Multitracer Technology to Petroleum Reservoir Studies	2	1080
229	Multicomponent Labeled Tracer Technology: Characterization of Coupled Transport and Chemical Interactions in Petroleum Reservoirs	2	650
283	Pipeline Safety	2, 3, 4, 5	4500
291	Airborne Remote Sensing of Natural Gas Leaks	2	1065
337	Leak Detection Using Horizontal Logging and Electromagnetic Sensor Techniques	2	500

## GAS STORAGE

64	Microparticle Analysis by Laser Spectroscopy	2	1080
71	Application of Multitracer Technology to Petroleum Reservoir Studies	2	1080
205	Thermoacoustic Natural Gas Liquefier	7	850

Index	Project Title	Sub-Topics	Funding (\$K)
229	Multicomponent Labeled Tracer Technology: Characterization of Coupled Transport and Chemical Interactions in Petroleum Reservoirs	2	650

## ENVIRONMENTAL & REGULATORY

1	Trainable Electrocatalytic Cermet Gas Microsensors Program		530
6	Capturing Carbon Dioxide Emissions From Flue Gas Streams		500
8	Micro Laser Desorption Time-Of-Flight Mass Spectrometer		900
17	Recovery of Hydrogen from Hydrogen Sulfide		3095
19	Using Geographic Information Systems to Site Gas Pipelines		750
26	Magnetic Separation and Recovery of Solids	13	300
71	Application of Multitracer Technology to Petroleum Reservoir Studies	5	1080
144	Large-Eddy Simulation of Separating Turbulent Flow Using the Finite Element Method	8	500
151	Quantitative Gas Leak Detection / Pressure Safety Training	5	1100
176	Optimization Methods for Reservoir Management	9	1500
177	Seismic Hazard Assessment for Santa Barbara Channel Offshore Platforms	14	250
178	Battery-powered Portable Micro-machined DNA Detector	12	1600
184	Electrical Resistance Tomography for Subsurface Imaging and Leak Detection	5	1120
202	Microwave Driven Chemistry	10	3000
283	Pipeline Safety	8, 10, 14	4500
285	Airborne Geophysical Surveying	5, 7, 8, 14	2405
291	Airborne Remote Sensing of Natural Gas Leaks	5, 7, 8, 14	1065
302	Tracer Technology	5, 8, 9	8000
308	Advanced Mass Spectrometry for the Characterization and Quantitative Analysis of High Molecular Weight Materials	4, 14	3500
335	Fluid/Rock Interactions - Mineral Dissolution and Precipitation Kinetics, Sorption, and Surface Charge Speciation	9, 12	1800
336	Organic Destruction/Re-Use and Recycling Methodologies	10	2300
338	The Origin and Fate of Toxic Combustion By-Products in Process Heaters	10	2140
345	The Development of a Real-Time Video Imaging System for Natural Gas Leaks	5,10	800
358	Replacement of Liquid H <sub>2</sub> SO <sub>4</sub> and HF Acids with Solid Acid Catalysts in the Paraffin Alkylation Process	10	765
362	Electromagnetic Reservoir Characterization	10	3700
366	Flow Visualization Laboratory for Multiphase Flow Processes	6	5000
367	Increased Effectiveness Of Hydraulic Fracturing Through Advanced Computational Technology (ACTI)	1, 2	825
371	Shallow Directional Drilling Development for Environmental Use	12	1600
375	Macroscopic Transport in Geologic Media: A Lattice Gas Automata Study	9	500
381	Reduction of Nitrogen Oxide Emissions for Lean Burn Engine Technology	10	2000

# Project Index By Laboratory

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Index	NPC Technology Need Category	Project Title	91-95 Funding (\$K)
<b>Argonne National Laboratory</b>			
1	Gas Processing (6, 12), Environmental & Regulatory	Trainable Electrocatalytic Cermet Gas Microsensors Program	530
2	Environmental & Regulatory (12)	Restoring Wetlands After Pipeline Installation	400
3	Environmental & Regulatory (12, 14)	Evaluation of Contaminated Sites Using Heavy Metal Speciation Techniques	335
4	Gas Processing (6)	Gas Chromatography/Matrix-Isolation/Fourier Transform Infrared Spectroscopy	300
5	Gas Processing	Reformers for Fuel Cells	350
6	Gas Processing (2,8), Environmental & Regulatory	Capturing Carbon Dioxide Emissions From Flue Gas Streams	500
7	Gas Processing (6)	Continuous Fiber Ceramic Composites: Testing and Evaluation	120
8	Oil Processing & Refining (20,19), Environmental & Regulatory	Micro Laser Desorption Time-Of-Flight Mass Spectrometer	900
9	Oil Processing & Refining (25, 4)	Ab Initio Studies of Reactive and Non-Reactive Potential Surfaces	1000
10	Oil Processing & Refining (1,7)	Synthesis and Characterization of Molecular Sieve Materials	300
11	Environmental & Regulatory (12, 14)	Integrated Spatial Analysis Techniques for the Gas Industry	1300
12	Oil Processing & Refining (2)	Development of Ceramic Membranes for Partial Oxidation of Methane Into Syngas	1475
13	Environmental & Regulatory (4, 5)	Trace-Level Organic Analysis	800
14	Environmental & Regulatory (10,14)	Nuclear Counting Technique	1750
15	Environmental & Regulatory (14, 5)	Application of Dynamic Stability to Liquid-Filled Tanks	350
16	Environmental & Regulatory (14, 5)	Computer Software for Seismic Response of Liquid-Filled Tanks	450
17	Gas Processing (2, 7), Environmental & Regulatory	Recovery of Hydrogen from Hydrogen Sulfide	3095
18	Gas Gathering	Information/GIS System to Understand the Natural Gas Industry and Infrastructure	300
19	Gas Gathering, Environmental & Regulatory	Using Geographic Information Systems to Site Gas Pipelines	750
20	Oil Processing & Refining (21, 24)	Fundamental Chemistry of Coals	3690
21	Environmental & Regulatory (2, 12)	Integrated Electrodialysis/Reverse Osmosis Process for Produced Water Treatment	260
22	Oil Processing & Refining (16,17), Gas Processing	High-Performance, Compact Evaporators and Condensers	1230
23	Gas Processing (6)	Hot-Gas Filters	200
24	Oil Processing & Refining (1,25)	Molecular Sieve Materials Research	300
25	Environmental & Regulatory (11)	Recycling Waste Lubricating Oils	300
26	Oil Processing & Refining (19, 4, 11), Environmental & Regulatory (13)	Magnetic Separation and Recovery of Solids	300
27	Oil Processing & Refining (25)	Computer Software for Fluid/Solids Systems Hydrodynamics and Erosion	2000

<b>Index</b>	<b>NPC Technology Need Category</b>	<b>Project Title</b>	<b>91-95 Funding (\$K)</b>
28	Production (3, 4)	Development of Environmentally Acceptable Microbial Corrosion Control Methods	525
29	Drilling & Completion(8), Production, Deepwater Offshore, Arctic Region Activities, Oil Processing & Refining, Gas Processing	Mechanical Properties of Materials	2000
30	Oil Processing & Refining (20, 21)	Process Chemistry of California Crudes	400
31	Production (3), Oil Processing & Refining (3,5)	Development of Environmentally Acceptable Microbial Corrosion Control Methods	1680
32	Drilling & Completion (8)	Thin Diamond Films Deposited by Microwave-Enhanced Chemical Vapor Deposition	950
33	Oil Processing & Refining (19), Gas Processing (6)	Analytical Support Services/Methods Research and Development Provided by the Analytical Chemistry Laboratory	3500
34	Oil Processing & Refining (21,1)	Improved Resid Upgrading	1650
35	Environmental & Regulatory (12, 6)	Designing a Remediation Plan to Restore Drinking Water From a Contaminated Site	575
36	Oil Processing & Refining (1,21), Gas Processing	Fluid Catalysis Program	1340
37	Oil Processing & Refining (21,20)	On-Line Nuclear Magnetic Resonance Sensor System for Upgrading Residuum and Heavy Oil	1750
38	Oil Processing & Refining (21,3)	Fouling Mitigation in Processing of Residuum and Heavy Oil	1110
39	Oil Processing & Refining (3,12)	Organic-Fluid Fouling	2400
40	Oil Processing & Refining (25,6)	Generation of a Validated Computational Capability to Support Advanced Fluid Catalytic Cracker (FCC) Development	5565
41	Oil Processing & Refining (3,5), Gas Processing	Creep Testing of Structural Materials	300
42	Environmental & Regulatory (12)	In-Situ Bioremediation by Electrokinetic Injection	100
43	Oil Processing & Refining (6,19), Gas Processing	Particle and Droplet Removal from Gas Streams	250
44	Oil Processing & Refining (4,7)	Conversion of Spent Catalysts into Marketable Products	160
45	Oil Processing & Refining (21,25)	Fluidized-Bed Upgrading of Heavy Oils and Resids	855
46	Environmental & Regulatory (5,7)	Gas Sensors for Environmental Control Technologies	490
47	Oil Processing & Refining (25, 21)	Analysis and Modeling of Multi-Dimensional, Multi-Phase, Multi-Species, Turbulent Reacting Flow Using ICOMFLO Computer Code	450
48	Environmental & Regulatory (5, 10)	Passive and Active Millimeter-Wave Spectrometry for Detection of Trace Gases From Remote Locations	2250
49	Environmental & Regulatory (12)	Establishing "Banks" to Replace Wetlands Lost to Industrial Development	600
50	Environmental & Regulatory (12)	STRATEX for Treatment of Soils	325
51	Environmental & Regulatory (2,12)	Solvent Extraction Processes for Removal of Inorganic Components From Aqueous Streams	2230
52	Environmental & Regulatory (2, 12)	Magnetically Assisted Removal of Soluble Contaminants From Liquid Streams	400
53	Environmental & Regulatory (12, 9)	Implementing a Systems Approach to Remediate a Gasoline-Contaminated Site	350
54	Environmental & Regulatory (10, 2)	Development and Application of Novel TiO <sub>2</sub> Photocatalysts for Treating Combined Wastes	300
55	Environmental & Regulatory (12)	Ultrasonic Soil and Groundwater Cleanup	330

Index	NPC Technology Need Category	Project Title	91-95 Funding (\$K)
56	Oil Processing & Refining (6,25)	Evaluation of FCC Feed Nozzles	1500
57	Environmental & Regulatory (5, 6)	Pipeline Leak and Rupture Assessment	800
58	Environmental & Regulatory (14, 6)	South Louisiana and Mississippi Delta Subsidence and Wetlands Losses	700
59	Environmental & Regulatory (14)	Land Loss in the Deltaic Plain of Louisiana	1100
60	Environmental & Regulatory (12, 14)	Pipeline Right-Of-Way Research Program	2300
61	Environmental & Regulatory (12)	Bioremediation of Contaminated Soil by Enhanced Phytoremediation	400
62	Deepwater Offshore (9, 16), Oil Processing & Refining	Fluid Forces Acting on Tube Arrays in Crossflow	220
63	Environmental & Regulatory (2)	Integrated Electrodialysis/Reverse Osmosis Process for Produced Water Treatment	260
<b>Number of Projects: 63</b>		<b>Laboratory Project Funding Total (\$K):</b>	<b>63400</b>

### Brookhaven National Laboratory

64	Development (4, 21), Gas Gathering (2), Gas Storage (2) Environment & Regulatory (5)	Microparticle Analysis by Laser Spectroscopy	1080
65	Production (24), Oil Processing & Refining (27)	Combustion Kinetics & Reaction Pathways	3030
66	Environmental & Regulatory (9, 14), Oil Processing & Refining (8), Exploration (2)	EPA/DOE Interagency Project on Environmental Pathway Modeling	550
67	Gas Processing	Fischer-Tropsch Synthesis with Fine Particle Catalysts	320
68	Oil Processing & Refining (11)	Biodegradation of Selected Organic Compounds and Complexing Agents of Radionuclides and Metals	1340
69	Oil Processing & Refining (11)	Advanced Biochemical Processes for Geothermal Brines	1020
70	Drilling & Completion (4)	Geothermal Materials Development	1840
71	Development (4, 21), Gas Gathering (2), Gas Storage (2), Environmental & Regulatory (5)	Application of Multitracer Technology to Petroleum Reservoir Studies	1080
72	Exploration	Design of a Robust Numerical Model for Multiphase Flow	150
73	Environmental & Regulatory (4, 14), Production	Produced Water Risk Assessment and Programmatic Support	440
74	Environmental & Regulatory (10, 14)	Drinking Water Standards	390
75	Gas Storage	Adsorbent/Natural Gas Vehicle Storage Systems	3250
76	Environmental & Regulatory	Conversion of Waste Sulfur from Petroleum and Natural Gas Production into Cost Effective, Beneficial, and Environmentally Safe Secondary Products	240
77	Environmental & Regulatory (14)	Comprehensive Assessment	440
78	Production (3), Deepwater Offshore (8)	Mechanisms of Metal-Environment Interactions	1820
79	Environmental & Regulatory	Materials Characterization & Innovative Technology Group (MCIT)	2000

<b>Index</b>	<b>NPC Technology Need Category</b>	<b>Project Title</b>	<b>91-95 Funding (\$K)</b>
80	Production (18)	Economic Feasibility of Biochemical Processes for the Upgrading Of Crudes and the Removal of Sulfur, Nitrogen, and Trace Metals From Crude Oil - Benchmark Cost Establishment of Biochemical Processes on the Basis of Conventional Downstream Technologies	540
81	Environmental & Regulatory	Development and Testing of BLT-EC, a Coupled Finite-element Geochemical Transport Code	900
82	Development (5, 18, 22), Oil Processing & Refining (1)	Measurement of Fluid Flow and Fluid-Rock Interactions Using Synchrotron Computed Microtomography	380
83	Drilling & Completion (4)	In Situ Containment and Stabilization of Buried Waste	870
<b>Number of Projects: 20</b>		<b>Laboratory Project Funding Total (\$K):</b>	<b>21680</b>

### Idaho National Engineering Laboratory

84	Exploration	Locating and Numerically Modeling Geopressed Hydrocarbon Reservoirs and Associated Pressure Seals in Soft, Clastic Sediments	440
85	Oil Processing & Refining (8)	Use of an Environmental Risk Based Approach for Industrial Design	240
86	Development (2)	Interactive Computer Visualization of TETRAD Results	100
87	Oil Processing & Refining (1)	Improved Catalyst Development	1330
88	Exploration (3, 14), Development (3, 16)	Large Downhole Seismic Sensor Array	1200
89	Environmental & Regulatory (5, 14)	Above-Ground Storage Tank Leak Detection System Certification Facility	110
90	Arctic Region Activities (3, 2, 1)	Alaska North Slope Oil and Gas Resource - Exploration, Development, Production, and Environmental Issues	1100
91	Oil Processing & Refining (4, 21)	Plasma Upgrading of Heavy Oil and Residuum	950
92	Oil Processing & Refining (12, 13, 3)	Industrial Plant Life Extension and Integrity Evaluations	200
93	Gas Gathering (5), Production (6), Deepwater Offshore (6)	Measurement of Component Ratio in Oil/Water/Gas Mixtures and Determination of Flow Regime	150
94	Gas Gathering (5), Oil Processing & Refining (16, 17)	Complex Multi-Fluid Flow Analysis	1000
95	Environmental & Regulatory (10, 12)	Removal of Organic Contaminants from Solid Materials	110
96	Environmental & Regulatory (12)	Development and implementation of enhanced bioremediation of hydrocarbons in the petroleum industry: production, refinery, distribution systems	300
97	Environmental & Regulatory (10)	Hydrothermal Oxidation of Toxic Materials	3000
98	Production (21)	Microbial Enhanced Oil Recovery and Reservoir Fundamentals	4000
99	Environmental & Regulatory (9, 10)	Large-Scale Infiltration Study	6000

<b>Index</b>	<b>NPC Technology Need Category</b>	<b>Project Title</b>	<b>91-95 Funding (\$K)</b>
100	Environmental & Regulatory (6, 9, 11, 14), Production (2, 16, 17, 18, 19), Development (4)	US Air Force Installation Restoration Program	10000
101	Environmental & Regulatory (10)	Development of Biofilters for the Treatment of Hazardous Gases and Vapors	590
102	Oil Processing & Refining (19)	Polyphosphazene Membranes for Chemical Separations	760
103	Environmental & Regulatory (10)	Heavy Metals and Halocarbon Removal from Aqueous Waste Streams	500
104	Exploration (3, 4), Drilling & Completion (11)	Vertical Seismic Profiling While Drilling	300
105	Oil Processing & Refining (15)	Human Centered Performance Systems	3600
<b>Number of Projects: 22</b>		<b>Laboratory Project Funding Total (\$K):</b>	<b>35980</b>

### Lawrence Berkeley Laboratory

106	Gas Storage (3)	Gas Storage in Aquifers	100
107	Development (10, 14, 29, 30)	LBL/Industry Fractured Reservoir Performance Definition Project	1300
108	Development (9, 3, 8, 10)	Influence of Clay and Clay Fluid Interaction on Seismic Wave Attenuation in Reservoir Rocks	400
109	Production (23, 18)	Feasibility of Steam Drive in Diatomite	400
110	Development (9, 5, 6, 13)	Effects of Heterogeneity on the Mechanical Properties of Rock	300
111	Environmental & Regulatory (10)	Low Temperature Catalysts for the Oxidation of Methane	125
112	Development (9, 13)	Laboratory and Theoretical Analysis of Transport Paths in Single Natural Fractures	300
113	Development (3, 9, 10, 12, 14)	Energy Partitioning of Seismic Waves in Fractured Rock	300
114	Development (3)	Application of Guided Waves to the Detection and Characterization of Continuous Flow Units and Bounding Surfaces	500
115	Exploration (14, 1)	Subsalt Imaging with Marine Magnetotellurics	350
116	Development (10, 14, 17)	Surface-to-Borehole Electromagnetic Surveying (Vertical Electromagnetic Profiling)	120
117	Development (10, 14, 29, 30)	Geophysical Measurements Facility	400
118	Production (16)	Mechanisms of Mobility Control with Foams	1500
119	Environmental & Regulatory (10)	Airborne Emissions Monitoring and Analysis	200
120	Development (1, 6, 9, 10, 11, 12)	Characterization of Fractured Reservoirs	3000
121	Development (9)	Analysis and Reduction of Well Failures in Diatomite Reservoirs	350
122	Oil Processing & Refining (9)	Solid Superacid Catalysts for Isomerization and Alkylation	230
123	Production	Optimal Fluid Injection and Producibility in Fractured, Low-Permeability Reservoirs	250

Index	NPC Technology Need Category	Project Title	91-95 Funding (\$K)
124	Environmental & Regulatory (5, 6)	Design, Construction, and Application of a Very-Early-Time Electromagnetic (VETEM) System for Detailed Mapping of the Shallow Subsurface	305
125	Environmental & Regulatory (9, 2, 6, 9, 15)	Analog Site for Characterization of Fractured Rock	634
126	Environmental & Regulatory (4, 8, 9, 12, 14)	Site Remediation Analysis and Decision Support	800
127	Oil Processing & Refining (9, 11)	Development of Solid Acid Catalysts for Gasoline Alkylation	840
128	Oil Processing & Refining (9, 11)	Development of Poison Resistant, Low Deactivation Rate, Platinum-Based Bimetallic Catalysts	300
129	Oil Processing & Refining (7, 9, 23)	Synthesis and Characterization of Heterogeneous Catalysts for the Petroleum Industry	475
130	Oil Processing & Refining (2, 1, 4)	Catalytic Membranes for Paraffin Activation and Hydrogen Transport	425
131	Environmental & Regulatory (10)	Fractionation and Cycling of Selenium in the Biogeochemical System of Suisun and San Pablo Bays	800
132	Development (10)	Multifrequency Electromagnetic (EM) Imaging for Reservoir Characterization	785
133	Production	Subsidence, Analysis, and Control	200
134	Exploration (1, 7), Development (4, 8)	Integrated Isotopic Studies of Fluid Flow Processes and Time Scales in Sedimentary Basins	500
135	Development (25, 30, 31, 33)	Advanced Flux Visualization and Virtual Reality for Reservoir Engineering	200
136	Development (10, 15)	Electromagnetic (EM) Imaging through Steel-Well Casing	200
137	Development (10, 14, 29, 30)	High-frequency Seismic-Acoustic Imaging	1000
138	Development (10, 14, 29, 30)	Subsurface Imaging for Characterizing the Effects of Natural Heterogeneity on Transport Properties	1420
139	Gas Processing	Transition Metal-Catalyzed Conversion of CO, NO, H <sub>2</sub> , and Organic Molecules to Fuels and Petrochemicals	260
140	Environmental & Regulatory (8, 14)	Airborne Emissions and Air Quality	500
141	Development (1, 6, 10, 14, 12)	Definition of Reservoir Heterogeneities	799
142	Development (25, 30, 31) Exploration (14, 16, 10)	Geothermal Reservoir Engineering	2000
143	Environmental & Regulatory (10, 12)	Control and Measurement of Toxic and Hazardous Compounds	1000
<b>Number of Projects: 38</b>		<b>Laboratory Project Funding Total (\$K):</b>	<b>23568</b>

### Lawrence Livermore National Laboratory

144	Deepwater Offshore (9, 16), Environmental & Regulatory (8), Production (22)	Large-Eddy Simulation of Separating Turbulent Flow Using the Finite Element Method	500
145	Environmental & Regulatory (9), Development (25),	High-Performance Computing Strategies for Subsurface Flow and Chemical Migration	2100

Index	NPC Technology Need Category	Project Title	91-95 Funding (\$K)
146	Environmental & Regulatory (7, 10, 8, 14)	Chemical Kinetics of Refinery Toxic Emissions and the Clean Air Act	2000
147	Production (23, 24)	Chemistry of Diatomite Dissolution and Silica Precipitation during Steam Flooding	100
148	Exploration (1, 7)	Petroleum Geochemistry and Basin Modeling Project	1800
149	Environmental & Regulatory (7), Oil Processing & Refining (1)	Increased Efficiency and Pollution Reduction in Engine Systems	3000
150	Environmental & Regulatory (15)	Naturally Occurring Radioactive Materials (NORM) Analysis for Oil and Gas Operations	600
151	Gas Storage (2), Environmental & Regulatory (5)	Quantitative Gas Leak Detection / Pressure Safety Training	1100
152	Development (23)	EQ3/6, Software for Modeling Rock/Water Interactions	1500
153	Oil Processing & Refining (2)	Production Of Hydrogen From Municipal Solid Waste	850
154	Development (8, 9)	Analysis of Wellbore Stability, Seal Integrity, and Rock Fracture in the Subsurface Using Statistical Models.	600
155	Production (3), Oil Processing & Refining (12)	Corrosion Sensors	200
156	Environmental & Regulatory (2, 10)	Portable Electrochemical Sensor for Environmental Monitoring and Process Control	1000
157	Environmental & Regulatory (12, 6, 9, 2)	In Situ Microbial Filters	8280
158	DEVELOPMENT (10)	Electromagnetic methods for reservoir characterization and process monitoring	5500
159	Environmental & Regulatory (7)	Advanced Infrared Imaging Sensors	4180
160	Drilling & Completion (5)	Design, Testing, and Improved Manufacturing of Well Perforation Devices	200
161	Deepwater Offshore (16), Oil Processing & Refining (12)	Integrity Testing of Offshore Structures	1000
162	Oil Processing & Refining (22, 23, 24, 25, 27)	Computational Modeling of Hydrocarbon Chemical Kinetics	1000
163	Development (8, 19, 23), Production (3, 4, 6, 17, 19), Oil Processing & Refining (1, 7, 25)	Atomic Scale Electrochemical Modeling	800
164	Environmental & Regulatory (7)	Plasma Processing of Diesel Engine Exhaust	3000
165	Arctic Region Activities (1, 2, 5, 7)	Site Characterization for Exploration and Production Systems	120
166	Exploration (14, 3, 4)	Synthetic Seismic Data (SSD) Calculations - part of the GONII project	500
167	Production (27, 25)	Perforation Dynamics in Geological Media	700
168	Oil Processing & Refining (6)	Granular Flow	4900
169	Development (22, 5)	Evaluation of Geologic Specimens with CT	7000
170	Oil Processing & Refining (4), Production (24)	Oil Shale Technology	5000
171	Environmental & Regulatory (7)	Gas Phase Sensors	310
172	Development	Oil and Gas Well Log Imaging	2000
173	Environmental & Regulatory (9)	3-D Simulation of Multiphase Contaminant Transport and In Situ Remediation of Low Permeability Soils Using an Alternating Current Based Ohmic Heating Technique	385
174	Development (18)	Laboratory Analysis of Rock Core Using Electrical Resistance Tomography	50

<b>Index</b>	<b>NPC Technology Need Category</b>	<b>Project Title</b>	<b>91-95 Funding (\$K)</b>
175	Exploration (4, 6, 10, 12), Development (3, 9, 11)	Velocity Analysis, Parameter Estimation, and Constraints on Lithology for Transversely Isotropic Sediments	600
176	Development (33); Environmental & Regulatory (9)	Optimization Methods for Reservoir Management	1500
177	Deepwater Offshore (16), Environmental & Regulatory (14)	Seismic Hazard Assessment for Santa Barbara Channel Offshore Platforms	250
178	Production (21), Environmental & Regulatory (12)	Battery-powered Portable Micro-machined DNA Detector	1600
179	oil Processing & Refining (12)	Compact Analytical Neutron Interrogation System	100
180	Oil Processing & Refining (23)	Biomimetic Catalysts for the Conversion of Methane to Methanol	3000
181	Exploration (1), Development (2)	Massively Parallel Computing	1000
182	Oil Processing & Refining (25, 21, 4)	Heavy Crude Oil Processing	1550
183	Environmental & Regulatory (2, 10, 11)	Capacitive Deionization	1800
184	Development (10), Environmental & Regulatory (5)	Electrical Resistance Tomography for Subsurface Imaging and Leak Detection	1120
185	Oil Processing & Refining (26)	Economic Analysis and Modeling	600
186	Environmental & Regulatory (12)	Dynamic Underground Stripping	10500
187	Development (15, 14, 20)	Computer Simulation of Nuclear Well Logging Devices	800
188	Development, Production	Oil and Gas Data Infrastructure	2500
189	Environmental & Regulatory (10, 12)	Portable Micro-machined Gas Chromatograph	480
190	Oil Processing & Refining (12)	Quantifying Corrosion Damage	7800
<b>Number of Projects: 47</b>		<b>Laboratory Project Funding Total (\$K):</b>	<b>95475</b>

## Los Alamos National Laboratory

191	Development (33)	Development of a Uniform Resource Characteristics Service	300
192	Exploration (15, 2)	Facility for Information Management, Spatial Analysis, and Visualization	10000
193	Environmental & Regulatory (10, 7,14)	Advanced Lidar Systems for Pollution Monitoring	5000
194	Environmental & Regulatory (10, 5, 7)	A Simple New Monitor For Air Emissions	3100
195	Oil Processing & Refining (1, 7)	Synthesis and Evaluation of New Mixed Metal Nitride Catalysts for Petroleum Refining and Specialty Chemical Manufacturing	100
196	Development (16, 3, 8, 10)	Mapping Conductive Fractures Using a Through-Tubing Geophone Receiver Array (Slimline Through-Tubing Geophone Receiver Array)	780
197	Environmental & Regulatory (11)	Microcellular Foams for the Separation of Heavy Metal-Ions from Waste Streams	500
198	Environmental & Regulatory (8, 14)	Atmospheric Transport and Fate of Pollutants Over Complex Terrain	5250
199	Development (16, 3, 8, 10)	Advanced Sensor Technology for Microholes and Other Seismic Applications	225

Index	NPC Technology Need Category	Project Title	91-95 Funding (\$K)
200	Development (16, 3, 8, 10)	Advanced Instrumentation for Fracture Mapping/Microseismic (Downhole Microprocessor for Mono-cable Telemetry Systems)	265
201	Deepwater Offshore (11)	Fatigue Failure of Top Drive Drilling Rigs to Jarring Operations	175
202	Oil Processing & Refining (1, 11), Environmental & Regulatory (10)	Microwave Driven Chemistry	3000
203	Deepwater Offshore (16, 9)	Damage Detection and Health Monitoring of Structures and Mechanical Systems	1400
204	Development (25,2,6), Exploration (15)	National Information Infrastructure Technologies Applied to Database Synthesis and Remote Problem-Solving for the Carpinteria Reservoir Re-Development Project	100
205	Gas Gathering (1), Gas Storage (7)	Thermoacoustic Natural Gas Liquefier	850
206	Environmental & Regulatory (12, 2, 11), Oil Processing & Refining (11)	An Intelligently Controlled Three-Phase Centrifuge for Petroleum Waste Separation	1830
207	Drilling & Completion (5, 1, 6), Production (5, 18, 25)	Ultrasonic Reduction of Wellbore Deposits and Formation Damage	550
208	Exploration (4, 3)	Testing Advanced Computational Tools for 3D Seismic Analysis Using the SEG/EAGE Model Dataset	775
209	Oil Processing & Refining (25,6)	Computer Simulation of Reactive Multiphase Flow	2100
210	Environmental & Regulatory (9, 6, 12, 14)	Modeling Transport and Remediation of Soil and Groundwater Contaminants	5000
211	Oil Processing & Refining (1, 19, 25)	Modeling and Simulation of Hydrocarbon Catalysis in Zeolites.	2300
212	Development (10), Production (25)	Binary Liquid Explosive and Initiator System for Wellbore Applications	1000
213	Exploration (2), Development (33)	Modeling Ocean Currents and Eddies for Offshore Operations	150
214	Development (25, 1, 27)	Innovative Gridding and Solution Techniques for High-Performance Reservoir Simulation	2100
215	Environmental & Regulatory (15, 4, 14)	Naturally Occurring Radioactive Materials (NORM) Analysis For Oil And Gas Operations	120
216	Exploration (3, 4)	Gulf of Mexico Sub-Salt Seismic Imaging Project	1625
217	Development (33, 25)	Prepare Information for the Los Alamos/Petroleum Recovery Research Center Electronic Information System as a Means for Communications and Data Transfer to Independent Gas and Oil Producers	500
218	Drilling & Completion (5, 1, 3), Development (9, 8) , Production (25, 13)	Coupled Rock/Fluid Mechanics Numerical Simulations Applied to Well Completions	1650
219	Development (16, 3, 8, 10)	Microseismic Fracture Mapping and Determination of Fluid Flow Paths in a Producing Reservoir	1500
220	Oil Processing & Refining (26, 3)	Neural Networks for Chemical Process Control	1300
221	Exploration (4, 3)	New Methods for Modeling and Processing Seismic Data	900
222	Drilling & Completion (5), Production (25)	Perforator Design and Testing	150
223	Development (25, 5, 8, 30)	Pore-Scale Flow and Examination of Effects of Scaling on Improved Oil Recovery Processes	1400

<b>Index</b>	<b>NPC Technology Need Category</b>	<b>Project Title</b>	<b>91-95 Funding (\$K)</b>
224	Development (25, 33)	Reservoir Studies and Information Delivery Tools for Independent Oil Producers	1600
225	Development (27, 25, 33)	Scale-Up in Heterogeneous Reservoirs	175
226	Exploration (4, 3), Development (3)	Society of Exploration Geophysicists Synthetic Seismic Database	1500
227	Development (14, 16, 20)	Computer Simulation in Support of Nuclear Well-Logging	1200
228	Drilling & Completion (5), Production (25)	Advanced Perforator Technology	1800
229	Development (4, 8, 21, 25, 30), Gas Gathering (2), Gas Storage (2)	Multicomponent Labeled Tracer Technology: Characterization of Coupled Transport and Chemical Interactions in Petroleum Reservoirs	650
230	Drilling & Completion (10, 1, 2, 9, 12, 13)	Multi-Phase Fluid Simulator for Underbalanced Drilling (Hydrodynamic Modeling of Multi-Phase Drilling Fluid Flow to Simulate Underbalanced Drilling)	600
231	Development (25,28), Exploration (13)	Sunrise: A National Information Infrastructure Prototype	3500
232	Development (25,2)	Parallel Object Oriented Methods and Applications	1250
233	Environmental & Regulatory (9,6)	Lithology Characterization for Remediation of Underground Pollution	875
234	Development (25), Exploration (13)	The Development of a General Reservoir Simulation for Massively Parallel Computers	875
235	Development (25, 28, 33)	Advanced Reservoir Management (ARM) for Independent Oil and Gas Producers	6500
<b>Number of Projects: 45</b>		<b>Laboratory Project Funding Total (\$K):</b>	<b>76520</b>

### National Institute for Petroleum and Energy Research

236	Development	Characterization of Fractured Rock to Produce Remaining Oil in Place.	300
237	Development (2), Production (3, 2, 11)	Field Demonstrations in High Priority Reservoir Classes	17736
238	Development	Integrated Geoscience/Engineering Methods of Optimal Reservoir Upscaling	3827
239	Environmental & Regulatory	Natural Gas Technology Enhancements	3000
240	Environmental & Regulatory	AMFA Fleet Fuel and Oil Analyses	278
241	Environmental & Regulatory	Establishing California Air Resources Board Reactivity Rating for Ethanol	185
242	Drilling & Completion	Drilling, Completion and Re-Completions (Underbalanced Drilling, Wellbore Stability, Coiled Tubing and Slimhole Drilling)	475
243	Exploration, Drilling & Completion	Risk-Based Decision Management	321
244	Environmental & Regulatory	California Pipeline and Gathering Line Assessment	650
245	Oil Processing & Refining	Processing and Utilization Research - Thermodynamic and Thermophysical Property Measurements	500

Index	NPC Technology Need Category	Project Title	91-95 Funding (\$K)
246	Oil Processing & Refining	Conduct Round Robin Tests on Heavy Crude and Bitumen	150
247	Production	Chemical Methods for Improved Oil Recovery	2000
248	Oil Processing & Refining	Processing and Utilization Research - Analysis and Remediation of Contaminated Soil and Groundwater	200
249	Environmental & Regulatory	Area of Review Variance Program	650
250	Production	Biotechnology for Improved Oil Recovery	2417
251	Environmental & Regulatory	Biodiesel, Commercialization of a Renewable Fuel	695
252	Oil Processing & Refining	Processing and Utilization Research - Analysis of the Refining Industry	547
253	Oil Processing & Refining	Development of Analytical Methodology for Analysis of Heavy Crudes: Catalytic Cracking Behavior of Compound Classes in Petroleum Resid	1500
254	Environmental & Regulatory	Impacts of Alternative Fuels on Air Quality	278
255	Oil Processing & Refining	Processing and Utilization Research - Nuclear Power Training Unit Diesel Fuel Testing	100
256	Environmental & Regulatory	Safety and Environmental Management Program	240
257	Oil Processing & Refining	Processing and Utilization Research - Additives for Coke Reduction during Heavy Oil Processing	445
258	Oil Processing & Refining	WFO - Petroleum Product Surveys	225
259	Oil Processing & Refining	Processing and Utilization Research - Upgrading and Environmental Concept	643
260	Oil Processing & Refining	Processing and Utilization Research - OER and Thermodynamic Properties for Polycyclic Systems by Non-Calorimetric Methods	3000
261	Production	Gas Flooding Methods for Advanced Oil Recovery	2060
262	Production	Thermal Methods for Advanced Oil Recovery	833
263	Development	Relative Permeability - Development of Relative Permeability measurement Methodology and Correlations of Pore Characteristics with Multiphase Relative Permeability and Capillary Pressure Functions	1507
264	Oil Processing & Refining	Processing and Utilization Research - Naval Air Warfare Center - Jet Fuel Support	250
265	Oil Processing & Refining	Processing and Utilization Research - Navy Petroleum Office - Fuel Reclaiming	100
266	Environmental & Regulatory	Monitoring Tulsa Public Schools Alternative Fuel Fleet	315
267	Oil Processing & Refining	Processing and Utilization Research - Process Engineering Property Measurements on Heavy Oils	10000
268	Environmental & Regulatory	Monitoring of Tinker Air Force Base Alternative Fuel Fleet	900
269	Environmental & Regulatory	Safety and Environmental Management Demonstration Program	660
270	Oil Processing & Refining	Strategic Petroleum Reserve Supporting Research	3750
271	Development	Imaging Techniques Applied to the Study of Fluids in Porous Media	2163
272	Environmental & Regulatory	Regulatory Streamlining	1000
273	Oil Processing & Refining	Crude Oil Analysis Database	225

Index	NPC Technology Need Category	Project Title	91-95 Funding (\$K)
274	Oil Processing & Refining	Processing and Utilization Research - Defense Fuel Supply Center Problem Fuel Chemistry	750
275	Exploration	Exploration Keys Used to Reduce Risk in Exploration Prospect Generation in Selected U.S. Basins	1500
<b>Number of Projects: 40</b>		<b>Laboratory Project Funding Total (\$K):</b>	<b>66375</b>

### Oak Ridge National Laboratory

276	Oil Processing & Refining (2, 16, 18, 4)	Renewable Hydrogen Production for Fossil Fuel Processing	500
277	Oil Processing & Refining (16, 18, 4)	Separations Concepts	300
278	Environmental & Regulatory (1, 2, 3, 4, 9)	In Situ Vitrification	2000
279	Gas Processing (2, 3, 8), Oil Processing & Refining (1, 4, 16)	Heterogeneous Catalysts Related to Energy Systems	3520
280	Exploration (15), Arctic Region Activities (2, 3, 5, 7)	Joint High-Performance, High-Resolution Ocean Circulation Modeling for Enhancing Offshore Oil and Gas Exploration and Production	350
281	Environmental & Regulatory (14)	Programmatic Environmental Assessment for the Oil Research Program	250
282	Environmental & Regulatory (4, 10, 12, 14), Gas Processing (6)	Mercury Air/Surface Exchange in the Environment	1100
283	Production (3, 4, 6, 9, 12, 15), Arctic Region Activities (5, 7), Deepwater Offshore (1, 2, 4, 5, 6, 8, 15), Gas Gathering (2, 3, 4, 5), Oil Processing & Refining (14, 15), Environmental & Regulatory (8, 10, 14)	Pipeline Safety	4500
284	Gas Processing (2, 3, 8), Oil Processing & Refining (4, 6, 21)	Advanced Bioreactor Systems for Gaseous Substrates	300
285	Exploration (8, 15), Environmental & Regulatory (5, 7, 8, 14)	Airborne Geophysical Surveying	2405
286	Oil Processing & Refining (15, 5), Deepwater Offshore (1, 4, 5, 6, 7)	ANS Flow blockage Computational Fluid Analysis and Experimentation	1300
287	Oil Processing & Refining (3, 15, 19, 25), Production (3, 4)	ANS and HFIR Thermal and Hydraulic Analysis and Experimentation	12000
288	Environmental & Regulatory (7, 8, 10, 14)	METER and AENEC Programs	600
289	Environmental & Regulatory (7, 8, 10, 14)	Prediction of Air Pollution Dispersion/Transformation/Fate	3000
290	Oil Processing & Refining (24, 27, 28, 20, 21)	Low Emissions Diesel Fuels	1050
291	Exploration (8, 10), Environmental & Regulatory (5, 7, 8, 14), Gas Gathering (2)	Airborne Remote Sensing of Natural Gas Leaks	1065
292	Environmental & Regulatory (3, 6, 9, 14), Exploration (4)	Seismic Reflection Acquisition, Processing and Source Comparison	575
293	Environmental & Regulatory (3, 6, 9, 12, 14)	The Seasonal SOIL Compartment Model (SESOIL) and Computational Fluid Dynamics Modeling	135
294	Gas Processing (3), Oil Processing & Refining (16, 18, 4)	Removal of Heteroatoms form Crude Oil	900
295	Oil Processing & Refining (16, 18, 1, 2, 4, 6, 21)	Advanced Bioreactor Concepts and Development	1400

Index	NPC Technology Need Category	Project Title	91-95 Funding (\$K)
296	Exploration (3, 4, 6, 10, 13), Development (2, 12)	Advance Computational Tools for 3-D Seismic Analysis using the SEG/EAGE Model Dataset	2550
297	Environmental & Regulatory (7, 8, 10)	Environmental Regulations and Compliance Requirements for Clean Air Act and Other Regulations	4500
298	Environmental & Regulatory (1, 2, 10, 12, 14)	In Situ Chemical Oxidation of Organic Contaminants in Soil and Groundwater	555
299	Oil Processing & Refining (16, 17, 6, 23)	Development of Materials for Black Liquor Recovery Boilers for Pulp and Paper Mills	550
300	Oil Processing & Refining ((16, 18, 1, 6, 21, 23), Production (1, 2, 3, 4, 16, 21)	Biological Catalysts in Organic Media	1100
301	Environmental & Regulatory (3, 6, 9, 12, 14)	Remediation of DNAPL Compounds in Low Permeability Media	1000
302	Development (4, 21, 23, 24), Environmental & Regulatory (5, 8, 9)	Tracer Technology	8000
303	Oil Processing & Refining (15, 20, 27, 28)	Fuel Models	500
304	Production (25, 26), Development (26)	Computational Simulation of Hydrofracturing	155
305	Environmental & Regulatory (3, 4, 7, 14)	Quantitative Assessment of Environmental Risks	5000
306	Production (11, 16, 18, 23)	Enhanced Recovery of Petroleum Using High-Power Microwaves	2300
307	Environmental & Regulatory (7, 14), Oil Processing & Refining (8)	Estimating the Externalities of Fuel Cycles Associated with Electric Power Production	4000
308	Oil Processing & Refining (20, 24, 28), Development (5, 18, 30), Environmental & Regulatory (4, 14)	Advanced Mass Spectrometry for the Characterization and Quantitative Analysis of High Molecular Weight Materials	3500
309	Oil Processing & Refining (17, 5, 15), Arctic Region Activities (4, 5, 6), Deepwater Offshore (4, 5, 7, 8)	Heavy-Section Steel Technology and Irradiation Programs	5000
310	Development (5, 7, 8, 9, 17, 23), Drilling & Completions (3), Production (25)	Borehole Geophysical Logging	975
311	Exploration (7), Development (4, 5, 6, 14, 18, 21, 22, 23, 24, 28), Production (4, 5)	Experimental and Analytical Geochemistry	1890
312	Environmental & Regulatory (5, 7, 8, 10, 14)	Applied Analytical Mass Spectrometry (Emissions/Process Monitoring, Field Instrumentation, Residuum/Product Characterization)	3500
313	Gas Processing (4), Oil Processing & Refining (16, 17, 2, 6, 23)	High Pressure Heat Exchange System - Advanced Materials for Steam-Methane Reforming	1600
<b>Number of Projects: 38</b>		<b>Laboratory Project Funding Total (\$K):</b>	<b>83925</b>

### Pacific Northwest Laboratory

314	Environmental & Regulatory (5, 6)	The Effects of the Exxon Valdez Oil Spill on Pacific Herring	3500
315	Environmental & Regulatory (4, 5)	Effects of Petroleum Products on Bull Kelp; Perform Field Assessment of Possible Damages to Eelgrass in Faadalgo Bay, WA; Investigate Effects of Oil on Kelp <i>Nereocystis Leutkeana</i> ; Analyses Using Seimpermeable Membrane Devices	201

Index	NPC Technology Need Category	Project Title	91-95 Funding (\$K)
316	Environmental & Regulatory (7, 8)	Low-Temperature Catalytic Gasification of Wet Wastes	1905
317	Environmental & Regulatory	Investigation of Self-Help Oil-Spill Response Techniques and Equipment and Effects of Petroleum Contaminated Waterways on the Spawning Migration of Pacific Salmon	173
318	Oil Processing & Refining (11)	Catalytic Hydrotreating of Biomass Pyrolysis Oils	160
319	Oil Processing & Refining (11)	Nanophase Catalyst Synthesis and Reaction Mechanisms	1585
320	Environmental & Regulatory (9, 10)	Conduct Literature Review on Polychlorinated Biphenyl (PCB) Sorption from Gas Line Condensates into Soils	106
321	Environmental & Regulatory (4, 5)	Predicting TPH Biodegradation & Leaching in Contam. Soils Using State-of-the-Art Hydrocarbon Charact. Evaluate Chem. & Phys.Properties in Solids, Water, & Oil Samples Great Lakes; Evaluate Environmental Monitoring Program for Legovan Amuay Oil Refinery	117
322	Oil Processing & Refining (7)	Superacidic Solid Acid Catalysts	680
323	Environmental & Regulatory (5)	U. S. Coast Guard Human Factors Engineering	3943
324	Environmental & Regulatory (4, 6, 7, 12); Oil Processing & Refining	Petroleum Sludge Treatment; Spent Catalyst Processing	1100
325	Environmental & Regulatory (5, 6)	Toxicological Monitoring of Ballast-Water Effluent Discharge	300
326	Environmental & Regulatory (4, 5)	Perform Field Assess of Possible Damage to Eelgrass in Fidalgo Bay, WA During Oil Spill Cleanup, Investigate Effects of Oil on Kelp Nereocystis Luetkeana, Conduct Analyses Using SPMD to Estimate Bioconcentration Potential of Oil Additives in Aquatic Life	152
327	Environmental & Regulatory (5, 6)	Conduct Histopathological Evaluation and Body Burden Analysis of Alaska Salmon Potentially Affected by the Exxon Valdez Oil Spill	100
328	Environmental & Regulatory (5, 6)	Alyeska Sediment Studies	250
329	Environmental & Regulatory	Soil Washing for Removal of Heavy Metals and Radionuclides	1214
<b>Number of Projects: 16</b>		<b>Laboratory Project Funding Total (\$K):</b>	<b>15486</b>

### Sandia National Laboratories

330	Oil Processing & Refining (4, 20, 24, 25, 27)	Molecular Modeling of Macromolecular Structure of Complex Hydrocarbons and Fuels	750
331	Environmental & Regulatory (10, 11, 12)	Photocatalytic Detoxification of Organic Contaminants	3200
332	Drilling & Completion (8)	Advanced Synthetic-Diamond Drill Bit Technology for Hard-Rock Drilling	1500
333	Drilling & Completion (6, 1, 3, 5, 10), Production (11, 13, 25)	Near Wellbore Mechanics (ACTI)	1700

Index	NPC Technology Need Category	Project Title	91-95 Funding (\$K)
334	Environmental & Regulatory (9, 5), Drilling & Completion (11), Development (4)	Monitoring of Contaminants, In-Situ Remediation, Subsurface Barriers, and Landfill Covers Using Tracers	970
335	Development (8), Environmental & Regulatory (9, 12), Exploration (9), Drilling & Completion (2, 6)	Fluid/Rock Interactions - Mineral Dissolution and Precipitation Kinetics, Sorption, and Surface Charge Speciation	1800
336	Oil Processing & Refining (11,4), Environmental & Regulatory (10)	Organic Destruction/Re-Use and Recycling Methodologies	2300
337	Environmental & Regulatory (5), Gas Gathering (2)	Leak Detection Using Horizontal Logging and Electromagnetic Sensor Techniques	500
338	Oil Processing & Refining (11), Environmental & Regulatory (10)	The Origin and Fate of Toxic Combustion By-Products in Process Heaters	2140
339	Oil Processing & Refining (1, 4, 19), Gas Processing (4, 5, 6)	Design and Development of Smart Membranes for Small Molecule Separations	2100
340	Drilling & Completion (11), Development (31)	Acoustic Telemetry	2700
341	Development (10, 3), Exploration (3, 10, 14, 16)	Three Component Borehole Seismic Source	3160
342	Environmental & Regulatory (10), Gas Processing (6)	Laser-Spark Spectroscopy for Continuous Metal Emissions Monitoring	1800
343	Drilling & Completion (9,11)	Downhole Instruments for Slim, High-Temperature Wells	2000
344	Environmental & Regulatory	Transport and Fate of Oil Spilled in a Marine Environment	600
345	Gas Gathering (2), Environmental & Regulatory (5,10)	The Development of a Real-Time Video Imaging System for Natural Gas Leaks	800
346	Development (14, 2, 9, 25, 33)	Geomechanics of Petroleum Reservoirs	1400
347	Oil Processing & Refining (1, 6, 7, 12, 16, 22)	Catalyst Assessment and Reactor Hydrodynamics for Indirect Liquefaction	2500
348	Drilling & Completion (3), Production (11, 25)	Hydraulic Fracturing Diagnostics	3500
349	Environmental & Regulatory (6), Development (31)	In Situ Permeable Flow Sensor	1520
350	Development (9, 2, 5, 14, 18), Exploration (1, 9)	Rock Mechanics Investigations	2070
351	Deepwater Offshore (9, 16)	Advanced Computational Models for Deep Water Oil and Gas Production (ACTI)	650
352	Oil Processing & Refining (1, 4, 11, 25)	Conversion of Carbon Dioxide Using Biomimetic Catalysts	1500
353	Drilling & Completion (9)	Slimhole Drilling for Geothermal Exploration and Reservoir Assessment	5000
354	Drilling & Completion (3), Production (11, 13, 25)	Hydraulic Fracturing	600
355	Oil Processing & Refining (1, 25)	Study of Catalysts Using ab initio Codes on Massively Parallel Computers.	1050
356	Development (7, 17, 18)	Natural Fractures	1800
357	Development (10, 3), Exploration (3, 10, 14, 16)	Advanced Borehole Seismic Receiver	3100
358	Oil Processing & Refining (9, 1, 7, 16), Environmental & Regulatory (10)	Replacement of Liquid H2SO4 and HF Acids with Solid Acid Catalysts in the Paraffin Alkylation Process	765
359	Drilling & Completion (13)	Geothermal Drilling Organization	2000
360	Environmental & Regulatory (12, 9)	Numerical Modeling of Thermal Enhanced Vapor Extraction Remediation Technology	2500
361	Development (3, 10), Exploration (4, 14)	Single-well Imaging of Salt Dome Flanks (ACTI)	1550

Index	NPC Technology Need Category	Project Title	91-95 Funding (\$K)
362	Development (10, 6, 14), Environmental & Regulatory (10), Exploration	Electromagnetic Reservoir Characterization	3700
363	Development (2), Exploration (5, 9, 11)	Computational Geomechanics for Geologic Structure and Reservoir Mechanics (ACTI)	1250
364	Environmental & Regulatory (9, 5)	Natural Geochemical Attenuation and Chemical Manipulation to Stabilize Groundwater Contaminants	580
365	Production (10, 3, 5, 7, 8)	Applied Production Technology	1700
366	Development (8), Environmental & Regulatory (6)	Flow Visualization Laboratory for Multiphase Flow Processes	5000
367	Drilling & Completion (6, 1, 3), Development (9, 26), Production (11, 25), Environmental & Regulatory (1, 2)	Increased Effectiveness Of Hydraulic Fracturing Through Advanced Computational Technology (ACTI)	825
368	Exploration (4, 3, 10, 13)	3-D Seismic Imaging of Complex Geologies: Remote and Rapid Processing of Terabyte Data Sets (ACTI)	1650
369	Oil Processing & Refining (1, 21, 22)	Highly Dispersed Catalysts	1200
370	Development (9, 3), Deepwater Offshore (1, 16)	Seafloor Earthquake Measurement System (SEMS)	700
371	Drilling & Completion (13), Environmental & Regulatory (12)	Shallow Directional Drilling Development for Environmental Use	1600
372	Oil Processing & Refining (12, 3, 6), Production (5)	Advanced Thermally Stable Jet Fuels and Field Measurement of Oil Properties	2660
373	Oil Processing & Refining (1,7,16,22)	Catalyst Development for Direct Liquefaction and Dehydrogenation Processes	4350
374	Environmental & Regulatory (4, 6, 9, 14)	Risk-Based Decision Analysis Tools for Remedial Alternatives Selection Based on Probabilistic Flow and Transport Simulators	2200
375	Production (17), Environmental & Regulatory (9)	Macroscopic Transport in Geologic Media: A Lattice Gas Automata Study	500
376	Oil Processing & Refining (22, 23, 25)	Catalysts for the Conversion of Light Hydrocarbons to Alcohols	1125
377	Oil Processing & Refining (22, 4, 21, 16)	Advanced Direct Liquefaction Concepts for Improved Efficiency and Economics in the Refining of Coal-Derived Liquids	715
378	Drilling & Completion (4, 3, 13)	Lost Circulation Technology	3000
379	Gas Processing (4, 8)	Microengineered Polymer-Derived Adsorbents for Natural Gas	300
380	Exploration (4), Development (33)	Gas and Oil National Information Infrastructure (GONII)	4500
381	Oil Processing & Refining (1, 16), Environmental & Regulatory (10)	Reduction of Nitrogen Oxide Emissions for Lean Burn Engine Technology	2000
382	Oil Processing & Refining (21, 25)	Simulation of Residual Oil Hydroprocessing Units on Massively Parallel Supercomputers	800
383	Gas Storage (7)	U.S. Strategic Petroleum Reserve Geotechnical Support	16500

Number of Projects: 54

Laboratory Project Funding Total (\$K): 116380



Index: 1

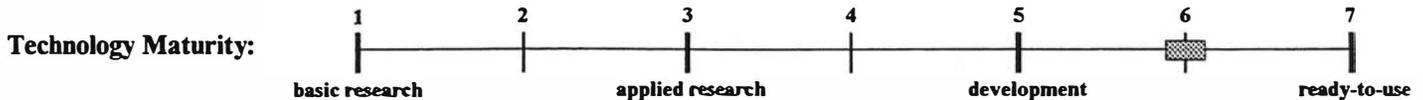
Category: Gas Processing (6, 12), Environmental & Regulatory

Laboratory: Argonne National Laboratory      Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Trainable Electrocatalytic Cermet Gas Microsensors Program

**Description:** The electrocatalytic gas microsensors program has been developing an "active" gas sensing technique for use with its cermet (ceramic metallic) microsensor. The sensor technology brings together three established complimentary technologies to produce a single miniature microsensor that responds uniquely to a wide variety of gases and mixtures, with the added capability of being trainable for interest gases. The microsensors are fabricated using economical thick-film screening techniques and cermet materials. A cyclic voltammetry active measurement technique is used in conjunction with the microsensor to produce an electrical signature of the gas or mixture it is exposed to, and neural network-artificial intelligence (AI) techniques are used to identify and quantify the gas or mixture in near-real time. The support for the sensor has been reduced to a single microcontroller chip with embedded data acquisition and AI processing code. The current thick-film sensors are 2 x 3 mm in size and can operate on a network or individually with a miniature support system. Thin-film versions are being developed that are 1/100th that size. The current project in this 7 year old program involves tuning the microsensor for CO2/O2 detection for closed-circuit underwater breathing apparatus, to improve operational safety and extend dive times. An industrial partner (NeuralWare) is interested in the applied AI spin-off technology (neural network integrated circuit) being developed and is assisting in developing neural network code for those applications. Early work had investigated the application of this technology for arms control and treaty verification. New work has begun developing the sensor for emissions control, CO monitoring, and textiles processing control. The project is assisted by several departments at ANL including Energy Systems Division (sensor and AI system design), Materials Science Division (advanced cermet materials preparation), Chemical Technology (data processing and analysis), and Electronics.

91-95 Funding (\$K): 530      Dates: 1994 - 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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 Naval Surface Warfare Center: John Kady: Phone: (708) 235-5112, Fax: (708) 235-5112, e-mail: KADY\_JOHN@ccmail.ncsc.navy.mil  
 NeuralWare: Ms. Berni

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 2

Category: Environmental & Regulatory (12)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

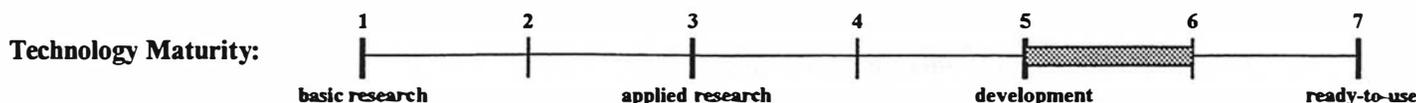
Title: Restoring Wetlands After Pipeline Installation

**Description:** An Argonne National Laboratory study documented the impacts of natural gas pipeline ROWs on 15 wetland communities. Pipelines involved ranged in age from 1 to 31 years since installation and traversed a variety of wetland types. During a single site visit, data were collected on the plant communities which established on the ROW and those in the undisturbed wetlands adjacent to the ROW. Any modification of the general topography, water flow patterns, and percent coverage of surface water were recorded.

The study revealed that ROWs associated with pipelines installed during the last several years under recent wetland regulations normally are revegetated with dense and diverse plant communities within several years after site closure. The plant communities that develop on the ROWs are similar to those occurring in the adjacent natural areas in terms of species richness, wetland indicator values, and percentages of native species. These plant communities develop readily from naturally available propagules without soil amenities or artificial seeding. Traditional ROW maintenance by periodic mowing to exclude large, woody vegetation allows the development of ROW plant communities consisting of an herb stratum composed predominantly of plant species found in the adjacent natural areas. Little evidence was observed to indicate that ROWs degrade the wetland by providing avenues for invasive and nonnative plant species. Most impacts are temporal in nature, decreasing with time.

Argonne's study verified that current environmental regulations and pipeline technology limit impacts of pipelines through wetlands both spatially and temporally. The current recommendation to seed ROWs through wetlands with annual ryegrass in the types of wetlands surveyed is not necessary and may only serve to delay establishment of native vegetation. This knowledge should both facilitate the protection of wetlands and avoid unnecessary effort on the part of regulatory agencies and gas distribution companies..

91-95 Funding (\$K): 400      Dates: 1991-1994



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: Pat Wilkey Division: ES Phone: (708) 252-6258

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 3

**Category:** Environmental & Regulatory (12, 14)

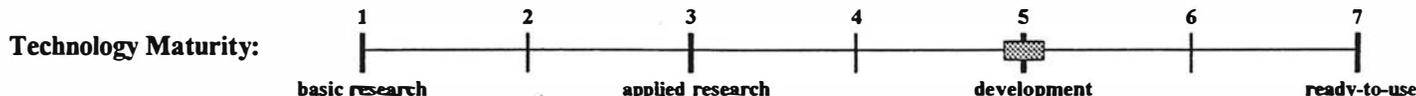
**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** Evaluation of Contaminated Sites Using Heavy Metal Speciation Techniques

**Description:** Until recently, heavy metal speciation techniques have been used primarily as characterization and analytical tools for determining the concentrations and speciation of heavy metals present in soils. These projects investigated the use of chelant extraction for removing heavy metals from contaminated soils. Objectives of these studies included: (1) Determining the heavy metal speciation (exchangeable, carbonate, reducible oxides, organically-bound, and residual), (2) Determining the feasibility of chelant extraction for removing heavy metals from soils using soil washing techniques, (3) Determining optimum pH conditions and extractant concentrations for maximum metal removal, and (4) Determining the leachability of the metal residual present in the soil after soil washing (using the Toxicity Characteristics Leaching Procedure -- TCLP). The sequential extraction technique has been used in conjunction with soil washing operations at ANL. The project establishes the relationship between heavy metal speciation and heavy metal removal, as well as TCLP and heavy residuals in the soil as it relates to clean-up criteria.

**91-95 Funding (\$K):** 335      **Dates:** 1994 - 1995



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

**Key Personnel:** ANL: Robert W. Peters: Phone: (708)252-7773, FAX: (708)252-9281, E-mail: ROBERT\_PETERS@QMGate.ANL.GOV

**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 4

Category: Gas Processing (6)

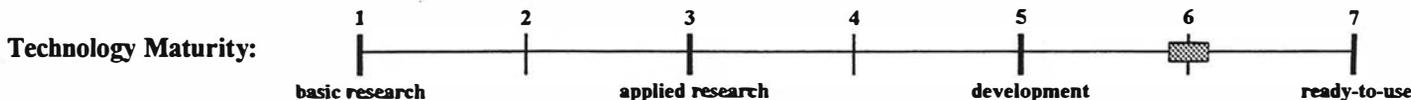
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Gas Chromatography/Matrix-Isolation/Fourier Transform Infrared Spectroscopy

Description: Gas Chromatography/Matrix-Isolation/Infrared Spectroscopy (GC/MI-IR) combines the ability of capillary GC to separate the components of complex mixtures with the high sensitivity and specificity of MI-IR. In the GC/MI-IR technique, as developed at Argonne National Laboratory, a GC column effluent containing 1% argon travels through a glass-lined transfer line and is sprayed directly on a cryogenic collector. The collector, a mirror-finished, gold-plated carousel, is slowly rotated by a computer controlled stepping motor. This action produces a strip of frozen argon in which the sample molecules, which are surrounded by the argon matrix, retain their capillary column separation. Once the sample is trapped in the matrix, the infrared spectra of the compounds numbering a hundred or more can be measured. The MI-IR spectra are free of band-broadening or perturbations caused by rotation or intermolecular forces, such as hydrogen bonding. The GC/MI-IR has nearly the same sensitivity as GC/MS, and the data complement mass spectral data. The GC/MI-IR is ideal for distinguishing between organic isomeric compounds.

91-95 Funding (\$K): 300 Dates: 1991-present



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Gerald T. Reedy Division: CMT/ACL Phone: (708) 252-3599

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 5

**Category:** Gas Processing

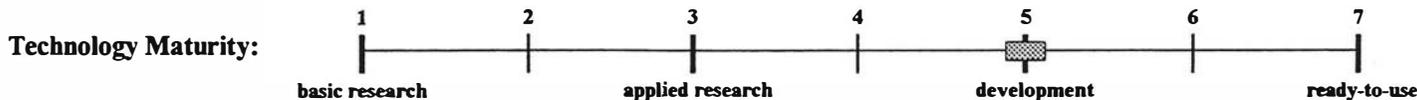
**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** Reformers for Fuel Cells

**Description:** Fuel cell powered vehicles require an on-board source of hydrogen. Alternative fuels such as methanol, ethanol, and natural gas have greater energy density than hydrogen. With alternative fuels, on-board reformers are needed to convert the fuel into hydrogen and supply it to the fuel cell on demand. Steam reforming and partial oxidation reforming are two of the techniques available for this conversion; each has its advantages and limitations. Our research investigates the potential of each technique. Different system designs are investigated through the use of theoretical models. For either method, catalysts are required, which must be tested for activity and selectivity. Based on these analytical and experimental results, compact, lightweight reformers are designed and tested. A bench-scale partial oxidation reformer for methanol is currently being evaluated for use with fuel cell propulsion systems.

**91-95 Funding (\$K):** 350      **Dates:** 1992-present



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

**Key Personnel:** Michael Krumpelt Division: CMT Phone: (708) 252-8520 Fax: (708) 252-4176 E-mail: krumpelt@cmt.anl.gov

**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 6

**Category:** Gas Processing (2,8), Environmental & Regulatory

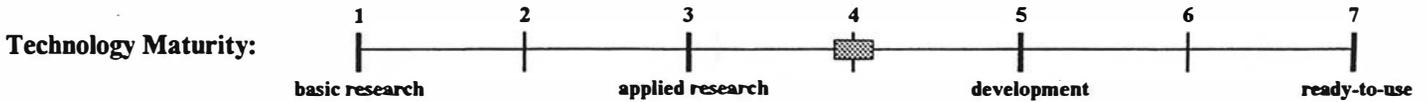
**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** Capturing Carbon Dioxide Emissions From Flue Gas Streams

**Description:** Because of concern about the greenhouse effect, future regulations may require coal-fired power plants to capture and sequester carbon dioxide (CO<sub>2</sub>). Argonne and the Massachusetts Institute of Technology reviewed methods and identified research, development, and demonstration needs for capturing CO<sub>2</sub> from conventional pulverized-coal-fired power plants, integrated coal-gasification combined-cycle plants, and fuel-cell plants. (The fuel cell is still in the design stage but is expected to be widely used in the next two decades.) In another project, funded by Morgantown Energy Technology Center, Argonne defined how capturing CO<sub>2</sub> affects present designs for the integrated coal-gasification combined-cycle plants and fuel-cell plants. Results indicate that capturing CO<sub>2</sub> from combined-cycle and fuel-cell power plants is less complicated, less energy intensive, and less costly than from conventional coal-fired power stations.

**91-95 Funding (\$K):** 500      **Dates:** 1992-1994



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

**Key Personnel:** Edward J. Daniels Division: ES Phone: (708) 252-5279 Fax: (708) 252-3443 E-mail: ed\_daniels@qmgate.anl.gov  
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**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 7

**Category:** Gas Processing (6)

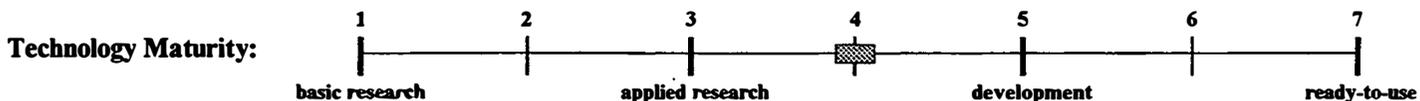
**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** Continuous Fiber Ceramic Composites: Testing and Evaluation

**Description:** We have developed state-of-the-art mechanical testing and microstructural evaluation facilities for continuous fiber ceramic composites (CFCCs). We routinely evaluate mechanical properties (stress-strain plots, first matrix cracking strain, ultimate strength, work of fracture, fiber/matrix interfacial strength) of composites at room and elevated temperatures. We have established a special technique to evaluate in-situ fiber strength in composites to assess fiber damage during processing and in service. Application of these techniques and test procedures includes process optimization and reliability prediction of ceramic composites for use in high-temperature structural applications such as advanced heat engines, heat exchangers, and hot-gas filters.

**91-95 Funding (\$K):** 120      **Dates:** 1991-present



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

**Key Personnel:** J.P. Singh Division: ET Phone: (708) 252-5123 Fax: (708) 252-3604 E-mail: jp\_singh@qmgate.anl.gov

**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



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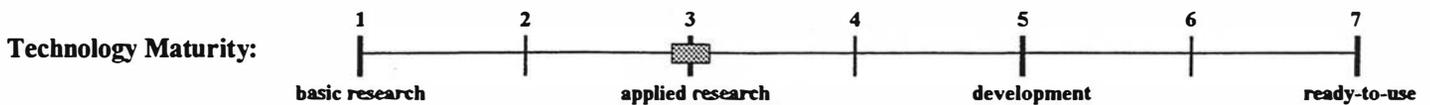
Category: Oil Processing & Refining (20,19), Environmental & Regulatory

Laboratory: Argonne National Laboratory      Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Micro Laser Desorption Time-Of-Flight Mass Spectrometer

**Description:** The objective of this work is to develop an economical (\$3,000-\$6,000/unit), mass produced, micro (4-10 cm flight tube), laser desorption laser photo ionization time-of-flight mass spectrometer (LD-LP-TOF-MS) prototype for on-site monitoring of nuclear related materials. The prototype will be hand-portable, completely self contained (i.e., including all system components, such as high vacuum pump, computer, source, detector, sample port, etc.). The unit will weigh 15-18 pounds and be the size of a thick notebook, approximately 4"x11"x9". The work scope encompassed in this proposal includes background studies with a model laboratory unit, the design and manufacture of a fully functional prototype, and ultimately a field evaluation of the prototype's performance. Specifically, the work scope can be described as five main tasks. Task 1 includes a design study and the development of a laboratory micro linear and micro angular reflectron LD-LP-TOF-MS. In Task 2, system performance will be determined using standards and molecules of programmatic interest. In Task 3, the most promising linear or reflectron prototype will be manufactured. In Task 4, appropriate packaging will be added to provide a highly portable, fully automated, notebook-size TOF-MS. In Task 5, field testing of the prototype will be performed. The resulting instrument will be capable of analyzing effluents without sample preparation, with sub ppm to ppb sensitivities, and with near real-time response (<10 ms, ignoring data interpretation or archiving time). The system will be capable of operating manually for on-site inspections, and modified at a later time for use in perimeter monitoring or aboard a plane or drone. Additionally, this device can be readily applied to a variety of refinery applications including real-time chemical reaction monitoring, intelligent process control, and environmental sensing.

91-95 Funding (\$K): 900      Dates: 1994 - 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: A. C. (Paul) Raptis: Phone: (708) 252-5930, FAX: (708) 252-3250, E-mail: ac\_raptis@qmgate.anl.gov

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



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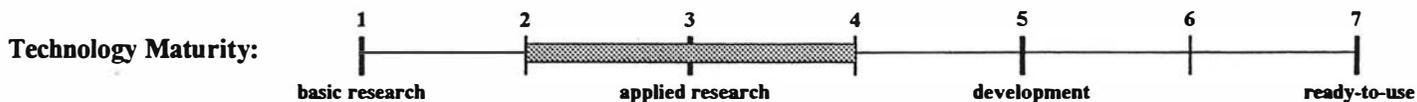
**Category:** Oil Processing & Refining (25, 4)

**Laboratory:** Argonne National Laboratory **Contact:** Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230 eichamep@smtplink.eid.anl.gov

**Title:** Ab Initio Studies of Reactive and Non-Reactive Potential Surfaces

**Description:** State-of-the-art, ab initio, electronic structure techniques are being used to characterize both reactive and nonreactive potential surfaces involving small gas phase molecules. The focus of the work at Argonne is on species and reactions important to hydrocarbon combustion. These methods can be used to accurately predict thermodynamic properties of small molecules (i.e. heats of formation, geometries, and vibrational frequencies) and rates of reaction (including temperature and pressure dependencies).

**91-95 Funding (\$K):** 1000 **Dates:** 1992-present



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

**Key Personnel:** Lawrence Harding Division: CHM Phone: (708) 252-3591 Fax: (708) 252-4470 E-mail: harding@tcg.anl.gov

**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 10

Category: Oil Processing & Refining (1,7)

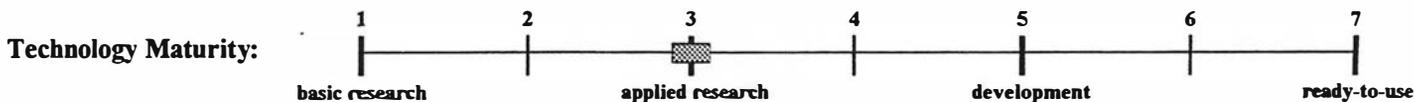
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Synthesis and Characterization of Molecular Sieve Materials

Description: Argonne National Laboratory is engaged in research aimed at the identification/characterization of new types of molecular sieve materials with tailored catalytic properties. This research involves studies of molecular sieve crystallization processes and the preparation of molecular sieves with specially modified frameworks or intracrystalline inclusion compounds. Unique facilities and methods employed in this work include synchrotrons (for a variety of x-ray studies), the intense pulsed neutron source at ANL (for structural and dynamical studies), and state-of-the-art quantum mechanical codes (for structure and property predictions, e.g., proton affinities). Recent applications-oriented research has included the development of molecular sieve-based bifunctional catalysts for methane activation to produce higher hydrocarbons and the tailoring of molecular sieve properties to produce catalysts suitable for automotive exhaust treatment, i.e., to reduce nitrogen oxide emissions.

91-95 Funding (\$K): 300      Dates: 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lennox E. Iton Division: MSD Phone: (708) 252-5536  
Lawrence A. Curtiss Division: MSD/CMT Phone: (708) 252-7380

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 11

Category: Environmental & Regulatory (12, 14)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Integrated Spatial Analysis Techniques for the Gas Industry

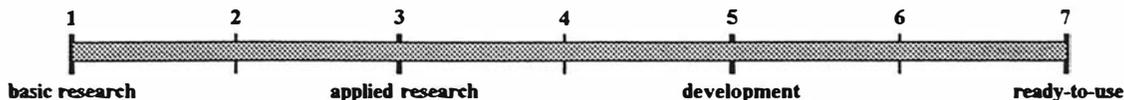
**Description:** The federal government has designated 6.4 million acres of desert, mostly in California, as a critical habitat for the desert tortoise, a threatened species. Argonne National Laboratory has evaluated the potential of low-altitude airborne remote- sensing technology as a means of monitoring desert ecosystems and characterizing the desert tortoise's habitat over Pacific Gas & Electric Company's (PG&E's) 300-mile gas pipeline rights-of-way (ROWs) in the California Mojave Desert. PG&E must acquire information on environmental conditions in the area continuously to satisfy regulations governing access to the ROWs for pipeline maintenance. Argonne comparatively analyzed and evaluated selected imaging sensors, including airborne video, photo CD, conventional color infrared (CIR) photography, a digital CCD camera, and Positive Systems' ADAR-5500 multispectral imaging sensor. The study has shown that airborne remote sensing is a cost-effective approach to monitoring and characterizing habitat over large desert areas and can provide critical information for maintenance activities in a timely manner.

This project evaluates the use of interactive multimedia technology to communicate spatial information to nontechnical audiences. As a demonstration project for the gas industry, ANL researchers are integrating GIS still imagery and animations with computer-aided design graphics, scanned maps, photos, video clips, text, and sound to create a multimedia application that presents environmental assessment information related to a hypothetical gas-pipeline right-of-way construction project. The end user will be able to explore information at different levels of complexity, and the multimedia application will provide the user with immediate feedback. This effort will also include realistic and accurate visual simulations of the post-construction appearance of the pipeline ROW. When completed, these applications will be transferred to CD-ROM in both Macintosh- and Windows-compatible formats for distribution.

91-95 Funding (\$K): 1300

Dates: 1993-present

Technology Maturity:



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 12

Category: Oil Processing & Refining (2)

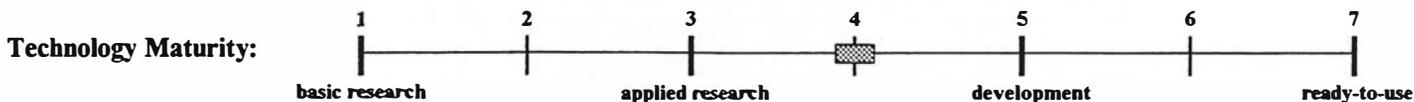
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Development of Ceramic Membranes for Partial Oxidation of Methane Into Syngas

**Description:** The goal of this cooperative research program is to develop economically attractive and environmentally friendly technology based on dense ceramic membranes to upgrade the basic hydrocarbon fuel such as natural gas (contains >95% methane) into high-value-added products. The first step in upgrading natural gas is to convert it into syngas (CO + H<sub>2</sub>). Syngas is the feedstock for variety of value-added-products such as easily transported liquid fuels and MTBE. The conventional conversion process (steam reforming or partial oxidation with O<sub>2</sub>) are very energy and capital intensive. In this program we are developing dense ceramic membrane that uses air as the source of oxidant for methane-conversion reactions and this eliminates the need for an oxygen plant. The cost of syngas generation is significantly reduced. Our membranes operate with out any external electrodes or external circuitry. Experimental issues being addressed include the selection of suitable ceramic material, fabrication into desired forms, reactor design, performance evaluation, and economic analysis. ANL's expertise in selection, fabrication and characterization of ceramics and the IPNS facilities are used. Amoco is evaluating the performance of the membranes in actual methane conversion reactors. It is expected that this novel technology will be scaled-up and commercialized.

91-95 Funding (\$K): 1475      Dates: 1993 - 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 13

**Category:** Environmental & Regulatory (4, 5)

**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** Trace-Level Organic Analysis

**Description:** The Analytical Chemistry Laboratory at ANL has well-established capabilities for analyzing volatile and semivolatile organic compounds, polychlorinated biphenyls, and pesticides at trace levels in environmental and mixed waste samples in soil/sludge and aqueous matrices. Purge-and-trap/gas chromatography/mass spectrometry is used for determining volatiles. Gas chromatography/mass spectrometry and high performance liquid chromatography/mass spectrometry are used for determining semivolatiles. Gas chromatography/electron capture detection is used for determining polychlorinated biphenyls and pesticides. The data can be used for characterization or for regulatory purposes.

**91-95 Funding (\$K):** 800      **Dates:** 1991-present

**Technology Maturity:**

1	2	3	4	5	6	7
basic research	applied research		development		ready-to-use	

**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

**Key Personnel:** Amrit S. Boparai Division: CMT/ACL Phone: (708) 252-7710 Fax: (708) 252-5655 E-mail: boparai@cmt.anl.gov

**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 14

Category: Environmental & Regulatory (10,14)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Nuclear Counting Technique

Description: The Analytical Chemistry Laboratory (ACL) employs a variety of instruments that measure nuclear decay events. These include intrinsic Ge detectors for gamma ray spectrometry, gas proportional counters for gross alpha and beta particles, liquid scintillation counting for alpha and beta particles, and alpha pulse detectors for alpha spectrometry. These techniques can be used to quantify the radionuclide content in all types of media.

91-95 Funding (\$K): 1750      Dates: 1991-present



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Delbert L. Bowers Division: CMT/ACL Phone: (708) 252-4354

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 15

Category: Environmental & Regulatory (14, 5)

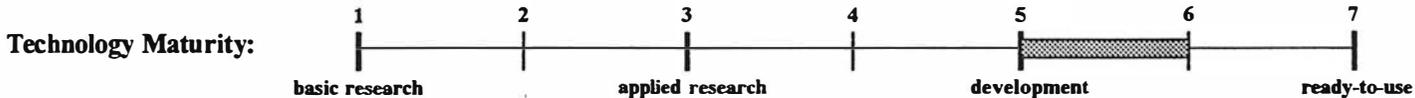
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Application of Dynamic Stability to Liquid-Filled Tanks

**Description:** The dynamic stability of liquid-filled tanks under seismic excitation was studied. The fluid and the structure were modeled using a Galerkin finite element method, and the resulting system of coupled Hill's equations was analyzed for modes of parametric instability. The formulation was incorporated into a computer code, then the couplings among various fluid-structure vibrational modes were identified under different types of seismic excitation. Comparison of the simulation results revealed excellent agreement for the major failure modes. The formulation was later extended to take into account the effect of the geometrical imperfections in the structure. With this modification, the appearance of almost all the modes observed during the experiments could be explained. This approach can be used to determine different failure modes of wine, oil, and water storage tanks under earthquake conditions. By performing parametric studies, design guidelines to reduce the risk of dynamic buckling in storage tanks may be established. This type of approach may prove itself useful in understanding the behavior of fuel tanks in aerospace technologies.

91-95 Funding (\$K): 350      Dates: 1991-1993



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

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Aziz Uras Division: RE Phone: (708) 252-5847

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 16

Category: Environmental & Regulatory (14, 5)

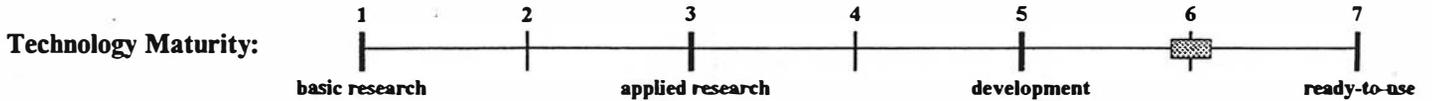
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Computer Software for Seismic Response of Liquid-Filled Tanks

Description: The U.S. Department of Energy (DOE) environmental management (EM) has initiated a high-level waste (HLW) storage tank safety program. One of the objectives of the safety program is to develop seismic design and evaluation criteria for use in assessing the seismic response of existing underground HLW storage tanks. DOE-EM has chosen Argonne to study the effect of liquid viscosity on the seismic response of underground high-level waste storage tanks. The computer software developed at Argonne has successfully solved the problem. The results proved to be useful not only at Hanford, but also at other DOE sites. The computer software developed at Argonne has the following additional features: (1) it can consider the tank wall flexibility, (2) it can consider the soil-fluid-structure interaction, and (3) it can consider the nonuniform density liquid. This computer software can also be used in the oil refinery and winery industries.

91-95 Funding (\$K): 450      Dates: 1991-present



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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R. Aziz Uras Division: RE Phone: (708) 252-5847

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 17

**Category:** Gas Processing (2, 7), Environmental & Regulatory

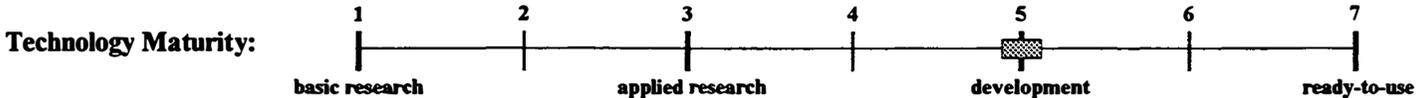
**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** Recovery of Hydrogen from Hydrogen Sulfide

**Description:** The objective of this research is to develop a refining process that will recover H<sub>2</sub> from H<sub>2</sub>S waste streams. This unique process uses plasma chemistry to dissociate H<sub>2</sub>S into H<sub>2</sub> and S. Back reaction of the products to H<sub>2</sub>S is minimized by in situ, cyclonic separation and a rapid quench of the products. Data obtained in Argonne's plasma-chemistry laboratory have shown that process conversions of 80 to 90 % per pass and process energy requirements between 12 & 16 kcal/gmole are possible. Furthermore, experiments with water and carbon dioxide concentrations typical of acid-gas streams from refinery operations and natural gas production have demonstrated that these components are compatible with the plasma-chemical process. In response to industrial concerns about hydrogen safety, plasma-reactor operating pressures in excess of atmospheric pressure have also been demonstrated. A preliminary economic evaluation indicates that the plasma-chemical process will be substantially cheaper to operate than the conventional sulfur recovery technology and that the sulfur emissions will also be lower. The very favorable economics stem from the ability of the plasma process to recover the hydrogen chemical value contained in the H<sub>2</sub>S waste stream while also recovering high-purity sulfur.

**91-95 Funding (\$K):** 3095      **Dates:** 1991 - 1995

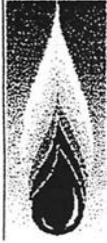


**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

**Key Personnel:** John Harkness: Phone: (708) 252-7636, Fax: (7708) 252-9728, e-mail: John\_Harkness@qmgate.anl.gov

**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 18

**Category:** Gas Gathering

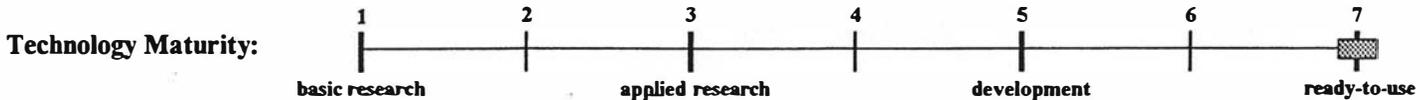
**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** Information/GIS System to Understand the Natural Gas Industry and Infrastructure

**Description:** GASMAP (The Geographic Analysis System for Market Assessment and Planning) is a geographic information system (GIS) encompassing the natural gas transmission, distribution, storage and production industries. Data on gas companies provided by various governmental data sources is linked to maps of pipelines, points on the pipelines, service territories of local distribution companies, cogeneration units, electric utility plants, and storage fields. GASMAP covers the U.S., and a user can zoom from a national map level down to a street block level of detail. GASMAP can assist the gas and electric industries in analysis of the natural gas infrastructure system. Argonne's approach is unique in that its comprehensive data system contains information on over 2,500 gas companies and its ability to link these databases to geographical points on a map. With the deregulation of the natural gas industry, companies need information to help with decision making. Applications include demand forecasting, assessing bottlenecks on routing issues, and information on competitors. GASMAP is an on-going project with a working prototype.

**91-95 Funding (\$K):** 300      **Dates:** 1993-present



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

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**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 19

**Category:** Gas Gathering, Environmental & Regulatory

**Laboratory:** Argonne National Laboratory

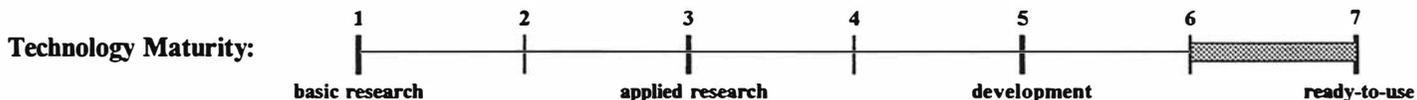
**Contact:** Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** Using Geographic Information Systems to Site Gas Pipelines

**Description:** Current methods for siting a natural gas pipeline route and obtaining permits can take up to three years. Argonne and gas industry researchers are applying a geographic information system (GIS) to reduce the effort needed to gather and assess data when planning pipeline rights-of-way. The GIS combines spatial data (population centers, land cover, wildlife habitats, hydrography, soils, and transportation routes) on the area of interest in layers. During analysis, layers can be combined or weighted on the basis of environmental and engineering characteristics associated with siting, permitting, construction, maintaining, and monitoring rights-of-way. The GIS-based approach determines least-cost and alternative rights-of-way and significantly reduces permitting time, typically to less than a year, with commensurate cost savings.

Using GIS methods, Argonne researchers have created a Right-of-Way Erosion Evaluation Program (REEP) that will allow land planners and engineers to quickly evaluate the potential for watershed erosion during and after the installation of a gas pipeline right-of-way (ROW). REEP is an enhancement of earlier work conducted at Purdue University. This program integrates a watershed simulation model called ANSWERS (Areal Nonpoint Source Watershed Environmental Response Simulation) with a GIS called GRASS (Geographic Resources Support System). REEP has an entirely X-Windows user interface, which improves the automation of soil and land cover data input derived from GRASS map layers. In addition, REEP provides an option to interactively place potential gas pipeline ROWs into the watershed before running the watershed simulation. This option allows land planners and engineers to evaluate the effects of ROW placement on watershed behavior during and after construction.

91-95 Funding (\$K): 750      Dates: 1992-1994



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

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**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 20

Category: Oil Processing &amp; Refining (21, 24)

Laboratory: Argonne National Laboratory

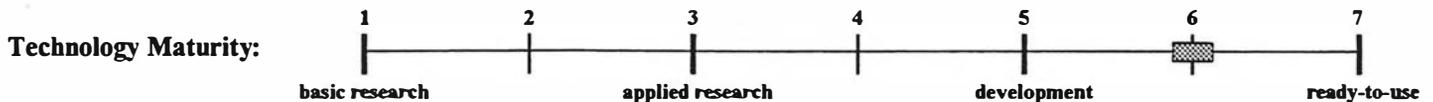
Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Fundamental Chemistry of Coals

**Description:** This program seeks to elucidate the chemical and physical structure of the Argonne Premium Coal Samples and their macerals on a global basis and on the molecular level. The prime objective is to establish statistically accurate, rank-dependent models for the Argonne Premium Coal Samples. Extraction and selective chemical procedures are used in combination with a complementary array of powerful instrumental techniques. The instrumental approaches include laser desorption, high-resolution, and tandem mass spectrometry; NMR spectroscopy and imaging; synchrotron X-ray spectroscopy, imaging and scattering; and neutron scattering. The emphasis is on large molecules common to both coal and heavy petroleum. Mass spectrometric methods have been developed to provide accurate molecular weight distributions for complex mixtures of polar molecules. This work has been supported by the results from small angle neutron scattering which show that most of the soluble molecules are very aggregated. High resolution MS is being used to identify heteroatomic molecules, which are important with respect to processing and environmental considerations. The first high resolution chemical images of coals and carbons have been obtained by soft X-ray methods. Also, this approach promises to be useful for studying catalysts. The synthetic program is designing clays and catalytic materials especially tailored for the conversion of these large molecules. Novel approaches to preparing pillared clays are being used and have been patented. The fundamental information derived from these studies will be used to guide the development of new processes to utilize America's coal and heavy petroleum.

91-95 Funding (\$K): 3690

Dates: 1994 - 1995



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

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**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 21

Category: Environmental & Regulatory (2, 12)

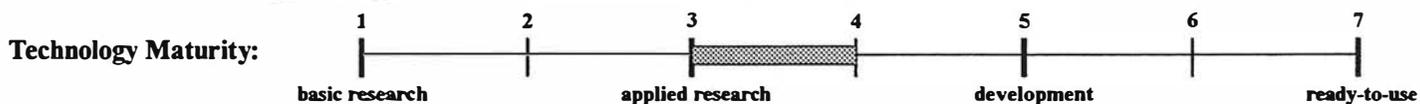
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Integrated Electrodialysis/Reverse Osmosis Process for Produced Water Treatment

**Description:** The project goal is to evaluate the technical and economic feasibility of an integrated electrodialysis (ED) / reverse osmosis (RO) process to treat produced waters (hydrocarbon-contaminated brine) generated by natural gas production. This process combines ED and RO in a synergistic manner to reduce the volume of the salt water waste by concentrating the salts and to generate a clean water stream for beneficial uses. In laboratory screening experiments key ED parameters (e.g., salt removal and current efficiency) were measured using produced water samples from gas production sites. Results of the ED and RO laboratory screening experiments will form the basis for a coordinated program consisting of more extensive laboratory experimentation, economic feasibility analyses, and optimization of the integrated ED-RO process. Techniques to reduce membrane fouling are being developed. After successful completion of laboratory-scale development and process demonstration, a field demonstration at a gas production site will be performed. A costing model is being developed to do sensitivity analyses of process parameters and conditions. Argonne will develop a preliminary design of the field demonstration unit and provide economic analysis support to ReTec. Project results will be incorporated into a knowledge base being developed by ReTec for use in identifying the optimal produced water treatment method for the specific conditions at a given site.

91-95 Funding (\$K): 260      Dates: 1994 - 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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 ReTec: Lonny Lawrence: Phone: (412) 826-3340, Fax: (412) 826-3409  
 GRI: Thomas Hayes, Phone: (312) 399-8325, Fax: (312) 399

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



**Index:** 22

**Category:** Oil Processing & Refining (16,17), Gas Processing

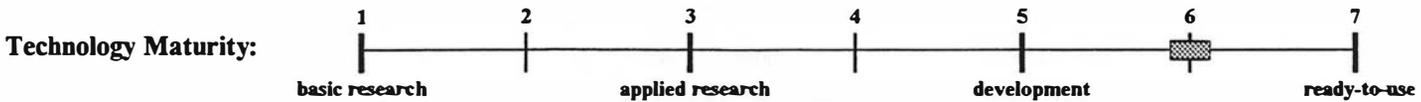
**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** High-Performance, Compact Evaporators and Condensers

**Description:** The goal of this program is to develop the technology base required for the design and optimization of high-performance, compact evaporators and condensers, for application in the refining, process, and transportation industries. Compact heat exchangers are defined as heat exchangers having a high heat transfer surface area density ratio (typically greater than 700 m<sup>2</sup>/m<sup>3</sup>). Such heat exchangers possess numerous features including small size, low weight, reduced fluid inventory, and fast response. The program is focusing on experimental studies of two-phase flow and heat transfer in small, circular and noncircular channels which are representative of compact heat exchanger geometries. High-performance compact evaporators are being studied under a DOE/OIT-sponsored program and a new CRADA with Modine Manufacturing Company, while high-performance compact condensers are being investigated in an existing CRADA with Modine. The technical approach involves study of the effect of flow passage geometry and size on the two-phase flow and heat transfer and the development of design correlations for two-phase pressure drop and heat transfer; mechanistic studies are being performed in a flow visualization test apparatus that includes ultra-high-speed video. It is expected that the developed technology base will provide the basis for the development of industry standards. Applications to the refining industry that are being considered include select separation processes where combined heat and mass transfer would benefit the process.

**91-95 Funding (\$K):** 1230      **Dates:** 1994 - 1995



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

**Key Personnel:** ANL: Martin W. Wambsganss: Phone: (708) 252-6144, FAX: (708) 252-5210, E-mail: M\_Wambsganss@qmgate.anl.gov

**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 23

Category: Gas Processing (6)

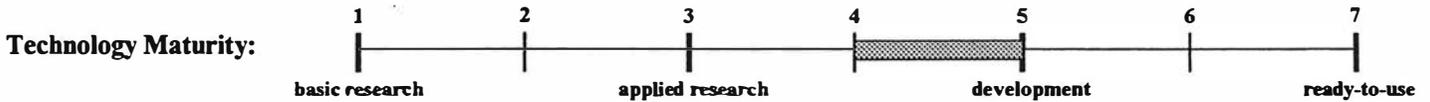
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Hot-Gas Filters

Description: We have developed state-of-the-art facilities, techniques, and test procedures to evaluate the structural reliability of hot-gas filters made of monolithic ceramics and ceramic-fiber-reinforced composites. We conduct mechanical testing to assess filter reliability, and perform stress and fracture mechanics analyses to establish structural requirements for candidate filter materials. Hot-gas filters are critical elements for the success of combined-cycle power generation with coal gasification.

91-95 Funding (\$K): 200 Dates: 1991-1994



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 24

Category: Oil Processing &amp; Refining (1,25)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

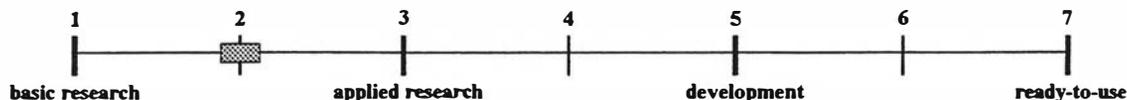
Title: Molecular Sieve Materials Research

**Description:** This program combines synthesis and characterization of molecular sieve materials with formulation of novel encapsulates for both basic studies and potential applications. Substantial implementation of theory and modelling is made to complement our fundamental understanding of chemical and physical properties of molecular sieves and the details of their shape-selective catalytic behavior. Novel synthesis methods, new material compositions, novel material forms, and novel catalysts are potential outgrowths of this research. Acid zeolites and zeolites incorporating transition metal clusters are important catalysts in central refinery processes involving hydrocarbon cracking and transformation reactions (alkylation, reforming, etc.). In recent and current work, we have pursued the development of ab initio theoretical treatments of Brønsted acidity and base protonation interactions in zeolites using large cluster models, the development of computer simulations of adsorption and intracrystalline diffusion of hydrocarbons in zeolites by molecular dynamics methods with large scale models, and the development of novel encapsulated clusters to be tested as HDS and HDN catalysts. Ab initio theoretical studies of the mechanisms of alkane cracking reactions in zeolites are in progress, and we expect to develop a complete fundamental analysis of the basis of molecular shape-selectivity in alkane cracking by the combination of ab initio theory and molecular dynamics simulations.

91-95 Funding (\$K): 300

Dates: 1995

Technology Maturity:



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

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**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 25

**Category:** Environmental & Regulatory (11)

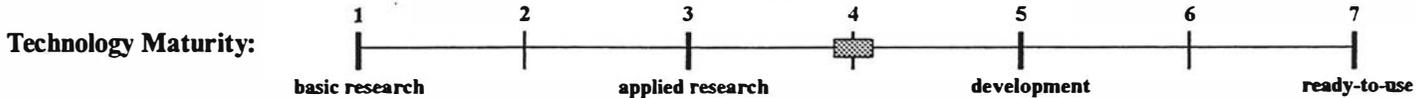
**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** Recycling Waste Lubricating Oils

**Description:** Conservative estimates are that at least 1.4 billion gallons of used lubricating oils are available for recycling each year. Only 2 percent of this oil is currently being recycled. Argonne researchers are assessing the opportunities and requirements for developing new technologies that would increase the recycling of lubricating oils in all market sectors. An R&D program will be undertaken to develop the needed technology. Successful development of novel technologies and methods could conserve as much as 175 trillion Btu per year, thereby displacing the equivalent of 30 million barrels of oil. These techniques could also reduce illegal dumping of up to 200 million gallons of used lubricants per year.

**91-95 Funding (\$K):** 300      **Dates:** 1993-1995



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

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**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 26

Category: Oil Processing & Refining (19, 4, 11), Environmental & Regulatory (13)

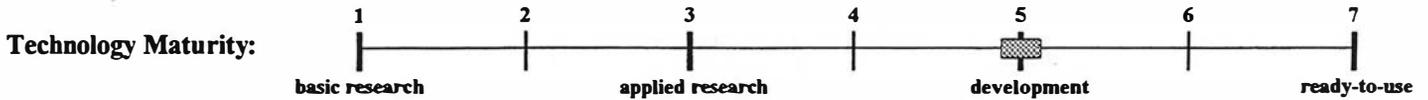
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Magnetic Separation and Recovery of Solids

Description: Argonne is developing two techniques for separation of materials using the magnetic properties of materials. The Open Gradient Magnetic Separator (OGMS) is an extension of Argonne's widely-recognized expertise in the development of superconducting magnets. The OGMS is being used to separate metal-contaminated solids such as catalysts in order to improve their performance and reduce waste. In related work, ANL personnel are developing the basic technology and applications for using specially designed magnetic particles that can remove dyes and chemicals from process or waste streams. This technology offers a unique, cost-effective approach for recovering valuable materials and harmful chemicals.

91-95 Funding (\$K): 300      Dates: 1993-present



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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R.D. Doctor Division: ES Phone: (708) 252-5913

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 27

Category: Oil Processing & Refining (25)

Laboratory: Argonne National Laboratory

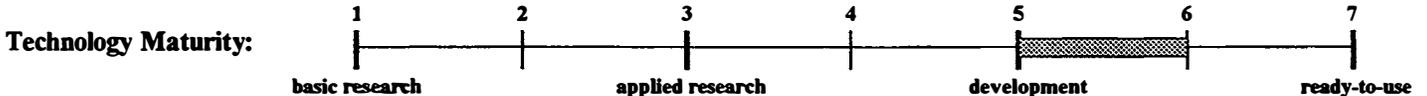
Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Computer Software for Fluid/Solids Systems Hydrodynamics and Erosion

**Description:** ANL has developed a computer code named FLUFIX to predict hydrodynamics in complex fluidized-bed combustor (FBC) systems. This code is based on a hydrodynamic model of fluidization and can predict frequency of bubble formation, bubble size and growth, bubble frequency and rise-velocity, solids volume fraction and gas and solids velocities for both atmospheric and pressurized bubbling and circulating FBCs. The results of the hydrodynamic model are used as inputs to ANL's EROSION computer program which contains various erosion models, including ANL's unique monolayer energy dissipation (MED) erosion model. Babcock & Wilcox (B&W) in close collaboration with ANL has developed the FORCE2 computer code, which is a three-dimensional transient and steady-state version of FLUFIX. ASEA Babcock PFBC funded the B&W work. ANL has implemented the FORCE2 computer program on its CRAY-XMP vector supercomputer and has performed quality assurance and validation. A computer code, SLUFIX, has been developed for liquid/solids slurry flow. This SLUFIX code extends the FLUFIX computer code, which has been successfully used to predict the hydrodynamic behavior of gas/solids flow.

91-95 Funding (\$K): 2000

Dates: 1991-present



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology, Erosion/Corrosion, Slurry Transport



Index: 28

Category: Production (3, 4)

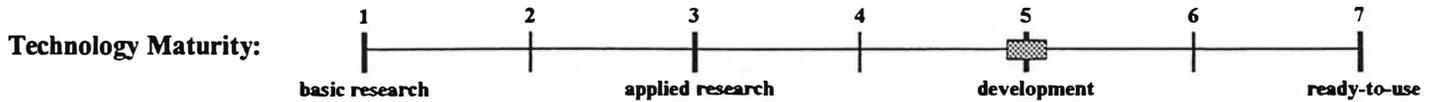
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Development of Environmentally Acceptable Microbial Corrosion Control Methods

**Description:** This project will develop environmentally acceptable alternatives to the use of toxic chemicals for the control of microbiologically-influenced corrosion (MIC) on carbon steel. The purpose of the DOE/ANL program is to develop the next generation of mitigation approaches and reduce the current dependence and large cost of chemical treatment. The goals include (1) the selection and/or development of inexpensive carbon steels that are MIC-resistant, (2) the development and transfer to industry efficient delivery systems of "alternative" less toxic biocides, and (3) calibration and testing of MIC detection methods and proprietary treatment approaches with industry cooperators. ANL will use experimental Test Loops (TL) to study effects or biocide treatments, sulfide inclusions and electrochemical monitoring of MIC processes. General and localized corrosion of carbon steel coupons from these TLs will be characterized with advanced surface analysis techniques at ANL: XPS, AES, XRD, XDS, Raman and FTIR spectroscopy. Microbial characterization and mapping will also be conducted. The Partners primary research activities will be field oriented at an actual underground gas storage facility. SOCAL and collaborators will screen different biocides and metallurgies under field test loop conditions and in actual gas storage wells. SOCAL and industrial collaborators will also conduct side-by-side comparisons under field conditions of commercially available on-line electrochemical corrosion monitoring probes in order to identify the most promising probes or set of probes for early detection of localized pit corrosion in wells and pipelines used by the gas storage and transmission industry.

91-95 Funding (\$K): 525      Dates: 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 29

**Category:** Drilling & Completion(8), Production, Deepwater Offshore, Arctic Region Activities, Oil Processing & Refining, Gas Processing

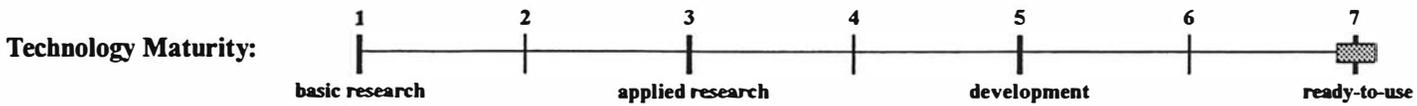
**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** Mechanical Properties of Materials

**Description:** This completely modern mechanical-properties testing facility includes an Instron 8562 Testing Machine with an electromechanical actuator and an 8502 Testing Machine with a servo-hydraulic actuator, each on a 250 kN load frame. Both machines possess full digital control; data acquisition and processing; load, position, and strain control operation; and wave generation capability. Capabilities of the 8562 machine include conventional and very low-rate, long-time tests at temperatures up to 1650°C in a Centorr vacuum furnace. The 8502 machine includes an environmental chamber and is ideally configured for testing elastomers in the stress relaxation and cyclic modes. The laboratory includes a fully-equipped metallographic preparation facility, scanning and optical electron microscopy, and a heat-treating furnace with an inert gas purge gas system. Computer programs include databases for advanced energy system design and for mechanical property modeling. Recent applications of the 8562 system include studies of the high-temperature mechanical behavior of structural stainless steels in relation to microstructural evolution, and measurements of the plastic flow behavior of railroad rail steels in connection with predicting rail life. The 8502 system is currently being used to measure elastomer shear strength and energy dissipation capacity for seismic damping applications.

**91-95 Funding (\$K):** 2000      **Dates:** 1991-1995



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

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**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 30

Category: Oil Processing & Refining (20, 21)

Laboratory: Argonne National Laboratory

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eichamep@smtplink.eid.anl.gov

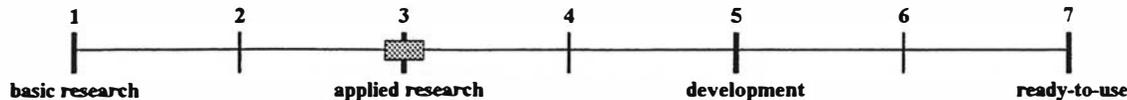
Title: Process Chemistry of California Crudes

**Description:** The overall objective of this research program is to develop new catalytic processes that will convert the non-volatile molecules in the heavy crude from the Midway Sunset field into the equivalent of a high quality Alaskan North Slope crude. Entirely new catalysts including subnanophase small metal clusters and synthetic pillared, layered clays will be explored in the course of this research. The effectiveness of the catalysts will be established by comparing their ability to convert the least reactive constituents of the heavy crude into desirable products. Thus, a key focus is the identification of the aromatic hydrocarbons and heteroatomic molecules of the resid that need to be converted to achieve our goal. There will be a close interplay between the results of the catalyst research and the characterization work with the specific objective of defining the effectiveness of the catalysts for heavy molecules with specific structural characteristics. The research plan was developed by directing ANL's current expertise in characterization and catalysis toward the fundamental problems that prevent the effective processing of heavy oils. Several characterization techniques including selective chemical degradation and high resolution chromatography will be coupled with very advanced laser desorption mass spectrometry, desorption high resolution mass spectrometry, and tandem mass spectrometry to determine which molecules in the heavy oils resist effective processing.

91-95 Funding (\$K): 400

Dates: 1995

Technology Maturity:



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 31

Category: Production (3), Oil Processing & Refining (3,5)

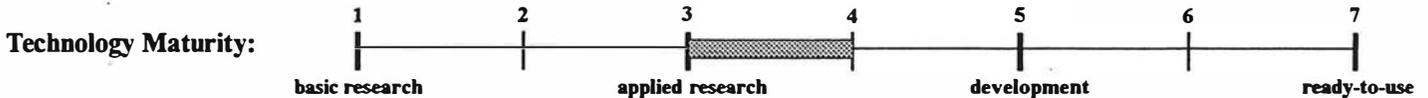
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Development of Environmentally Acceptable Microbial Corrosion Control Methods

Description: This project will develop environmentally acceptable alternatives to the use of toxic chemicals for the control of microbiologically-influenced corrosion (MIC) on carbon steel. The purpose of the program is to develop the next generation of mitigation approaches and reduce the current dependence and large cost of chemical treatment. The goals include (1) the selection and/or development of inexpensive carbon steels that are MIC-resistant, (2) the development and transfer to industry of efficient delivery systems of "alternative" less toxic biocides and (3) calibration and testing of of MIC detection methods and proprietary treatment approaches with industry cooperators.

91-95 Funding (\$K): 1680      Dates: 1994-present



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 32

Category: Drilling & Completion (8)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Thin Diamond Films Deposited by Microwave-Enhanced Chemical Vapor Deposition

Description: Thin diamond films can be grown on a variety of materials by microwave-enhanced chemical vapor deposition. The coating that is deposited has the characteristic sp<sup>3</sup> bonding structure of diamond. Items to be coated are placed in a vacuum chamber and exposed to a mixed hydrogen and methane gas plasma at relatively high temperatures to produce diamond films essentially free of hydrogen and contaminants. The films start growing as small crystallites (approximately 1-20 micrometers) that coalesce to form a continuous film. Variation of processing conditions allows the tailoring of smooth or rough diamond films.

91-95 Funding (\$K): 950      Dates: 1991-1993



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 33

Category: Oil Processing &amp; Refining (19), Gas Processing (6)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax:  
(708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Analytical Support Services/Methods Research and Development Provided by the Analytical Chemistry Laboratory

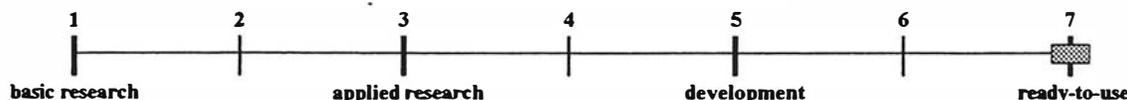
**Description:** Argonne's Analytical Chemistry Laboratory (ACL) provides a broad range of analytical chemistry support services to the scientific and engineering programs at ANL. In addition, the ACL conducts research in analytical chemistry, conducts instrument and methods development, and provides analytical services for governmental, educational, and industrial organizations. With a highly qualified staff and facilities that include most types of major analytical instrumentation, the ACL offers solutions to chemical analysis problems in materials characterization, process definition and control, environmental monitoring, and waste analysis. Inorganic materials are analyzed with a full range of classic wet-chemical and modern instrumental techniques, including plasma-emission and plasma-mass spectrometry. Elemental isotope abundances are measured by thermal-ionization or inductively-coupled-plasma-mass spectrometry. Organic compounds are identified and measured down to trace concentrations by a variety of chromatographic, mass spectroscopic, and infrared spectroscopy techniques [gas chromatography (GC), gas chromatography/mass spectrometry (GC/MS), Fourier transform infrared (FTIR)]. Radiological parameters involving alpha-, beta-, or gamma-emitting nuclides of all kinds are determined with an assortment of techniques that includes solid-state and gas proportional detectors, as well as liquid scintillation counting.

91-95 Funding (\$K):

3500

Dates: 1991-present

Technology Maturity:



Technology Transfer:

Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation:

List available through key personnel.

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Donald G. Graczyk CMT/ACL (70) 252-3489  
David W. Green Division: CMT/ACL Phone: (708) 252-4379  
Delbert L. Bowers Division: CMT/ACL

Lab Capabilities

Applied:

Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 34

Category: Oil Processing & Refining (21,1)

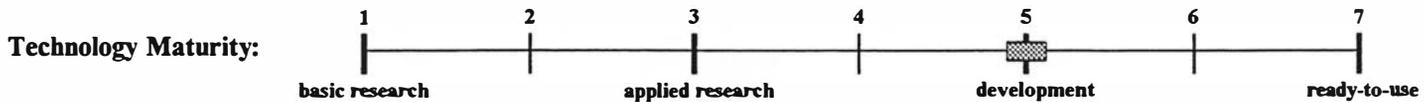
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Improved Resid Upgrading

**Description:** This project consists of several highly integrated tasks divided between Argonne National Laboratory and Amoco that focus on unique strengths in these two institutions. Key issues that control upgrading efficiency are being addressed. The resid asphaltenes are the molecules that are most difficult to upgrade and are least well characterized. They are being separated from the resid and characterized by using advanced techniques at ANL. Batch hydroprocessing reactions on a selected heavy residua are carried out in parallel work at Amoco. Several potentially effective catalysts will be studied. The objectives are to select the optimum catalyst and operating conditions for large- scale reactions. Products from selected experiments will be separated and characterized. Two additional tasks center on batch experiments. One task involves the use of in situ characterization methods to follow hydroprocessing at reaction temperature and pressure. Small-angle neutron scattering (SANS) is used to determine size reduction in real time to provide unique insight into these complex reactions. A high-temperature, high-pressure X-ray absorption spectroscopy (XAS) cell is employed to define the state of the catalyst and, possibly as important, the fate of vanadium and nickel that can poison the reaction catalyst. Another task concerns the discovery of the best catalyst on a small pilot-plant scale. Extensive characterization is being done on the products of the larger scale reactions to define the molecules in the resid that have reacted, as well as, those that have not been converted.

91-95 Funding (\$K): 1650      Dates: 1994 - 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 35

Category: Environmental & Regulatory (12, 6)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
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Title: Designing a Remediation Plan to Restore Drinking Water From a Contaminated Site

Description: A U.S. Air Force site in Johnson City, New York, may have contaminated the city's drinking water wells with trichloroethane and other hazardous compounds. Because of Argonne's expertise in field studies, contaminant transport modeling in complex hydrogeologies, and risk assessment of chemical compounds, the Air Force requested that the Laboratory design appropriate procedures and define required remediation. Argonne obtained data on the chemicals present, modeled groundwater flow, and installed wells to monitor drinking water quality. Results indicated that the Air Force facility contributed only a small fraction of the contaminants in the wells. Argonne also designed a remediation plan that satisfies city and state environmental regulatory agencies. This plan is expected to be incorporated at other Air Force facilities.

91-95 Funding (\$K): 575

Dates: 1991-1993



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 36

Category: Oil Processing & Refining (1,21), Gas Processing

Laboratory: Argonne National Laboratory

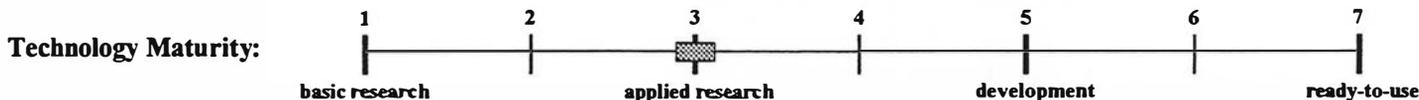
Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Fluid Catalysis Program

**Description:** The Fluid Catalysis Program uses an array of in situ high-pressure spectroscopic and kinetic techniques to explore and to develop new catalytic chemistry for the transformation of simple precursor molecules that serve as raw materials for many industrial processes. Precursors of interest include those of the Cl chemical industry, e. g., CH<sub>4</sub>, CO, CO<sub>2</sub>, and CH<sub>3</sub>OH; the ammonia synthesis precursors, N<sub>2</sub> and H<sub>2</sub>; and the ceramic precursors, e.g., (CH<sub>3</sub>)<sub>4</sub>Si, (CH<sub>3</sub>)<sub>3</sub>B, and Al<sub>2</sub>(CH<sub>3</sub>)<sub>6</sub>. Reaction types of interest include carbonylations, hydrogenations, hydroformylations, homologations, oxidations, polymerizations, and metatheses. Recent programmatic activities encompass (1) high-pressure NMR studies of homogeneous catalytic chemistry in supercritical fluids (Shell, Oxo, and Ziegler-type Processes), (2) catalytic and stoichiometric organometallic processes associated with the production of advanced materials (preceramic polymers, carbide fibers and films) and (3) the synthesis and development of extremely rugged homogeneous catalysts for the selective conversion (oxidation, oxidative coupling, or substitution) of methane and other hydrocarbons. The program has advanced toroidal detectors for NMR spectral and imaging studies at heretofore unattainable combinations of temperature and pressure. High-pressure NMR cells and techniques for the study of catalytic chemistry in supercritical H<sub>2</sub>O are being explored. Programmatic facilities include high-pressure NMR systems at 300 and 400 MHz, high-pressure FT-IR cells, and a variety of ancillary inert atmosphere and high-pressure equipment (autoclaves, pumps, circulators, monitoring devices, barricades, and safety devices).

91-95 Funding (\$K): 1340

Dates: 1994 - 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: ANL: Jerome W. Rathke: Phone: (708) 252-4549: FAX: (708) 252-9373, E-mail: rathke@cmt.anl.gov

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 37

Category: Oil Processing & Refining (21,20)

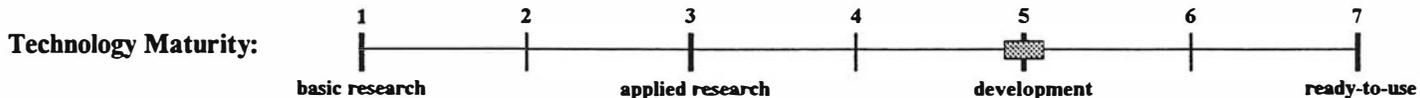
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: On-Line Nuclear Magnetic Resonance Sensor System for Upgrading Residuum and Heavy Oil

**Description:** This is a joint Cooperative Research and Development Agreement (CRADA) proposal between Amoco Corporation, Bio-Imaging Research, Inc. (BIR), and Argonne National Laboratory (ANL). The purpose of this program is to develop, demonstrate, and transfer technology for commercialization of on-line nuclear magnetic resonance (NMR) sensing and control technology for application to upgrading light oil residuum and heavy oil. Goals to be accomplished in this proposal include (1) development of on-line NMR sensor technology (NMR pulse techniques and prototype), (2) implementation of the NMR sensing and control system prototype in the plant environment, (3) implementation of this technology for a variety of upgrading processes and characterization needs (for both light oil residuum and heavy oil) over the lifetime of the proposal, and (4) transfer of the technology to BIR for commercialization. The benefits that will be achieved by implementation of NMR sensing technology are in the areas of environmental compliance, waste reduction, energy savings, increased U.S. competitiveness, and reduced dependence on foreign oil.

91-95 Funding (\$K): 1750      Dates: 1994 - 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: ANL: Stephen L. Dieckman: Phone: (708) 252-5628, FAX: (708) 252-3250, E-mail: sl\_dieckman@qmgate.anl.gov  
 Amoco Corporation: Michael L. Snoddy: Phone: (708) 420-5787, Fax: (708) 961-6250  
 Bio-Imaging Research Inc.: Timothy Fox: Phone: (708) 634-6

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 38

**Category:** Oil Processing & Refining (21,3)

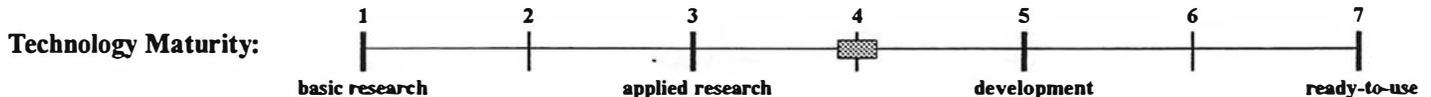
**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** Fouling Mitigation in Processing of Residuum and Heavy Oil

**Description:** The purpose of the CRADA work is to determine the major causes and threshold fouling conditions for feed/effluent heat exchangers used for hydrotreating gas oil. The focus of the CRADA work is generation of fouling precursor by the interactive reaction between sulfur and iron compounds present in gas oil derived from residuum and heavy oils. The work is coordinated between ANL, CRTC, and HTRI to obtain laboratory and field fouling data. The CRADA work will lead to the development of an analytical tool for applying the laboratory data to industrial conditions. The kinetics of precursor formation is being investigated at ANL using an autoclave-based fouling unit. The kinetic model will then be used to predict the rate of fouling deposition for the feed/effluent heat exchangers. The fouling data to be obtained at HTRI using the closed-flow loop apparatus will be used to validate the prediction method. It is believed that the fouling propensity can be significantly reduced by improving the heat/mass transfer processes for the two-phase flow of gas oil and recycled hydrogen. Therefore, an enhanced tube or tube insert will be used in the second phase of work to determine the relative rate of fouling deposition.

**91-95 Funding (\$K):** 1110      **Dates:** 1994 - 1995



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

**Key Personnel:** C. B. Panchal: Phone: (708) 252-8070, FAX: (708) 252-9728, E-mail: cb\_panchal@qmgate.anl.gov  
 CRTC: W. A. Ebert: Phone: (510) 242-3466, Fax: (510) 242-4647  
 HTRI: J. W. Palen: Phone: (409) 260-6227, Fax: (409) 260-6249

**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 39

Category: Oil Processing & Refining (3,12)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

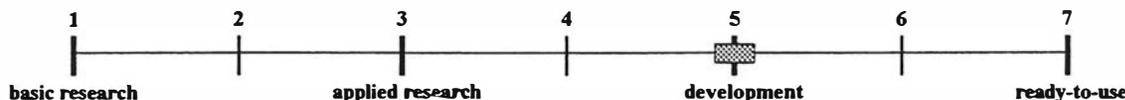
Title: Organic-Fluid Fouling

**Description:** This is an on-going project for the development of methodology for predicting the effects of physical parameters and determination of the threshold fouling conditions for petroleum products. Since FY94, the fouling project has been focused on the development of new and improved methods for mitigating fouling in the oil-refining industry. Considering the severity and complexity of the crude-oil fouling, the initial work was focused on product fouling. The crude-oil fouling work was started in FY95 in a cooperative work with Shell Development Co. CRTC provides the technical and programmatic support for the ANL work. The technology transfer is effectively carried out by working with HTRI and its refinery member companies. The major objectives for the ANL fouling project are to determine the major causes of fouling, develop methodology for predicting the threshold fouling conditions for different feed stocks, and develop new techniques to improve the effectiveness of chemical additives for preventing the fouling deposition. The three elements of the ANL fouling project are (1) development of prediction model incorporating the kinetic and fluid dynamic models, (2) laboratory experiments at ANL for the development of kinetic model for the formation of fouling precursors, (3) crude-oil fouling experiments at the Shell refinery in Woodriver, Illinois using the ANL field fouling unit.

91-95 Funding (\$K): 2400

Dates: 1991 - 1995

Technology Maturity:



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 40

Category: Oil Processing & Refining (25,6)

Laboratory: Argonne National Laboratory      Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
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Title: Generation of a Validated Computational Capability to Support Advanced Fluid Catalytic Cracker (FCC) Development

**Description:** Present and future environmental regulations are expected to have a major influence on the way the FCC can optimally contribute to the gasoline pool. A major incentive therefore exists to develop a better and more fundamental understanding of FCC operations and design in order to be able to adjust product yields. For example, current regulatory and market factors dictate that the FCC produce more oxygenate and alkylate precursors while reducing the yield of such undesirable products as heavy gasoline and LCO. The objective of this program is to develop an advanced analytical (design) capability that can be used to define and evaluate optimized operating conditions and potential hardware improvements (in areas such as injection nozzles, riser geometry, riser quench, etc.) that can produce the desired product mix. To achieve program goals, a multi-year, phased program is being pursued. The Phase I effort will focus on developing and validating a 3-D integrated kinetics-hydrodynamics model for evaluating the FCC riser. ANL will modify and extend its multiphase reacting flow codes to analyze short contact time riser designs. A cracking kinetics model will be developed from data taken on pilot-scale FCC units and integrated with a 3-D multiphase flow code. The modified code will be able to model interactions between solid, liquid, and gas phases. In Phase II, the 3-D analytical capability will be further validated with data taken from cold flow and full-scale FCC units. Also in Phase II, a simulation of the regenerator will be developed which will model pollutant (NOX, SOX) formation, coke combustion, etc. At the conclusion of the program, the validated 3-D analytical (design) tools and associated nonproprietary data bases will become available to all industry organizations interested in pursuing individual commercial opportunities for improving FCC performance.

91-95 Funding (\$K): 5565      Dates: 1993 - 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Chevron: John Paraskos: Phone: (510) 242-3105, Fax: (510) 242-2823  
UOP: Peter Knapik: Phone: (708) 391-2554, Fax: (708) 391-3737

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 41

Category: Oil Processing & Refining (3,5), Gas Processing

Laboratory: Argonne National Laboratory

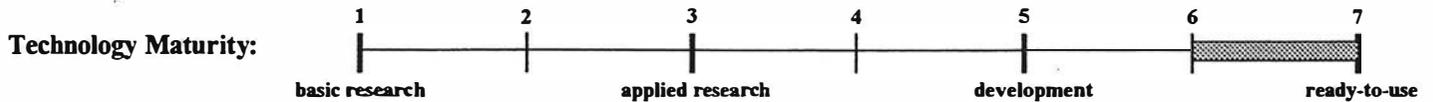
Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Creep Testing of Structural Materials

Description: Monotonic tensile creep (stress-rupture) tests can be conducted on a wide variety of structural materials at temperatures up to 1100°C. Test environments include air, inert gas, or several oxidizing, reducing, or sulfidizing gas mixtures specifically formulated to simulate the required test environment. Axial extensometry and digital data acquisition instrumentation provide a record of the complete strain history of the test specimen during the course of the test.

91-95 Funding (\$K): 300

Dates: 1991-1993



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 42

Category: Environmental & Regulatory (12)

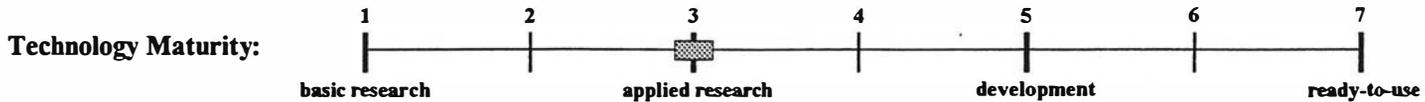
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: In-Situ Bioremediation by Electrokinetic Injection

**Description:** The purpose of this project is to investigate the use of electrokinetic soil processing technology for delivery of nutrients in conjunction with in-situ bioremediation. The project has three primary tasks under Phase I: (1) Efficient injection of nutrients across sandy, silty, and clayey soil exhibiting varying permeabilities and pore fluid conductivities, (2) Uniform distribution of nutrients across sandy, silty, and clayey soils, and (3) Directing nutrients across heterogeneities in layered and clayey soil. The Phase I project serves to demonstrate the proof-of-concept in order to pursue Phase II funding with DOE to perform a pilot-demonstration of electrokinetic injection scale-up and field demonstration at a selected site(s). ANL's role is to perform bench-scale proof-of-concept, 1-dimensional experiments, while Electrokinetics, Inc. will perform larger bench-scale experiments using a parallel plate apparatus (2-dimensional). This technology should stimulate and sustain in-situ bioremediation, and would significantly increase the potential of bioremediation at contaminated sites. The process will be applicable to wetlands, uplands, coastal regions, and locations that are relatively inaccessible (such as underneath existing buildings). The technique appears to have promise in cleaning up oil spills near leaking underground storage tanks. It can also be used in conjunction with injection of microbubbles (colloidal gas aphanes), surfactants, and Fenton's Reagent in deposits.

91-95 Funding (\$K): 100      Dates: 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: ANL: Robert W. Peters: Phone: (708)252-7773, FAX: (708)252-9281, E-mail: ROBERT\_PETERS@QMGate.ANL.GOV  
Electrokinetics, Inc.: Robert E. Marks: Phone: (504) 388-3992, Fax: (504) 388-3928

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 43

Category: Oil Processing & Refining (6,19), Gas Processing

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

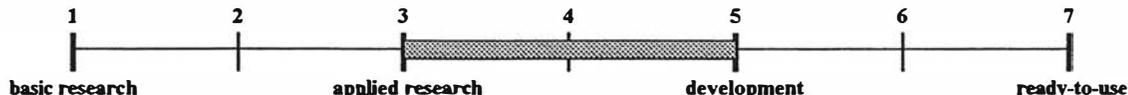
Title: Particle and Droplet Removal from Gas Streams

Description: The Aerosol Technology Group at ANL is involved in a variety of areas related to evaluating existing particle-control methods and developing new technologies. Recent programs include quantifying the capture efficiencies and mass loading characteristics for prefilters and high-efficiency particulate air (HEPA) filters, determining methods to measure and extend the useful lifetime of high-temperature ceramic filters that are subjected to cold cleaning pulses, and developing a heavy metal vapor removal technique based on condensation and thermophoretic deposition.

91-95 Funding (\$K): 250

Dates: 1994-present

Technology Maturity:



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 44

Category: Oil Processing & Refining (4,7)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Conversion of Spent Catalysts into Marketable Products

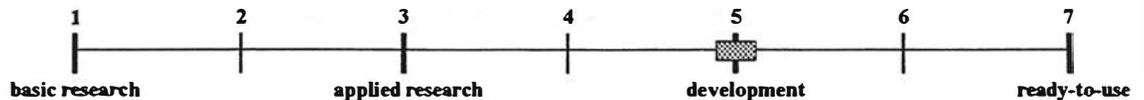
**Description:** Industries annually generate about 50 million tons of spent catalysts, much of which is contaminated with toxic metals. Federal regulations require that these wastes be disposed of in an environmentally sound manner that prevents the contamination of public drinking water by toxins leached from disposal landfills. The ANL program goal is to apply currently available vitrification technologies developed for nuclear waste disposal to the industrial sector so that spent catalyst waste materials can be converted into useful products. Vitrification would be used to produce marketable products that can be used as frits for glass making, abrasives, refractories, insulation, building materials, or color pigments. ANL will use its knowledge in glass formulation to develop laboratory-scale tests that convert the spent catalysts into glass, computer codes that aid in the formulation of glass materials, and use its extensive microanalytical capabilities to characterize the glass products that are formed. Miles Inc., a leading glass manufacture in the U.S., will scale-up laboratory tests into a pilot-scale vitrification facility that can convert the catalyst wastes into glass products. Successful demonstration of this process will result in the: (1) development of a process that reduces the amount of industrial wastes going to landfills, (2) conservation of resources by recycling metal components, and (3) development of economic benefits to catalyst users by providing a cost-effective disposal option for their wastes, and glass/ceramic manufactures by providing low-cost raw materials.

91-95 Funding (\$K):

160

Dates: 1995

Technology Maturity:



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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David Wronkiewicz: Phone: (708) 252-7362, FAX: (708) 252-5246, E-Mail: WRONKIEWICZ@CMT.ANL.GOV

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 45

Category: Oil Processing & Refining (21,25)

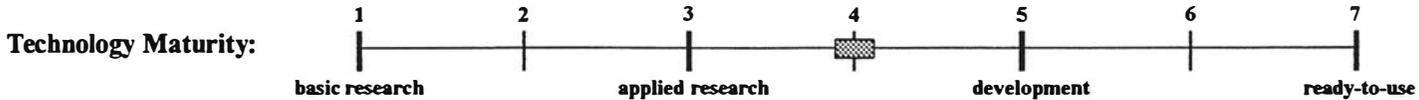
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Fluidized-Bed Upgrading of Heavy Oils and Resids

**Description:** The goal of this cooperative program is to investigate and demonstrate the feasibility and economic potential of a novel process technology for upgrading heavy oils and residual oils to feedstocks suitable for introduction as feedstocks to a petroleum refinery. Specific objectives are to demonstrate that the liquid(s) quality produced from the process will lower processing costs vis a vis costs normally associated with such liquids. The program is focusing on the potential upgrading of Midway Sunset Crude oil. Experimental issues being addressed include definition of process conditions to achieve quality improvements desired, hydrogenation of effluent liquids, and quality of products produced. California Synfuels is overseeing the experimental studies. ANL is developing an integrated 3-dimensional computational fluid dynamics (CFD) cracking kinetic model to interpret data obtained from the pilot pant and fluid characterization tests and to investigate scale-up issues. The code will be a derivative of the reacting multiphase flow code ICOMFLOW that the Laboratory has developed during the past 15 years. California Synfuels Research Corp. and Santa Fe Energy Resource, Inc. will utilize the data and information derived to evaluate the commercial viability of a 50,000 bbl/day field upgrader.

91-95 Funding (SK): 855      Dates: 1994 - 1995



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

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California Synfuels Research Corp.: Mr. Francis Dawson: Phone: (310) 375-7772, Fax: (310) 375-7772

**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 46

Category: Environmental & Regulatory (5,7)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

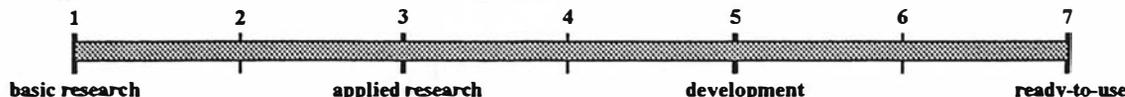
Title: Gas Sensors for Environmental Control Technologies

**Description:** Characterization of automobile and industry air emissions is needed to comply with strict state and federal regulations. Reliable microsensors capable of continuous monitoring for identification and quantification of air contaminants are needed. Argonne has developed new sensor technology with distinct, reproducible responses to a variety of organic gases. The prototype electrocatalytic gas sensors are constructed of rugged-cermet materials using thick-film techniques. The cermet materials are low cost and are capable of operating in high-temperature, corrosive environments. The sensors generate a unique electrical signal representative of a gas or gas mixture, "on demand" by using a cyclic voltammetry measurement technique and relying on neural network signal-processing algorithms to match these signals to a gas signature library. Organic material adsorbed on to the surface of the sensor can be burned off by flash heating the sensor with an incorporated thick film heating element. The current prototype has been tested successfully against a variety of organic gases and emissions mixtures, and has shown distinct signal responses to 100 ppm. Distinct responses to levels in the low ppm range are expected. A functional neural net has been developed which recognizes CO concentrations from the 100,000 to 100 ppm level.

91-95 Funding (\$K): 490

Dates: 1993-present

Technology Maturity:



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 47

Category: Oil Processing &amp; Refining (25, 21)

Laboratory: Argonne National Laboratory

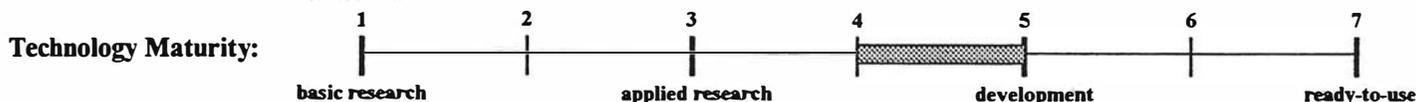
Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Analysis and Modeling of Multi-Dimensional, Multi-Phase, Multi-Species, Turbulent Reacting Flow Using ICOMFLO Computer Code

**Description:** ICOMFLO is used for detailed internal process analysis of individual flow system components. Such analysis may uncover problems in individual components or optimize the operation of those components, which can be critical to the overall operation of the entire system. This analysis may concentrate on component efficiency, or operational lifetime, which may be limited by fouling, erosion, etc., or minimization of pollutant production. ICOMFLO has been successfully applied to the analysis of coal-fired combustors in magnetohydrodynamic (MHD) power generation, air breathing jet engines with fuel spray injection, diesel engines, particle-laden nozzle flow, and the analysis of seed particle injection in the deswirl section of an MHD power train. Finally, the code is being applied to three-phase reacting flow in an FCC (fluid catalytic cracker) riser to aid in the development of technology used to process heavy residual oil into useful fuels or other petroleum products. The multi-dimensional, multiphase, multi-species, turbulent, reacting flow computer code solves conservation equations for gaseous species and solid particles/liquid droplets over a size spectrum. Associated submodels of the code include a unique integral reaction, two-parameter multiphase turbulence, droplet evaporation, and interfacial submodels. The integral reaction submodel provides much improved numerical stability allowing the code to be run efficiently on a fast personal computer. The code has been verified by comparison with experimental results for several applications. The code is operational on a CRAY supercomputer, a VAX minicomputer, and an IBM compatible personal computer (486 or better). The code may be used for either steady or unsteady flow computations.

91-95 Funding (\$K): 450

Dates: 1993-1995



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

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Steve Lottes Division: ES Phone: (708) 252-7014, Michael Petrick Division: ES Phone: (708) 252-5960

**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 48

**Category:** Environmental & Regulatory (5, 10)

**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** Passive and Active Millimeter-Wave Spectrometry for Detection of Trace Gases From Remote Locations

**Description:** The goal of this project is to investigate the potential and feasibility of millimeter-wave technology for continuous emission monitoring of process effluents. Both standoff monitoring of wide areas and in-situ monitoring of individual stacks are of importance. Additionally, the detection sensitivity and chemical selectivity of the technique are to be determined for common pollutants. Argonne National Laboratory is developing active radar-type and passive radiometer-type millimeter-wave systems in the frequency range of 200-300 ghz. A state-of-the-art millimeter-wave facility has been built for testing absorption and emission properties of gas-phase molecules. The laboratory measurements indicate that effluent chemicals can be measured with a sensitivity of tens of parts-per-million-meter using this technology. With a novel signal processing technique based on deconvolution, high specificity of detection has been shown for resolving individual chemicals from a mixture. Proof of principle has been tested by releasing chemicals in open air and detecting them in a standoff mode. Prototype sensors are being developed using a unique Russian backward-wave-oscillator technology. A crada is being initiated with Micro-Now Company for building a millimeter-wave gas analyzer.

**91-95 Funding (\$K):** 2250      **Dates:** 1994 - 1995



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

**Key Personnel:** Anl: A. C. (Paul) Raptis: Phone: (708) 252-5930, FAX: (708) 252-3250, E-mail: ac\_raptis@qmgate.anl.gov  
 Micro-Now Company: Mr. Clarence Arnow: Phone: (708) 677-4700, Fax: (708) 677-0394

**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 49

Category: Environmental & Regulatory (12)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
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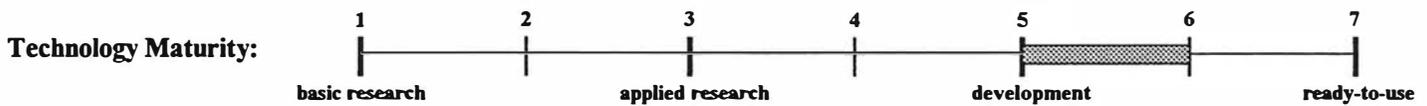
Title: Establishing "Banks" to Replace Wetlands Lost to Industrial Development

**Description:** Argonne National Laboratory under the funding of the Gas Research Institute, the Department of Energy, American Petroleum Institute, and Interstate Natural Gas Association of America evaluated the concept of wetland mitigation banking as a means for the oil and gas industry to achieve compliance with the "no net wetland loss" policy in a timely, cost-effective manner. The August 1993, Clinton wetlands policy statement included wetland mitigation as a part of the solution to protecting wetlands. The banking concept is also endorsed by the Chaffee bill being considered by the Congress of the United States. The program is divided into two phases; characterizing and evaluating the mitigation banking concept across the United States and developing a prototype mitigation bank(s) for the oil and gas industry. The first phase involved the following tasks:

- Define and Describe Key Terms & Issues
- Characterize Existing Banks
- Evaluate Technical Success of Mitigation Banking Efforts
- Cost Comparison: Mitigation Banking Vs. Traditional Mitigation

The ANL Wetland Mitigation Banking Program was designed to evaluate the state of the art in mitigation banking for the oil and gas industry. The research was to identify the most effective methods for creating, managing, and monitoring a wetland mitigation bank. The ultimate goal of the project is to create a prototype mitigation bank serving the oil and gas industry which can provide an area for research into unresolved questions on the technical and regulatory questions regarding mitigation banking for wetlands while adhering to the net loss policy for wetlands. The conclusions from this program were grouped into the four major categories of management, economic, regulatory, and ecology.

91-95 Funding (\$K): 600      Dates: 1991-1994



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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Pat Wilkey Division: ES Phone: (708) 252-6258

Lab Capabilities Applied: Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 50

**Category:** Environmental & Regulatory (12)

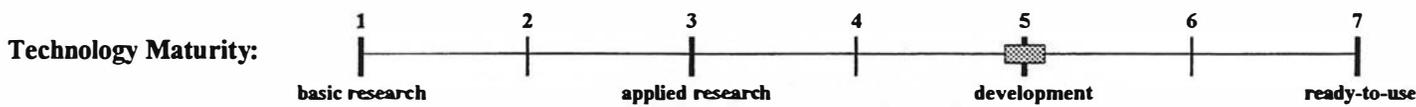
**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** STRATEX for Treatment of Soils

**Description:** The objective of this project was to develop and demonstrate an innovative technology for effective treatment of soils contaminated with volatile and semivolatile organics, and volatile metals (such as mercury and arsenic). This technology treats contaminated soils through a combination of thermal desorption, steam stripping, and solidification/stabilization (S/S). The thermal desorption and steam stripping remove the organic contaminants and the S/S renders the inorganic contaminants less mobile and permits the safe disposal of the treated soil. Two prototype treatment systems have been fabricated (involving a 1.0-ft dia x 1.0-ft long treatment chamber, and a 1.0-ft dia x 2.0-ft long treatment chamber). The organics/inorganics that have been removed from the soil are condensed and collected. Using soil spiked with hexadecane, removal efficiencies typically exceeded 98%. The technology is near-term ready for field demonstrations. Field demonstrations are needed to test the technology under industrial conditions and to obtain data for system scale-up and design, along with economic information. Because the technology is achieved chemically, it is a nonflame system, and thereby is not considered an incinerator/gasifier

**91-95 Funding (\$K):** 325      **Dates:** 1994



**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

**Key Personnel:** ANL: Robert W. Peters: Phone: (708)252-7773, FAX: (708)252-9281, E-mail: ROBERT\_PETERS@QMGate.ANL.GOV

**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 51

Category: Environmental & Regulatory (2,12)

Laboratory: Argonne National Laboratory

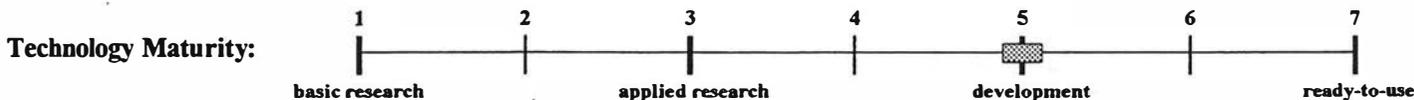
Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Solvent Extraction Processes for Removal of Inorganic Components From Aqueous Streams

Description: Solvent extraction processes and equipment are being developed for decontaminating waste streams and/or recovering valuable inorganic materials. Process development includes formulating and hydrolytic testing of organic solvent systems, batch testing extraction behavior of important feed components, modeling their extraction behaviors using sophisticated models for calculating distribution ratios based on aqueous-phase composition, modeling material balances for multistage countercurrent flowsheets based on the equipment type and known operation, and pilot demonstrating flowsheets in multistage centrifugal contactors. Equipment development includes improving and modifying the Argonne-design centrifugal contactor for specific applications. Most of our current activities are involved with DOE radioactive waste cleanup.

91-95 Funding (\$K): 2230

Dates: 1994 - 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: ANL: George F. Vandegrift: Phone: (708) 252-4513: FAX: (708) 252-5246: E-mail: george\_vandegrift@qmgate.anl.gov

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 52

Category: Environmental & Regulatory (2, 12)

Laboratory: Argonne National Laboratory

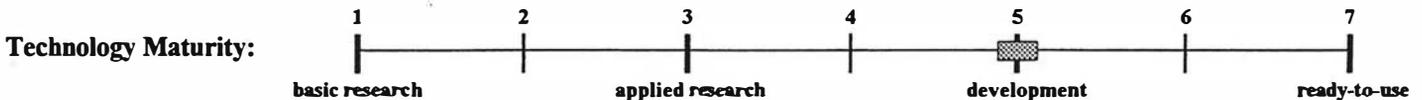
Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Magnetically Assisted Removal of Soluble Contaminants From Liquid Streams

Description: Argonne is developing methods to separate transuranics, heavy metals, and fission products from waste streams using magnetic microparticles. The ferromagnetic particles are coated with an organic complexant-containing solvent for the selective recovery of an inorganic species from solution. At present we are working on methods for the removal of contaminants (specifically transuranic elements, cesium, and strontium) stored in tanks at Hanford and other DOE sites. The greatest benefit of this technology is the simplicity of the operational method to separate the radionuclides and heavy metals from different types of wastes in a cost-efficient manner without the production of large secondary waste streams. The same processes can be adapted and applied for many types of industrial waste streams (e.g., textile, steel, and other metal industries).

91-95 Funding (\$K): 400

Dates: 1994 - 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: ANL: George F. Vandegrift: Phone: (708) 252-4513: FAX: (708) 252-5246: E-mail: george\_vandegrift@qmgate.anl.gov

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 53

**Category:** Environmental & Regulatory (12, 9)

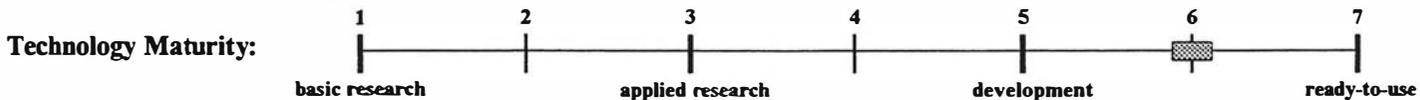
**Laboratory:** Argonne National Laboratory

**Contact:** Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

**Title:** Implementing a Systems Approach to Remediate a Gasoline-Contaminated Site

**Description:** Over the years, more than 10,000 gallons of gasoline, trichloroethylene, and benzene leaked into the subsurface at a U.S. Army base in Alexandria, Virginia. Because of Argonne's expertise in soil and groundwater chemistry, mechanical engineering, and numerical modeling, the Army requested a pilot-scale study to determine the feasibility of selected remediation techniques and critique a specific vapor-extraction design. Working with academia and private industry, Argonne designed and implemented a system for sampling, analysis, and risk assessment and adapted the U.S. Geological Survey's AIRFLOW model to simulate the performance of alternative remediation designs. During the technology demonstration, Argonne-installed horizontal wells removed about 500 gallons of gasoline. Argonne also learned that stimulating indigenous bacteria promotes bioremediation.

**91-95 Funding (\$K):** 350      **Dates:** 1991-1993

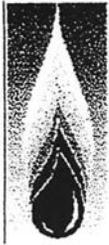


**Technology Transfer:** Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

**Key Documentation:** List available through key personnel.

**Key Personnel:** Tom Sydelko Division: ES Phone: (708) 252-3309

**Lab Capabilities Applied:** Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 54

Category: Environmental &amp; Regulatory (10, 2)

Laboratory: Argonne National Laboratory

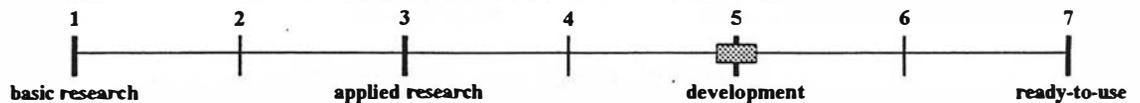
Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.govTitle: Development and Application of Novel TiO<sub>2</sub> Photocatalysts for Treating Combined Wastes

**Description:** This project has two major tasks: (1) the development and design of new photocatalysts, and (2) their application to contaminated waste streams. During FY1994, a colloidal reactor for controlled synthesis of nanoscale colloidal particles was developed and demonstrated. Cysteine and thiolactic acid have been used to change the surface characteristics of the TiO<sub>2</sub> photocatalysts. Bench-scale testing has been performed for waste streams containing lead and naphthalene, and lead and phenol. Removal rates of the lead were 2-3x faster and 9x faster for the cysteine- and thiolactic acid-modified photocatalysts, respectively, as compared to untreated TiO<sub>2</sub>. The presence of lead had little effect on the removal/degradation of naphthalene (or phenol); the presence of naphthalene resulted in a "lag-time" effect on the photoreduction of lead from solution. Our results indicate that simultaneous removal of organic compounds and heavy metals in aqueous solution can be achieved using a TiO<sub>2</sub> photocatalyst with UV light. The rates of organic and inorganic compounds is enhanced by surface modification of the TiO<sub>2</sub> photocatalyst. Using this technique, photooxidation (i.e., destruction of the organics) and photoreduction (i.e., removal/recovery of the heavy metals) occur simultaneously. We anticipate demonstrating the technology at an industrial site during FY1996.

91-95 Funding (\$K): 300

Dates: 1994 - 1995

Technology Maturity:



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: ANL: Robert W. Peters: Phone: (708)252-7773, FAX: (708)252-9281, E-mail: ROBERT\_PETERS@QMGate.ANL.GOV, Natalia K. Meskov: Phone (708)252-5234

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 55

Category: Environmental & Regulatory (12)

Laboratory: Argonne National Laboratory

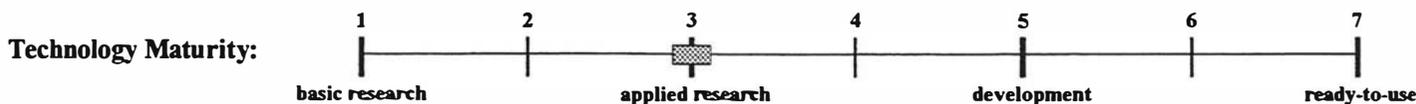
Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Ultrasonic Soil and Groundwater Cleanup

**Description:** A critical problem at many U.S. Department of Energy (DOE) and other government and industrial sites is the contamination of groundwater and soil with chlorinated organic compounds such as carbon tetrachloride (CCl4), trichloroethylene (TCE), perchlorethylene (PCE), polychlorinated biphenyls (PCBs), and pesticides. To address this issue, researchers at ANL are developing an innovative ultrasonic detoxification process that could ultimately be used to detoxify contaminated soil and groundwater at affected sites. ANL is one of the first research organizations to systematically test ultrasonic technology on the detoxification of contaminated soil and groundwater. Bench-scale batch and continuous-flow experimental systems have been set up in the laboratory. The results of initial experiments conducted at Argonne confirmed that the ultrasonic detoxification can be used to reduce the concentrations of CCl4 in water (to less than 2 ppb) and soil (to less than 1 ppm). A conceptual process design of an ultrasonic soil- detoxification system has been completed. In addition to the destruction of organic compounds, this process is also potentially able to remove radioactive compounds from the soil matrix, and these metals can be subsequently recovered. Preliminary cost estimates of the technology indicated that it would be less costly than incineration for treating soils and sludges contaminated with PCBs.

This project is aimed at developing a sonication device that can be placed in a well in order to destroy chlorinated hydrocarbons, chlorinated aliphatics, or polyaromatic hydrocarbons in-situ. Batch laboratory proof-of-concept experiments have been performed in which waters (deionized and the EPA artificial groundwater recipe) spiked with carbon tetrachloride (CCl4) and trichloroethylene (TCE) have been sonicated. Removal efficiencies greater than 95% have been achieved in less than 2 minutes. . Preliminary economic analyses indicate the treatment cost is about \$0.50-\$0.80/1000 gallons.

91-95 Funding (\$K): 330      Dates: 1991-1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: Jiann M. Wu Division: ES Phone: (708) 252-5786 Fax: z9708) 252-9281 E-mail: Robert W. Peters Division: ES Phone: (708) 252-7773

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 56

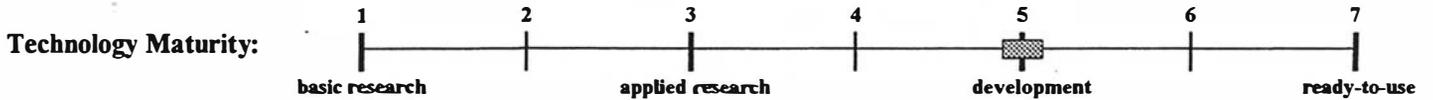
Category: Oil Processing & Refining (6,25)

Laboratory: Argonne National Laboratory      Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Evaluation of FCC Feed Nozzles

Description: Argonne and a consortium of oil refiners and nozzle vendors are entering into a cooperative research and development program. The purpose is to test commercial fluid catalytic cracking (FCC) feed nozzles, focusing on particle droplet size distributions and velocities, and to use this data to develop a mix zone hydrodynamic model of the interaction between atomized droplets, catalyst particles and the surrounding gas field. The goal is to design advanced FCC nozzles.

91-95 Funding (\$K): 1500      Dates: 1995-present



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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K. H. Im Division: TD Phone: (708) 252-5985  
V. J. Novick Division: TD Phone: (708) 252-6629 Fax: (708) 252-4007

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 57

Category: Environmental & Regulatory (5, 6)

Laboratory: Argonne National Laboratory

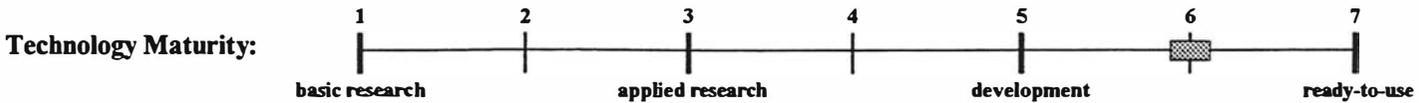
Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Pipeline Leak and Rupture Assessment

**Description:** On October 3, 1989, in an incident near Sabine Pass, Texas, the fishing vessel Northumberland struck and ruptured an off-shore, 16-in. diameter, natural gas transmission line, resulting in a fire and the loss of 11 lives. This incident has caused the pipeline and near-shore fishing industries to focus on the need to accurately locate and monitor subsea pipelines in shallow water. This report discusses the research needed in three areas associated with locating pipelines: sensors, delivery systems (remotely operated vehicles or ROVs), and the conditions that lead to pipeline exposure. Literature was surveyed, and experts working on determining pipeline burial conditions were consulted. The research on sensors and ROVs is leading to systems that will determine the present conditions of pipelines in shallow water.

The Rio Vista gas leak study evaluated methods for remotely sensing gas leaks from buried pipelines and developed methods to elucidate methane transport and microbial oxidation in soils. Remote-sensing methods were evaluated by staging gas leaks along an abandoned Pacific Gas and Electric (PG&E) gas field collection line in northern California and applying surface-based and airborne remote-sensing techniques in the field, including thermal imaging, laser imaging, and multispectral imagery. The remote-sensing techniques exhibited limitations in range and in their ability to correlate with ground truth data. To elucidate methane transport and microbial oxidation in soils, a study of a controlled leak permitted field testing of methods so that such processes could be monitored and evaluated. Monitoring and evaluation techniques included (1) field measurement of soil-gas concentrations, temperature, and pressures; (2) laboratory measurement of soil physical/chemical properties and activity of methane-oxidizing microorganism by means of field samples; and (3) development of preliminary numerical analysis technique for combined soil-gas transport/methane oxidation. Soil-gas concentrations at various depths responded rapidly to the high rate of gas leakage. The preliminary field, laboratory, and numerical analysis techniques tested for this study of controlled gas leak could be successfully applied to future studies of gas leaks.

91-95 Funding (\$K): 800 Dates: 1991-1992



Technology Transfer: Conference presentations, technical reports, Industry workshops, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: Patrick L. Wilkey, ES Division, Phone (708) 252 6258, Fax (708) 252-6407

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 58

Category: Environmental & Regulatory (14, 6)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: South Louisiana and Mississippi Delta Subsidence and Wetlands Losses

**Description:** Recent geologic literature from the petroleum industry indicates growth faults are episodically active, and during these episodes, saline fluids, oil, and gas migrate vertically up fault zones from deep seated geopressed sections into shallow aquifers. Data from south Louisiana indicate growth faults are not only active in the Holocene sedimentary section, but actively contribute to the subsidence of Louisiana wetlands. Argonne National Laboratory has successfully field-tested a method to detect the subcropping location of active growth faults, and determine whether a fault is sealing or non-sealing on the basis of bulk conductivity contrasts between aquifers on either side of these faults. Electromagnetics provide an inexpensive, non-invasive method to rapidly assess these conductivity contrasts. The implications of this study for the compartmentalization of hydro-geochemical regimes are profound, and challenge established models of simple diffusive flow between the marine and the terrestrial environment.

Argonne National Laboratory acoustic studies in Plaquemines, Terrebonne, and Lafourche Parishes, Louisiana have identified an anomalously low velocity zone in the upper 20-40 meters of sediment which appears to be present across widespread areas in the delta plain. The interval velocity of this zone varies with location but exhibits a range of values between 800 and 1200 m/s with a mean velocity of 1050 m/s. A mean gas volume of 12% was determined for this low-velocity zone from simultaneous attenuation and velocity modeling utilizing crosswell tomography techniques. The velocities in this area are attributed to variable gas concentrations of biogenic methane generated by the reduction of carbon in stacked deltaic peats under anaerobic, subsurface conditions. Sediments supported by gas are subject to rapid consolidation settlement. Delimiting the spatial dimensions of low-velocity zones aid in predicting future areas of subsidence. Implications of these studies include vertical gas-flux, in deltaic sediments, the release of greenhouse methane into the atmosphere during episodes of marine ravinement, and the built-in mechanisms which allow deltaic sequences to accommodate a new delta building event.

91-95 Funding (SK): 700 Dates: 1992-1994



Technology Transfer: Open literature publications, industry collaboration, technical reports, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: Lyle McGinnis, ES Division, Phone (708) 252-8722, Fax (708) 252-6407 Mike Thompson, ES Division, Phone (708) 252-9269, Fax (708) 252-6407 Gerald Kuecher, ES Division, Phone (708) 252-8893, Fax (708) 252-6407

Lab Capabilities Applied: Environmental Geophysics, Instrumentation and Non-Destructive Testing Instrumentation and non-invasive evaluation, fluid sciences, environmental



Index: 59

Category: Environmental & Regulatory (14)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Land Loss in the Deltaic Plain of Louisiana

Description: ANL is classifying the geomorphology and causes of land loss in southern Louisiana to determine the role oil and gas operations play. Based on Corps of Engineers geographic data over 40 years, land loss has been classified by a schema relating to interior and shoreline loss. Natural and man-made causes of loss are being evaluated and classified. The data will be summarized in Geographic Information Systems maps. The schema for geomorphology and land loss causes were developed through a committee involving natural resource agency, regulatory, academic, and industry personnel. Personnel for classification were experts in wetlands loss and southern Louisiana natural resources.

91-95 Funding (SK): 1100      Dates: 1991-1994



Technology Transfer: Open literature publications, industry collaboration, technical reports, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: Patrick L. Wilkey, ES Division, Phone (708) 252-6258, Fax (708) 252-6407

Lab Capabilities Applied: Remote Sensing, Geographic Information Systems, Advanced Data Processing, Decision Analysis



Index: 60

Category: Environmental & Regulatory (12, 14)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596. Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Pipeline Right-Of-Way Research Program

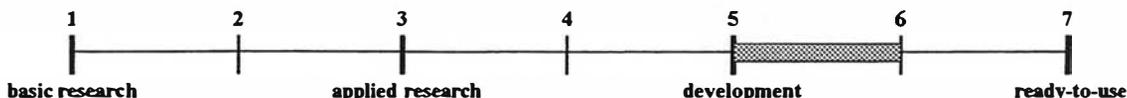
**Description:** Sponsored by the Gas Research Institute (Chicago, Illinois), Argonne National Laboratory has established field and laboratory research projects to develop and test construction and reclamation technologies to minimize the costs and mitigate the ecological impacts of pipeline installation. The program provides quantitative data that has been published in technical journals and used by the gas industry and others to increase the industry's understanding of the environmental effects of pipeline installation and right-of-way (ROW) rehabilitation.

The 10-year Right-of-Way Research Program has investigated the environmental impacts and mitigation techniques associated with the construction and maintenance of gas pipeline rights of way. The program has addressed several major topic areas involving pipeline rights of way. Areas of research include: Erosion Control, Geographic Information Systems, Soils and Revegetation, Bioremediation of Produced Waters, Vegetation Management, Remote Sensing, Wetlands Crossings, New Technologies, and Stream Crossings.

91-95 Funding (\$K): 2300

Dates: 1991-present

Technology Maturity:



Technology Transfer: Open literature publications, industry collaboration, technical reports, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: Patrick L. Wilkey, ES Division, Phone (708) 252-6258, Fax (708) 252-6407

Lab Capabilities Applied: Environmental Geophysics, Instrumentation and Non-Destructive Testing  
Instrumentation and non-invasive evaluation, fluid sciences, environmental



Index: 61

Category: Environmental & Regulatory (12)

Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

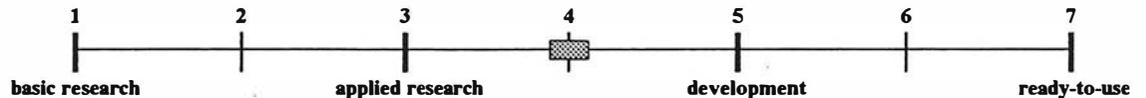
Title: Bioremediation of Contaminated Soil by Enhanced Phytoremediation

**Description:** This project investigates the coupled use of phytoremediation and chelant extraction to mobilize heavy metals in soil and hyperaccumulate in plants. Objectives of this study include: (1) Identification of the most promising conditions for successful application of the phytoremediation technology, (2) Obtain working samples of soil and plant specimens, (3) Perform laboratory treatability studies to identify conditions that increase to the maximum extent the mobility of the contaminant(s), measured by chemical analysis (sequential extraction and leaching), and (4) Evaluate the accumulation of contaminant(s) in plant tissues as a function of the treatment (soil condition) and plant species. ANS will assist ANL in conducting field demonstrations. This approach should greatly increase the role of bioremediation to treat heavy metal-contaminated sites with a low-cost technique.

91-95 Funding (\$K): 400

Dates: 1995

Technology Maturity:



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: ANL: M. Cristina Negri: Phone: (708)252-9662, FAX: (708)252-9281, E-mail: CRISTINA\_NEGRI@QMGate.ANL.GOV

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 62

Category: Deepwater Offshore (9, 16), Oil Processing & Refining

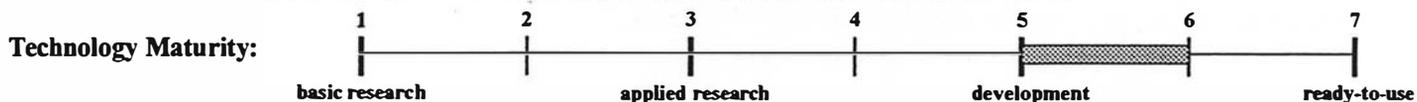
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Fluid Forces Acting on Tube Arrays in Crossflow

**Description:** A group of tubes submerged in crossflow can be subjected to dynamic instability, typically referred to as fluidelastic instability. If a system component consisting of multiple tubes is operated at a flow velocity above the critical value, severe damage to the component is likely to occur, often after only a short time. Therefore, operating at or above the critical flow velocity is not acceptable. This program is to evaluate existing fluid-force data, measure motion-dependent fluid forces, and complete the unsteady flow theory for fluidelastic instability of tube arrays in crossflow. A direct method of measurements for motion-dependent fluid forces acting on tube arrays has been developed at Argonne. This method is being applied to characterize the fluid-force coefficients including fluid stiffness and fluid damping for applications to various tube arrays in crossflow. Once fluid-damping and fluid-stiffness coefficients are characterized, the unsteady flow theory using the experimental fluid-force data, can be used to predict tube response under various conditions including random vibration, periodic oscillation, and chaotic motion. The potential benefits to be derived from this program are substantial: The existing test facilities at Argonne are very cost-effective and the extensive experience of Argonne staff in the subject area means that achievement of the goal is very likely. The unsteady flow theory will establish the applicable ranges of other simplified theories and provide the answers in the resolution of vibration problems in the components with multiple tubes in flow. The total budget for this program is \$219K (1994-\$100K and 1995-\$119K). It should be noted that in addition to this program, Argonne staff have close to 30 years of experience working in the areas of flow-induced vibration and fluid/structure interaction. Their work has included code development, modeling, experimentation, and design guide development, with application to nuclear internal and plant components, offshore structures, aerospace structures, and civil structures. One of the immediate applications of the results to the petroleum industry is deepwater offshore (risers) to withstand dynamic loading associated with waves, ocean currents, winds, and seismic activity.

91-95 Funding (\$K): 220      Dates: 1994-present



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

Key Personnel: Shoei-Sheng Chen, Energy Technology Division Tel./Fax: 708-252-6147/5568 (The author of a book, Flow-Induced Vibration of Circular Cylindrical Structures, which can be used in the petroleum industry)

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 63

Category: Environmental & Regulatory (2)

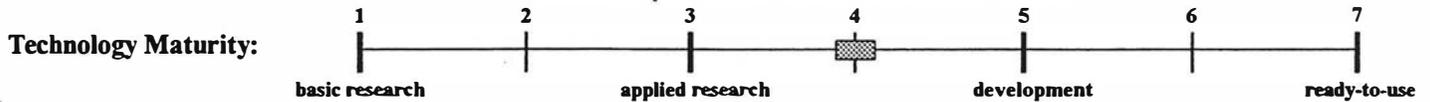
Laboratory: Argonne National Laboratory

Contact: Paul D. Eichamer, Jr. 800/627-2596.Fax: (708) 252-5230  
eichamep@smtplink.eid.anl.gov

Title: Integrated Electrodialysis/Reverse Osmosis Process for Produced Water Treatment

**Description:** The project goal is to evaluate the technical and economic feasibility of an integrated electrodialysis (ED) / reverse osmosis (RO) process to treat produced waters (hydrocarbon-contaminated brine) generated by natural gas production. This process combines ED and RO in a synergistic manner to reduce the volume of the salt water waste by concentrating the salts and to generate a clean water stream for beneficial uses. In laboratory screening experiments key ED parameters (e.g., salt removal and current efficiency) were measured using produced water samples from gas production sites. Results of the ED and RO laboratory screening experiments will form the basis for a coordinated program consisting of more extensive laboratory experimentation, economic feasibility analyses, and optimization of the integrated ED-RO process. Techniques to reduce membrane fouling are being developed. After successful completion of laboratory-scale development and process demonstration, a field demonstration at a gas production site will be performed. A costing model is being developed to do sensitivity analyses of process parameters and conditions. Argonne will develop a preliminary design of the field demonstration unit and provide economic analysis support to ReTec. Project results will be incorporated into a knowledge base being developed by ReTec for use in identifying the optimal produced water treatment method for the specific conditions at a given site.

91-95 Funding (\$K): 260      Dates: 1994 - 1995



Technology Transfer: Joint programs with industry, Open literature publications, licensing, INTERNET database, Tech Transfer Center

Key Documentation: List available through key personnel.

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ReTec: Lonny Lawrence: Phone: (412) 826-3340: Fax: (412) 826-3409  
GRI: Thomas Hayes: Phone: (312) 399-8325: Fax: (312) 399-8

Lab Capabilities Applied: Engineered Materials, Instrumentation and Nondestructive Evaluation, Thermal and Fluid Sciences, Engineering Mechanics, Process Efficiency and Waste Recycling, Controlled Systems, Environmental Control Technology



Index: 64

Category: Development (4, 21), Gas Gathering (2), Gas Storage (2) Environment & Regulatory (5)

Laboratory: Brookhaven National Laboratory Contact: I. N. Tang, 516-282-4517, tang1@bnl.gov

Title: Microparticle Analysis by Laser Spectroscopy

**Description:** The objective of this research program is to determine the fundamental properties that are essential in developing laser-based spectroscopic methods for microparticle analysis. Both the physics and the chemistry of these particulate matters govern the material processing in manufacturing industries, global climate change, combustion, and many other energy-related processes. Because of the minute physical size of these particles, it is imperative to develop ultra-sensitive analytical techniques for monitoring in situ the physical transformation and chemical reactions of these airborne particles. Laser Raman scattering is currently being investigated as a means for composition analyses of these particles. Areas of interests include: (1) determination of Raman scattering cross-sections for common ionic solids, such as oxyanions; (2) study of the chemistry of supersaturated solution droplets which can not otherwise be investigated with bulk samples; (3) sensitivity enhancement by resonance Raman scattering; and (4) mass spectrometric analysis of single micron-sized particles. Mass spectrometry is particularly suited for ultra-fine particles whose chemical characterization can not be accomplished by any other methods. It is anticipated that the research will lead to high sensitivity and wide selectivity of the spectroscopic methods specifically developed for microparticle analysis.

91-95 Funding (\$K): 1080 Dates: 1991-present

Technology Maturity:



Technology Transfer: Publication in Open Literature, Invited Talks, Conferences

Key Documentation: 1) Fung, K.H., Tang, I.N. Detection limits for sulfates and nitrates in aerosol particles by Raman spectroscopy. J. Aerosol Sci. 25(3), 479-85 (1994)  
2) Tang, I.N., Munkelwitz, H.R. Aerosol phase transformation and growth in the atmosphere. J. Appl. Meteorol. 33(7), 791-96 (1994).

Key Personnel: I. N. Tang, 516-282-4517, tang1@bnl.gov  
K. H. Fung, 516-282-3047, fung@bnlux1.bnl.gov

Lab Capabilities Applied: Laser Raman Scattering, Aerosol Chemistry, Microparticle Analysis, Spectroscopy



Index: 65

Category: Production (24), Oil Processing &amp; Refining (27)

Laboratory: Brookhaven National Laboratory

Contact: B. Klemm, 516-282-4022

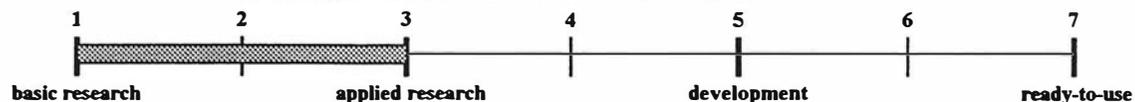
Title: Combustion Kinetics &amp; Reaction Pathways

**Description:** The scientific objectives of this program are: (1) the measurement of absolute rate constants for combustion-related reactions of fuel compounds and intermediate species; (2) the determination of pathways for multichannel reactions; and (3) the study of photoionization and thermochemistry of free radicals. The focus of the research is on fundamental aspects of combustion chemistry. This experimentally based project features three independent methods in a multi-technique approach that provides unique capabilities in performing reliable kinetic measurements over an exceptionally wide range in temperature, 300K to 2500K. Additionally, a discharge flow-photoionization mass spectrometer (DF-PIMS) experiment is used to identify primary products from multichannel reactions, to determine photoionization spectra for reactants and products, and to measure ionization energies of free radicals. The DF-PIMS apparatus was designed to be operated on the U-11 beam line at the National Synchrotron Light Source (NSLS) and thus take advantage of tunable vacuum ultraviolet light to achieve improved detection sensitivity and selectivity in monitoring free radicals.

91-95 Funding (\$K): 3030

Dates: 1991-present

Technology Maturity:



Technology Transfer: Publication in Open Literature, Workshops, Invited Talks

**Key Documentation:** 1) Kuo, S., Zhang, Z., Klemm, R.B., Liebman, J.R., Stief, L.J., Nesbit, F.L. Photoionization of hydroxymethyl (CD<sub>2</sub>OH and CD<sub>2</sub>OD) and methoxy (CD<sub>3</sub>O) radicals: Photoion yield spectra, ionization energies and thermochemistry. *J. Phys. Chem.* 98, 4026-33 (1994).

**Key Personnel:** R.B. Klemm, 516-282-4022  
J.W. Sutherland, 516-282-3053, jws@bnlux1.bnl.gov

**Lab Capabilities Applied:** Mass Spectrometry, Photoionization, Reaction Rates and Pathways, National Synchrotron Light Source, Combustion Chemistry



Index: 66

**Category:** Environmental & Regulatory (9, 14), Oil Processing & Refining (8), Exploration (2)

**Laboratory:** Brookhaven National Laboratory      **Contact:** P. D. Moskowitz, 516-282-2017, moskowi2@bnl.gov

**Title:** EPA/DOE Interagency Project on Environmental Pathway Modeling

**Description:** The U.S. Environmental Protection Agency Office of Radiation and Indoor Air and Office of Solid Waste and Emergency Response, and the U.S. Department of Energy Office of Environmental Management are sponsoring work at BNL to promote the appropriate and consistent use of mathematical models in the remediation and restoration process at sites containing, or contaminated with, radioactive materials. Specific activities undertaken in FY 1994 include: 1) the benchmarking of three ground-water models commonly used in R1/FS studies at EPA SUPERFUND sites, 2) preparation of a technical guide to ground-water model selection at sites contaminated with radioactive substances, and 3) a technical evaluation of three multimedia risk assessment models in use at these types of sites.

**91-95 Funding (\$K):** 550      **Dates:** 1991-present



**Technology Transfer:** Publication in Open Literature, Lectures, Conferences, Reports

**Key Documentation:** 1) Moskowitz, P.D., Pardi, R., DePhillips, M.P., and Meinhold, A.F. Computer models used to support clean-up decision making at hazardous and radioactive waste sites. Risks Analysis 12(4), 591-621 (1993).

**Key Personnel:** P.D. Moskowitz, 516-282-2007, moskowi2@bnl.gov

**Lab Capabilities Applied:** Mathematical Modeling, Technical Assessment



Index: 67

Category: Gas Processing

Laboratory: Brookhaven National Laboratory

Contact: D. Mahajan, 516-282-4985,  
dmahajan@bnl.gov

Title: Fischer-Tropsch Synthesis with Fine Particle Catalysts

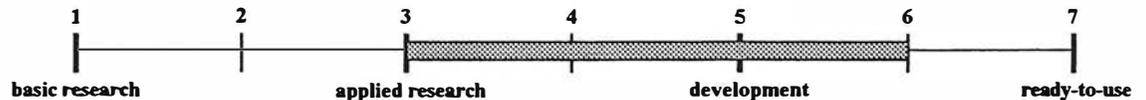
**Description:** The proposed approach seeks to build upon data generated during slurry-phase Fischer-Tropsch (F-T) synthesis effected at a lower temperature of 220°C by unsupported ultrafine particles (UFP) (mean Particle Diameter (MPD) < 100 nm) of Fe catalysts. Under conditions optimized for hydrocarbon production, these catalysts typically generate < 10 wt% oxygenates of which selectivity to C1-C4 linear alcohols exceeds 90%. From the F-T reaction, the intercepted metal species, which is active in high H<sub>2</sub>O concentration environment due to absence of water-gas shift (WGS) activity, is characterized via Extended X-ray Absorption Fine Structure (EXAFS) and Mössbauer spectroscopy to be solely magnetite (Fe<sub>3</sub>O<sub>4</sub>). In the suggested overall scheme, the following reaction sequence is anticipated: 1) temperature and pressure selection favorable for higher alcohols formation, 2) interception of hydrocarbon intermediates by CO<sub>2</sub> to increase oxygenates, 3) base promotion to enhance carbon-carbon coupling. Preblended CO<sub>2</sub>-rich synthesis gas (syngas) of composition normally available from carbonaceous sources (coal or natural gas) will be utilized.

Several projects including Department of Energy (DOE)/-industry cost-shared initiatives, administered through Pittsburgh Energy Technology Center (PETC), are aimed at addressing different aspects of economical production of isobutanol (isobutylene) from syngas. The presented approach will especially complement the DOE/Air Products and Chemicals, Inc. (APCI) effort in relation to the ongoing Alternative Fuels Development (AFD) program.

91-95 Funding (\$K): 320

Dates: 1991-1993

Technology Maturity:



Technology Transfer: Workshops, Reports, Publication in Open Literature, Invited Talks, CRADAS

**Key Documentation:** 1) Mahajan, D., Kobayashi, A., Gupta, N. Fischer-Tropsch synthesis catalyzed by ultrafine particles of iron: Cessation of water-gas shift activity. J. Chem. Soc., Chem. Commun., 795-96 (1994).

Key Personnel: D. Mahajan, 516-282-4985, dmahajan@bnl.gov

Lab Capabilities Applied: Chemical Sciences, Catalysis, Physical Measurements with X-Rays, Mossbauer Spectrometry





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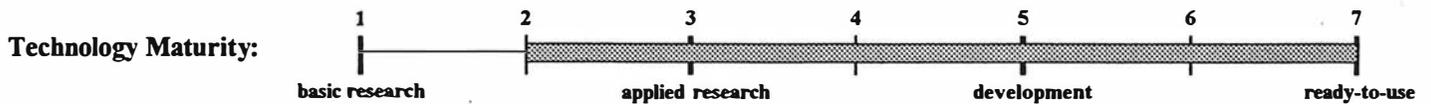
**Category:** Oil Processing & Refining (11)

**Laboratory:** Brookhaven National Laboratory      **Contact:** E. T. Premuzic, 516-282-2893; M. Lin, 516-282-3064

**Title:** Advanced Biochemical Processes for Geothermal Brines

**Description:** An R&D program to identify methods for the utilization and/or low cost environmentally acceptable disposal of toxic geothermal residues has been established at the Brookhaven National Laboratory (BNL). Laboratory work has shown that a biochemical process does meet the requirements. In this work, microorganisms which can interact with toxic metals (including trace radionuclides) found in geothermal residual brine sludges and which can convert them into soluble species for subsequent reinjection or concentration, have been identified. The biochemical activities of these organisms served as models for the development of technically and economically feasible detoxification processes leading to advanced biotechnology for geothermal waste treatment. The new biotechnology reduces significantly the cost of surface disposal of sludges derived from geothermal brines. A concurrent process for the concentration and recovery of valuable metals has also been developed.

**91-95 Funding (\$K):** 1020      **Dates:** 1991-1995



**Technology Transfer:** Reports, Invited Papers, Publication in Open Literature, CRADAs

**Key Documentation:** 1) Premuzic, E.T., Line, M.S., Jin, J.Z. Geothermal waste treatment biotechnology. Proc. Of Geothermal Program Review XI: "Geothermal Energy--The Environmentally Responsible Energy Technology for the Nineties.", Berkeley, CA, April 1993. BNL 48990, April 1993  
2) Premuzic, E. T. Advanced biochemical processes for geothermal brines - Annual Report. BNL 60291, February 1994.

**Key Personnel:** E. T. Premuzic, 516-282-2893  
M. Lin, 516-282-3064

**Lab Capabilities Applied:** Microbiology, Biochemistry, Instrumentation, Economic Analysis



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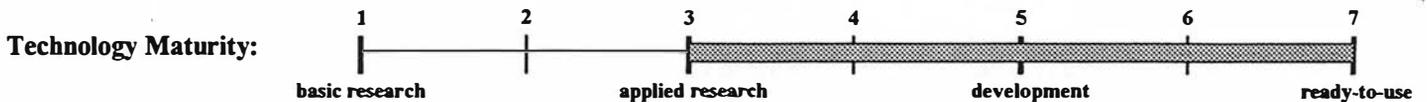
Category:

Laboratory:  Contact:

Title:

Description: This ongoing laboratory-based high payoff R&D program which is highly regarded by industry, is an important part of the Department of Energy/Geothermal Division Core Research Category, and it has already yielded several durable cost-effective materials of construction which are being used by the geothermal industry. During the period FY 1994 - FY 1995, R&D in the following areas will be continued: 1) advanced high temperature CO<sub>2</sub>-resistant lightweight well cementing materials, 2) high temperature chemical systems for lost circulation control, 3) thermally conductive corrosion resistant composites for heat exchange applications, and 4) corrosion mitigation at The Geysers. Activity 3 will be completed in FY 1994. Activity 2 will be completed in FY 1995, and two new activities "In Situ Conversion of Drilling Mud into Cement" and "Insulative, Corrosion Resistant Liners for Brine Transmission Piping Systems" initiated. In FY 1996, work on advanced cements (Activity 1) will be completed. Other materials problems will be addressed as their needs are identified by industrial advisory groups. All of the activities will be performed as cost-shared efforts with National Laboratories (Sandia National Laboratories, National Renewable Energy Laboratory), and industry. Successful developments will significantly reduce the cost of well drilling, completion and energy-extraction international competitiveness.

91-95 Funding (\$K):  Dates:



Technology Transfer:

Key Documentation: 1) Webster, R.P., Reams, W., Kukacka, L.E. Polymer concrete systems for use in the construction of steam-valve manholes. BNL 49623, September 1993.  
2) Webster, R.P., Reams, W., Kukacka, L.E. Development of polymer concrete liners and coatings for use in geothermal applications. BNL 49623, September 1993.

Key Personnel:

Lab Capabilities Applied:



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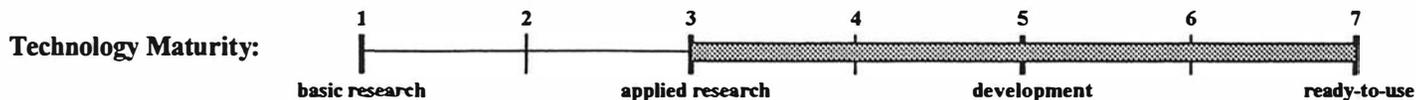
**Category:** Development (4, 21), Gas Gathering (2), Gas Storage (2), Environmental & Regulatory (5)

**Laboratory:** Brookhaven National Laboratory      **Contact:** G. Senum, 516-282-3896

**Title:** Application of Multitracer Technology to Petroleum Reservoir Studies

**Description:** The Tracer Technology Center (TTC) at Brookhaven National Laboratory (BNL) has developed a ultitracer perfluorocarbon-tracer (PFT) technology which, over the last fifteen years, has been applied to various atmospheric, hydrological, and subsurface applications. This five and one-half-year program is aimed at applying this technology to petroleum reservoir studies, i.e.: (a) exploiting the potential 1000-fold reduction in tracer costs for PFTs compared to radioactive tracers; (b) making use of the convenient sampling methodology which allows samples to be easily shipped; and demonstrating the applicability of multiple PFTs, having different volatilities, to the characterization and study of petroleum reservoirs. The areas to be pursued are: 1) demonstration of the PFT technology ability to determine the transport and dispersion of injected gas, oil, and water in petroleum reservoirs in cooperation with other petroleum researchers; 2) demonstration of the multi-PFT technology to determine the averaged residual pore oil saturation of petroleum reservoirs along the path of tracer transport; 3) develop new and unique tracers for petroleum reservoir studies which either are compatible with PFT technology of SF6 technology; 4) in conjunction with these field experiments: a) development and evaluation of tracer-injection techniques adapted to conditions of injection, b) validation of the effectiveness and representativeness of the sampling procedures for various phases extracted, and c) development of analytical-system modifications as needed; and 5) design unique and novel field experiments in conjunction with the University of Texas at Austin (UT/Austin) to fully demonstrate the capabilities of PFTs and tracer experiment in assisting the characterization of petroleum reservoirs for enhanced oil recovery (EOR). Field experiments are ongoing at the National Petroleum Reserve in California (NPRC).

**91-95 Funding (\$K):** 1080      **Dates:** 1991-present



**Technology Transfer:** Reports, Publication in Open Literature, Lectures, CRADAs, Patents

**Key Documentation:** 1) Senum, G.I., Fajer, R., DeRose, W.E., Harris, B.R., Ottaviani, W.L. Petroleum reservoir characteristics by perfluorocarbon tracers. Presented at SPE/DOE Eighth Symposium on Enhanced Oil Recovery, Tulsa, Oklahoma, April 22-24, 1992. SP/DOE 24137.  
 2) Shotts, D.R., Senum, G.I. A CO2 based analysis of a light-oil steamflood at NPR-1, Elk Hills, CA BNL 49759, November 1993.

**Key Personnel:** G. Senum, 516-282-3896  
 R. N. Dietz, 516-282-3059

**Lab Capabilities Applied:** Chemical Analysis, Tracer Technology



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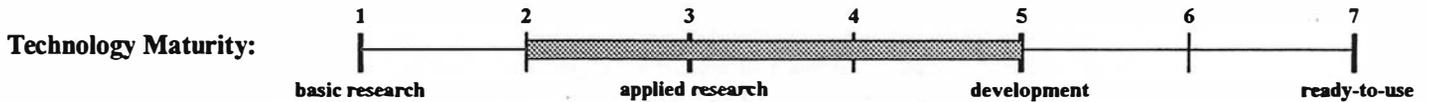
Category: Exploration

Laboratory: Brookhaven National Laboratory      Contact: H. B. Stewart, 516-282-4179, [stewart1@bnl.gov](mailto:stewart1@bnl.gov)

Title: Design of a Robust Numerical Model for Multiphase Flow

**Description:** The purpose of this task is to guide the design of computer software which implements a numerical model of multifield multiphase fluid dynamics applicable to the same class of problems as the existing KfK code IVA3. This will include (1) derivation of a multifield mathematical model, of a corresponding finite numerical approximation and solution procedure; (2) design of computer code to implement the model; (3) robustness, and accuracy; and (4) providing adequate documentation for all stages of the work, including a final report. The actual writing of computer code and execution of test computations will be the responsibility of KfK.

91-95 Funding (\$K): 150      Dates: 1993-1995



Technology Transfer: Reports, Publication in Open Literature, Seminars and Lectures

Key Documentation: Stewart, H.B., Wendroff, B. Two-phase flow: models and methods. J. of Computational Physics, 56(3), December 1994.

Key Personnel: H. B. Stewart, 516-282-4170, [stewart1@bnl.gov](mailto:stewart1@bnl.gov)

Lab Capabilities Applied: Mathematical Modeling, Numerical Simulations, Software Development, Fluid Dynamics



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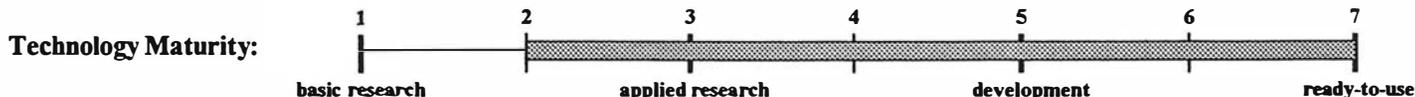
**Category:** Environmental & Regulatory (4, 14), Production

**Laboratory:** Brookhaven National Laboratory      **Contact:** L. D. Hamilton, 516-282-2004

**Title:** Produced Water Risk Assessment and Programmatic Support

**Description:** Offshore and coastal oil and gas production may result in the discharge of produced water and sand that can contain significant amounts of naturally occurring radioactive materials (NORM), organics and heavy metals. There is a concern that the discharge of these materials may result in impacts to human health and the environment. A comprehensive field study was initiated in FY 1992 by the U.S. Department of Energy (DOE), Office of Fossil Energy (FE) to characterize the health and ecological effects of produced water and sand discharges. This task involves support to DOE FE in this research effort and includes: (1) participation in the committee which oversees field study implementation; (2) review of U.S. Environmental Protection Agency (EPA) documents, regulations and guidelines; (3) development of approaches to human health and ecological risk assessment; and (4) development of human health and ecological risk estimates. Work in FY 1994 will include continuing programmatic support, completion of technical approaches to risk assessments, and development of initial estimates of individual human health risks. Efforts in FY 1995 and 1996 will include continuing programmatic support to DOE, improvements to the assessment of individual human health risk, and estimates of human population and ecological risk based on data collected in FY 1993 through FY 1995.

**91-95 Funding (\$K):** 440      **Dates:** 1991-1993



**Technology Transfer:** Publication in Open Literature and Reports, Lectures, Attendance at Conferences

**Key Documentation:** 1) Meinhold, A.F., Hamilton, L.D., Holtzman, S., Baxter, S.L. Human health risk assessment for radium discharged in produced water offshore - Phase II. BNL 60107, May 1994.

**Key Personnel:** S. Morris, 516-282-2018, morris3@bnl.gov  
P. Moskowitz, 516-282-2017, moskowi2@bnl.gov

**Lab Capabilities Applied:** Mathematical Modeling, Risk Assessment, Medical Science, Chemistry



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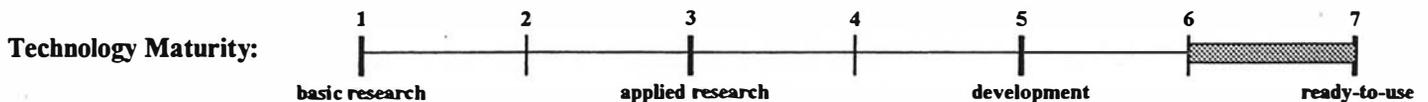
Category: Environmental & Regulatory (10, 14)

Laboratory: Brookhaven National Laboratory      Contact: S. Morris, 516-282-2018, morris3@bnl.gov

Title: Drinking Water Standards

Description: This task provides general technical support to the U.S. Department of Energy Office of environmental Guidance related to exposure and risk assessment issues. Work in FY 1993 and FY 1994 addressed exposure and risk associated with implementing proposed regulations for radionuclides in drinking water.

91-95 Funding (\$K): 390      Dates: 1992-1995



Technology Transfer: Reports, Publication in Open Literature, Seminars, Lectures

Key Documentation: 1) Morris, S.C., Rowe, M.D., Holtzman, S., and Meinhold, A.F. Review of technical justification of assumptions and methods used by the Environmental Protection Agency for estimating risks avoided by implementing MCLs for radionuclides. BNL 48482, Nov. 1992.  
2) Morris, S.C., Rowe, M.D. Holtzman, S., and Meinhold, A.F. National raditation exposures and risks caused by implementing EPA's proposed revised national primary drinking water regulations. BNL 49162, May 1993.

Key Personnel: S. Morris, 516-282-2018, morris3@bnl.gov

Lab Capabilities Applied: Mathematical Modeling, Medical Science, Chemistry



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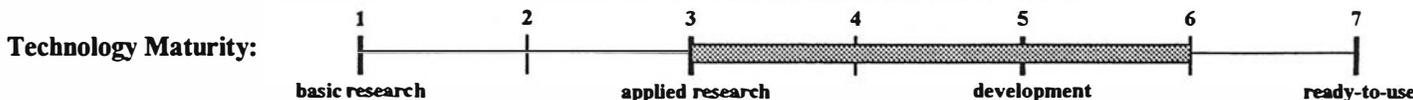
Category: Gas Storage

Laboratory: Brookhaven National Laboratory      Contact: J. Wegryzn, 516-282-7917

Title: Adsorbent/Natural Gas Vehicle Storage Systems

**Description:** Natural gas vehicles (NGV) are now penetrating the transportation sector. There are currently 30,000 NGVs operating in the United States, displacing 40 million gallons of petroleum fuel annually. Although this usage is small, when compared to the 130,000 million gallons of petroleum consumed annually in the United States, it has the potential for rapid growth within the next five years. However, before NGVs can substantially increase their marketshare, several technologies need development. These technologies are refueling stations, low cost emission reductions and on-board storage. Of these, on-board storage is the most significant since it limits the range of a vehicle and its market acceptability. Past studies have identified the cost/performance benefits of low pressure adsorbent natural gas (ANG) storage when compared to compressed natural gas (CNG) storage. These benefits are contingent on improving the storage density of ANG and lowering the conversion costs. Essentially the goal of this work is to exceed the storage density of 150 Vm/Vs with the use of low-cost adsorbents, where Vm is the delivered volume of methane at standard temperature pressure (STP) and Vs is the storage volume. A three-part federal program is outlined with this proposal to achieve this goal. The first part proposes a study into natural gas adsorbents, most notably activated carbons, in order to acquire adsorbents which out perform compressed gas storage systems. This work is followed by engineering development and laboratory testing of the storage system. The second task of the proposal is to convert and road test two OEM dedicated NGVs to ANG storage technology. The last task is a cost and technical feasibility study on the uses of conformable storage tanks.

91-95 Funding (\$K): 3250      Dates: 1992-present



Technology Transfer: Reports, Participation in National Committees, Exhibits, Seminars and Lectures, Publication in Open Literature

Key Documentation: Wegryzn, J., Wiesmann, H., and Lee, T. Low pressure storage of natural gas on activated carbon. Proc. Annual Automotive Technology Development Contractors' Coordination Meeting 1992, Dearborn, Nov. 1992, P-265, pp. 191-201. BNL 48685

Key Personnel: J. Wegryzn, 516-282-7917

Lab Capabilities Applied: Mathematical Modeling, Physical Absorption Measurements, Materials Science, Chemistry, Economic Analysis



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Category: Environmental & Regulatory

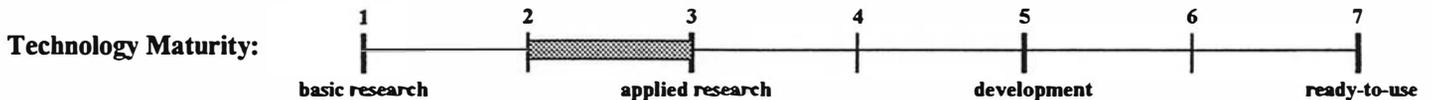
Laboratory: Brookhaven National Laboratory      Contact: Paul D. Kalb, 516-282-7644, kalb@bnl.gov

Title: Conversion of Waste Sulfur from Petroleum and Natural Gas Production into Cost Effective, Beneficial, and Environmentally Safe Secondary Products

**Description:** Large quantities of waste sulfur are currently generated by the cleanup of hydrogen sulfide in the production of petroleum and natural gas within the U.S. and worldwide. Waste sulfur is produced during both the pumping of crude oil from oil fields and in the refining of petroleum products. Presently, the sulfur has little commercial or social benefit and is either disposed of as waste or is sold at low cost to fertilizer manufacturers.

With techniques developed by the U.S. Bureau of Mines and Brookhaven National Laboratory, this waste sulfur can be successfully converted into a stable, durable alternative to concrete with numerous commercial applications. The sulfur is reacted with an organic oligomer to form a thermoplastic polymer with mechanical properties and chemical durability greater than conventional cement products. Its strength and resistance to harsh chemical environments makes sulfur polymer useful as a general construction material, paving material, coating material for tanks and pads, and for waste encapsulation of radioactive, hazardous and mixed wastes. The commercial cost of sulfur polymer produced in the U.S. is currently about \$0.12/lb., but if the large inventories of waste sulfur are better utilized, the anticipated cost of sulfur polymer can be dramatically reduced. This project will evaluate the feasibility of converting waste sulfur produced by Chevron Oil at the Carter Creek, WY oil fields, Chevron refinery operations throughout the U.S., and at other Chevron facilities worldwide by characterizing waste sulfur products, conducting bench-scale R&D to confirm optimal additive formulations and reaction rates, evaluating performance properties of sulfur polymer products, developing secondary use applications for sulfur polymer, and evaluating cost effectiveness and market potential.

91-95 Funding (\$K): 240      Dates: 1995 - Present



Technology Transfer: Not applicable

Key Documentation: 1) Kalb, P.D. and P. Colombo, Modified Sulfur Cement Solidification of Low-Level Wastes, BNL-51923, Brookhaven National Laboratory, Upton, NY, October 1985.  
2) Durability of Incinerator Ash Waste Encapsulated in Modified Sulfur Cement, BNL-45292, Brookhaven National Laboratory, Upton, NY, 1991.

Key Personnel: Paul Kalb, 516-282-7644, kalb@bnl.gov

Lab Capabilities Applied: Materials and final waste form process development, testing and demonstration.



Index: 77

Category: Environmental & Regulatory (14)

Laboratory: Brookhaven National Laboratory

Contact: M. D. Rowe, 516-282-2081, rowe2@bnl.gov

Title: Comprehensive Assessment

**Description:** This continuing program provides the U.S. Department of Energy (DOE) with state-of-the-science methods for analyzing energy systems and their health, environmental, and economic effects. It provides scientifically derived environmental data and information on health and environmental costs of alternative technologies and policies, and results of specific analyses requested by DOE. FY 1994 tasks in this program include: (I) continued refinement and application of the MARKET ALlocation (MARKAL) energy and environmental systems model and participation in the International Energy Agency (IEA) Energy Technology Systems Analysis Programme (ETSAP), which is evaluating alternatives for reducing worldwide emissions of CO2 from production and use of energy; and (ii) continued development of MARKAL-Macro Economic Growth Model (MACRO), which combines the MARKAL energy and environmental systems model with the MACRO economic growth model. Proposed tasks for FY 1995 include: (I) continued development and refinement of MARKAL-MACRO; (ii) analysis of potential impacts on the structure and costs of U.S. energy system of constraints imposed by endangered species legislation; (iii) continued development of state-of-the-science methods for energy policy analysis and assessing risks of energy technologies as requested by DOE; and (iv) continued oversight and analyses of pending health and environmental legislation or regulations requested by DOE.

91-95 Funding (\$K): 440      Dates: 1991-present



Technology Transfer: Publication in Open Literature, Lectures, Reports

**Key Documentation:** 1) Hamilton, L.D., Holtzman, S., Meinhold, A.F., Morris, S.C., Rowe, M.D., Daniels, J.I., Layton, D.W., Anspaugh, L.R. Lessons learned: Needs for improving human health risk assessment at U.S. DOE sites. BNL 60157, September 1993.  
 2) Rowe, M. D. Health risks in perspective: Judging health risks of energy technologies. BNL 49434, May 1994 (Rev.).

Key Personnel: Michael R. Rowe, 516-282-2081, rowe2@bnl.gov

Lab Capabilities Applied: Energy Systems Modeling, Risk Assessment, Economic Analysis



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Category: Production (3), Deepwater Offshore (8)

Laboratory: Brookhaven National Laboratory

Contact: H. S. Isaacs, 516-282-4516,  
isaacs1@bnl.gov

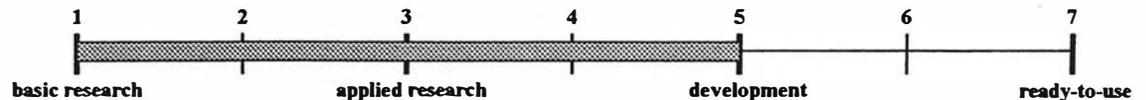
Title: Mechanisms of Metal-Environment Interactions

**Description:** This project is directed towards a fundamental mechanistic understanding of the initiation and propagation of localized corrosion of metals and alloys. The morphological changes which take place on metal surfaces during oxide film growth and reduction have been studied in situ using the Scanning Tunneling Microscope (STM) and the Atomic Force Microscope (AFM). This part of the project will now cease due to lack of funds. The passive oxide film can be modified chemically to reduce its susceptibility to localized attack. This may be achieved by alloying additions to the metal or addition of inhibiting ions to the environment. Structural and chemical changes in the oxide film formed using both these approaches are being studied using x-ray absorption spectroscopy at the National Synchrotron Light Source (NSLS). The action of inhibitors is being investigated in situ by mapping the change in the local corrosion currents using a scanning vibrating probe (SVP) method in addition to x-ray and rotating disc measurements. This powerful combination of in situ techniques is being used to give a complete picture of the mechanisms of localized corrosion and its prevention.

91-95 Funding (\$K): 1820

Dates: 1991-present

Technology Maturity:



Technology Transfer: Publication in Open Literature, Invited Talks, CRADAs, Workshops, Reports, Patents

**Key Documentation:** 1) Davenport, A.J., Isaacs, H.S., Bardwell, J.A., MacDougall, B., Frankel, G.S., Schrott, A.G. In situ studies of passive film chemistry using x-ray absorption spectroscopy. *Corrosion Science* 35(1-4), 19-25 (1993).  
2) Davenport, A.J., Sansone, M., Bardwell, J.A., Aldykiewica, A.J., Jr., Taube, M., Vitus, C.M. In situ multielement XANES study of formation and reduction of oxide film on stainless steel. *J. Electrochem. Soc.* 141(1), L6-L8 (1994).

**Key Personnel:** H. S. Isaacs, 516-282-4516, isaacs1@bnl.gov  
A. J. Davenport, 516-282-4410, davenpo1@bnl.gov

**Lab Capabilities Applied:** Materials Science, National Synchrotron Light Source, Advanced Corrosive Analysis and Corrosion Remediation, In situ Techniques for Corrosion Studies



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**Category:** Environmental & Regulatory

**Laboratory:** Brookhaven National Laboratory      **Contact:** C. J. Czajlowsli, 516-282-4420, czajkow@bnl.gov

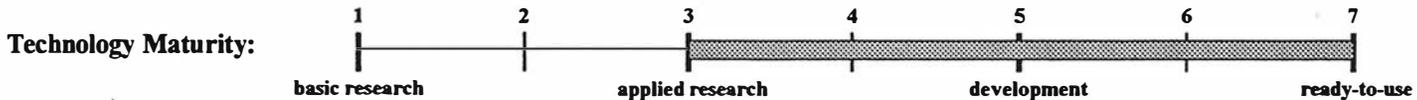
**Title:** Materials Characterization & Innovative Technology Group (MCIT)

**Description:** The MCIT Group has conducted numerous pipe and other component failure investigations with the U.S. Nuclear Regulatory Commission over the last 14 years. The four most recent are:

- 1) Surry Nuclear Power Plant Steam Pipe Rupture (single phase erosion/corrosion)
- 2) Mohave Power Station (Southern California Edison, stress rupture, 30 inch pipe)
- 3) Midland Power Plant (Detroit Edison, stress rupture failure)
- 4) Trojan Power Plant (Portland General Electric, single and 2-phase erosion/corrosion).

The MCIT Group has more than 10 years experience in conducting failure analyses, and evaluating materials in commercial and research nuclear plants and high energy accelerators. MCIT capabilities include mechanical testing, chemical analysis, nondestructive tests, and metallurgical evaluations. MCIT has conducted inspections and supported allegations investigations for NRC and DOE.

**91-95 Funding (\$K):** 2000      **Dates:** 1984-present



**Technology Transfer:** Journal Articles, ASM Publications

**Key Documentation:** 1) C. J. Czajlowsli, et al, "Thermal Embrittlement Test Method for Type 410 Stainless Steel," Proc. of the 27th IMS Annual Technical Meeting, Montreal, Canada, 24-27 July, 1994.

**Key Personnel:** Carl J. Czajkowski, 516-282-4420, czajkow@bnl.gov  
 Mel G. Cowgill, 516-282-2082, cowgill@bnl.gov  
 Biays S. Bowerman, 516-282-2946, bowerman@bnl.gov

**Lab Capabilities Applied:** Metallographic Preparation, Mechanical Testing, Transmission, Electron Microscopy, Scanning Electron Microscopy, Corrosion Testing and Analysis, Metallurgical Evaluations, Field Inspections



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Category: Production (18)

Laboratory: Brookhaven National Laboratory      Contact: E. T. Premuzic, 516-282-2893

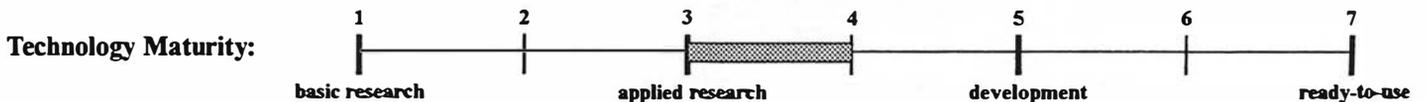
Title: Economic Feasibility of Biochemical Processes for the Upgrading Of Crudes and the Removal of Sulfur, Nitrogen, and Trace Metals From Crude Oil - Benchmark Cost Establishment of Biochemical Processes on the Basis of Conventional Downstream Technologies

Description: The Department of Energy/Fossil Energy (DOE/FE) has been supporting applied biotechnical research at Brookhaven National Laboratory (BNL) for several years, focusing on the development of biochemical processes for recovery of crudes with applications in the downstream oil processing industry. Three major promising applications have been identified. They all deal with reduction of impurities from crude oil. The three impurities are sulfur, nitrogen, and trace metals. Another potentially beneficial application of biochemical downstream processing of crude oil is the breakdown of heavy ends to lighter hydrocarbons and bioconversion of oil wastes for recycling.

The downstream biotechnological crude oil processing research performed thus far is of laboratory scale and has focused on demonstrating the technical feasibility of downstream processing with different types of biocultures under a variety of processing conditions. Quantitative economic analysis has not as yet been performed under DOE sponsorship. This important analysis is the topic of the presently proposed project which will investigate the economic feasibility of the various biochemical downstream processes which have achieved different stages of development, and appear to hold promise in upgrading of heavy crudes, such as those found in California (Monterey-type crudes), Arkansas, and Alabama.

The project will be a joint program between BNL and Energy Consultants International (ECI, Inc.). ECI has performed a multitude of economic feasibility studies for the national and international refining industry as well as funding institutions [International Monetary Fund (IMF), etc.]. ECI's extensive worldwide experience in marketing and oil processing will be applied in the biochemical processes evaluation of domestic and other heavy crudes used by the U.S. industry.

91-95 Funding (\$K): 540      Dates: 1994-present



Technology Transfer: Reports, CRADAs, patents, lectures

Key Documentation: 1) Premuzic, E.T., Lin, M.S. Effects of selected thermophilic microorganisms on crude oils at elevated temperatures and pressures - 1993 Final Report. BNL 60119, November 1993.

Key Personnel: E. T. Premuzic, 516-282-2893  
 M. Lin, 516-282-3064

Lab Capabilities Applied: Biochemistry, Biotechnology, Economic Analysis



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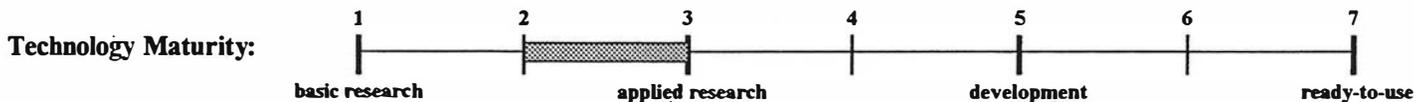
**Category:** Environmental & Regulatory

**Laboratory:** Brookhaven National Laboratory      **Contact:** Terry Sullivan, (516) 282-2840, [sullival@bnl.gov](mailto:sullival@bnl.gov)

**Title:** Development and Testing of BLT-EC, a Coupled Finite-element Geochemical Transport Code

**Description:** The computer code BLT-EC (Breach, Leach, Transport -Equilibrium Chemistry) is capable of modeling miscible flow and transport of several chemical species subject to thermodynamic equilibrium. It was originally developed to examine problems pertaining to low-level radioactive waste disposal facility performance where changes in pH, Eh, and other important chemical parameters are likely to occur due to the presence of metallic containers, cement structures and waste forms, and other degradable wastes. These changes in chemistry will alter the mobility of key radioactive contaminants and therefore, impact on their release and transport. The code will have pre- and post-processors available to assist in the implementation of the code and interpretation of the output.

**91-95 Funding (\$K):** 900      **Dates:** 1991 - 1995



**Technology Transfer:** Software will be available to all government agencies free of charge. A minimal charge is expected for non-government agencies.

**Key Documentation:** 1) MacKinnon, R.J., T.M. Sullivan, C.J. Suen, and S.A. Simonson, "BLT-EC (Breach, Leach, Transport, and Equilibrium Chemistry), a Finite-Element Model for Assessing the Release of Radionuclides from Low-Level Waste Disposal Units: Background, Theory, and Model Description," NUREG/CR-6340, 1995.

**Key Personnel:** Terry Sullivan, (516) 282-2840, [sullival@bnl.gov](mailto:sullival@bnl.gov)

**Lab Capabilities Applied:** Contaminant transport modeling, geochemical modeling, groundwater flow modeling, numerical analysis, finite element methods, visualization techniques.



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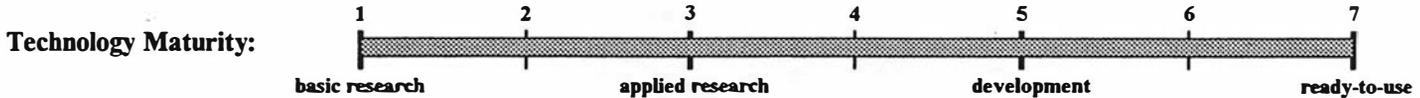
**Category:** Development (5, 18, 22), Oil Processing & Refining (1)

**Laboratory:** Brookhaven National Laboratory      **Contact:** K. W. Jones, 516-282-4588

**Title:** Measurement of Fluid Flow and Fluid-Rock Interactions Using Synchrotron Computed Microtomography

**Description:** This project is aimed at investigating fluid flow and fluid-rock interactions using synchrotron computed microtomography (CMT). Investigations of the microgeometry of rocks are being carried out since it is recognized that this is a key factor influencing these phenomena at pore-scale dimensions. Measurements on rocks flooded with oil and with oil displaced by brine are done to determine the interaction of the fluids with the rock pore volumes and to provide basic data for input into microscopic flow models. Apparatus for study of the kinetics of the displacement of one fluid by another is now be implemented. This will lead to the study of the flow processes in times short enough to observe the evolving interface between the fluids. These experiments require a high level of sophistication in the CMT apparatus. Attention is being paid to development of high-speed area detectors to improve the data acquisition rates and to the addition of three-dimensional imaging techniques to make the interpretation of the data more efficient. Ultimately, it will be necessary to use the experimental system developed at the National Synchrotron Light Source (NSLS) at high-brilliance/high-energy synchrotron sources such as the European Synchrotron Radiation Facility (ESRF) and the Argonne National Laboratory (ANL) Advanced Photon Source (APS) in order to reach the highest possible performance levels for study of the flow kinetics.

**91-95 Funding (\$K):** 380      **Dates:** 1992-present



**Technology Transfer:** Publication in Open Literature, Seminars, CRADAs, Reports

**Key Documentation:** 1) Coles, M.E., Spanne, P., Muegge, E.L., Jones, K.W. Computed microtomography of reservoir core samples. Presented at 1994 International Symposium of the Society of Core Analysts, Stavanger, Norway, September 1994, Society of Core Analysts Paper, SCA-9401.  
 2) Spanne, P., Thovert, J.F., Jacquin, C.J., Linquist, W.B., Jones, K.W., Adler, P.M. Synchrotron Computed Micromography of Porous Media: Topology and Transport. J. Phys. Rev. 73(14), 1994.

**Key Personnel:** K. W. Jones, 516-282-4588

**Lab Capabilities Applied:** X-Ray Scattering Experiment and Theory, Computed X-Ray Tomography, National Synchrotron Light Source, Geoscience



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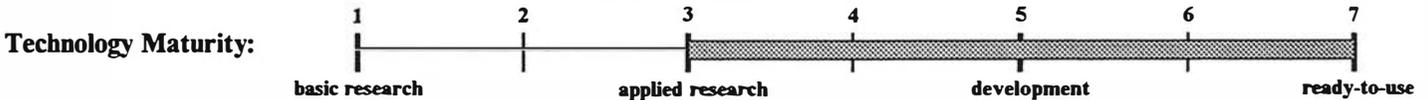
**Category:** Drilling & Completion (4)

**Laboratory:** Brookhaven National Laboratory      **Contact:** L. E. Kukacka, 516-282-3065

**Title:** In Situ Containment and Stabilization of Buried Waste

**Description:** The object of this program is to develop, demonstrate and implement advanced grouting materials for the in situ stabilization of contaminated soils. In addition, these grouts will be used for the in situ installation of impermeable, corrosion resistant caps and subsurface barriers around waste sites. Success will be measured by hydraulic and geochemical isolation of liquid and solid contaminants within the Chemical Waste Landfill (CWL) and Mixed Waste Landfill (MWL) at Sandia National Laboratory (SNL). To insure near-term (FY96) deployment and commercial utilization of these advanced material systems, the development effort focuses on materials compatible with commercially available placement technology. This mandates strong interactions with ongoing MWLID placement technology efforts at SNL and with grout placement companies. The task is divided into two subtasks: 1) In Situ Stabilization of Contaminated Soils: EPA-acceptable pumpable grout formulations that are curable at ambient temperature in dry and wet environments are being developed and their properties characterized. FY93 results from this test produced data needed for the planning of a larger-scale demonstration at the CWL in FY94. Concurrent with this effort, a similar work plan which focuses on the MWL site will be implemented. This work will be completed with a demonstration at the MWL in FY96 or 97. 2) Capping and Barrier Grouts Ongoing work which has developed inorganic-based materials with vastly superior properties which yield the potential of reducing costs by 1 to 3 orders of magnitude when compared to conventional grouts. Diffusion of contaminants from the sites and infiltration of water into the waste sites will be eliminated or reduced to less than regulatory limits. Additional anticipated benefits from this technology include 1) the reduction of health and environmental risks as compared to those resulting from the use of other remedial technologies such as exhumation, 2) reductions in cost compared to those of excavation, treatment, and disposal, 3) improved operations, thereby increasing regulatory agency and public acceptance, and 4) demonstration of technology broadly applicable to more than one DOE site.

**91-95 Funding (\$K):** 870      **Dates:** 1992-present



**Technology Transfer:** Reports, Workshops, Panels, Patents

**Key Documentation:** Allan, M., Kukacka, L. Grout treated soil for low permeability barriers around waste landfills. American Concrete Institute Materials J. 91(4), 355-61 (1994).  
 Allan, M., Kukacka, L. In situ containment and stabilization of buried waste. BNL 49709, October 1993.

**Key Personnel:** L.E. Kukacka, 516-282-3065  
 M.L. Allan, 516-282-3060

**Lab Capabilities Applied:** Composites, Materials Science, Chemistry, Materials Testing, Hydrology



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Category: Exploration

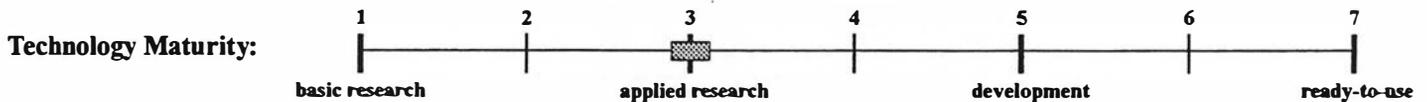
Laboratory: Idaho National Engineering Laboratory      Contact: R. E. Rice, 208-526-1992, rrr@inl.gov

Title: Locating and Numerically Modeling Geopressured Hydrocarbon Reservoirs and Associated Pressure Seals in Soft, Clastic Sediments

**Description:** Geopressured oil and gas fields in the Gulf of Mexico represent only 10% of the commercial reservoirs, yet account for approximately 50% of the cumulative Gulf production. This makes such resources attractive exploration targets; however, locating and identifying the resource remains difficult. A conceptual model for the formation of geopressured reservoirs has been developed. This model can explain various features of geopressured reservoir behavior, including seal formation, local structural features, faulting, and recharge/discharge of reservoir fluids. The seismic signature of a geopressured reservoir may also have unique characteristics that can be used in developing new interpretation methods for identifying such resources.

This project has three separate tasks: reservoir engineering, reservoir mechanics, and geophysics. The reservoir engineering task will focus on the formation and long-term behavior of pressure seals, including hydrocarbon reservoir charging and building a numerical model of the conceptual model. Geomechanics will consider the effects of geopressure on structural features and faulting, and geophysics will attempt to devise new methods of interpretation to identify the pressure seals. These projects are split between INEL, Sandia, and various universities. Overall project management will be maintained at INEL.

91-95 Funding (\$K): 440      Dates: 1995



**Technology Transfer:** Technical conferences, including Society of Petroleum Engineers and American Association of Petroleum Geologists. Additional manuscripts will be prepared for submittal to the relevant professional journals

**Key Documentation:** Proposal to Advanced Computer Technology Initiative

**Key Personnel:** G. M. Shook, 208-526-6945, ook@inl.gov

**Lab Capabilities Applied:** Reservoir Engineering and Analysis, Numerical Modeling, Seismic Interpretation, Geology, Hydrodynamics, Geomechanics, Geochemistry, Subsurface Fluid Flow



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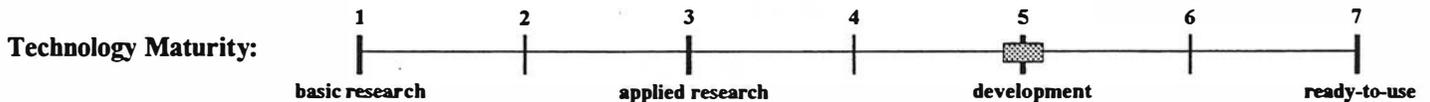
Category: Oil Processing & Refining (8)

Laboratory: Idaho National Engineering Laboratory      Contact: R. E. Rice, 208-526-1992, rrr@inel.gov

Title: Use of an Environmental Risk Based Approach for Industrial Design

**Description:** The goal of this cooperative, integrated effort is to develop an approach that incorporates existing data and state of the art techniques into a risk based framework to evaluate the impacts from emission sources (e.g., air from stacks) on environmental systems. Specific objectives are to develop an approach that uses indicators of environmental stress to develop monitoring and characterization systems that are more cost-effective than the current approach that is focused on sampling all media. Using an Environmental Risk Assessment approach allows the INEL to build consensus between regulatory agencies and industry and provides a means to minimize unwarranted environmental regulations. The approach focuses on identifying the sources of contaminants that are being emitted, their pathways into the environment, and potential impact to critical receptors. The approach also accounts for the fact that environmental systems have some degree of resiliency and can accommodate some minimum level of anthropogenic input.

91-95 Funding (\$K): 240      Dates: 1995



Technology Transfer: Publication in appropriate journal, presentation at technical meetings.

Key Documentation:

Key Personnel: R. P. Breckenridge, 208-526-0757, rpz@inel.gov

Lab Capabilities Applied: Regulatory Compliance, Risk Assessment, Environmental Computer Modeling, Hazards Identification/Accident Analysis, Safety Analysis, Technology Assessments, Remediation Goal Determination, Projected Emissions Analysis, Performance Objectives Analysis



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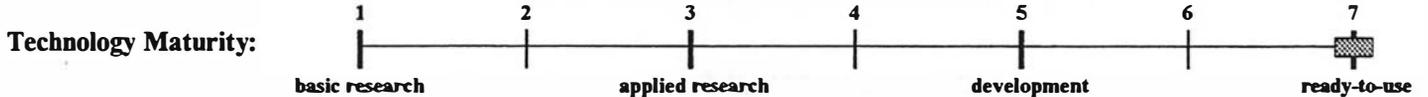
Category: Development (2)

Laboratory: Idaho National Engineering Laboratory      Contact: R. E. Rice, 208-526-1992, rrr@inel.gov

Title: Interactive Computer Visualization of TETRAD Results

Description: This project developed a real-time interactive tool for visualization of the 3D data resulting from TETRAD simulations of geothermal reservoir systems. The system is capable of displaying up to 27 different variables from the simulation, in a user selectable manner. One task was to develop modules that incorporated specific physics, such as steam tables, into the interactive system. The software runs on a wide variety of Unix workstations and is available on PC compatibles running Windows NT. The visualization occurs in true three dimensional space with the ability to extract any number of arbitrarily oriented two dimensional subsets. All the standard graphics and visualization capabilities are present including data driven axes, contour lines, iso-surfaces, vector descriptors, and both user and data driven annotations. There are also five separate volume rendering methods for direct viewing of the 3D data, all of which may be intermixed with the traditional geometry-based techniques mentioned above. Output is available in many fashions from interactive display on the workstation monitor, to high resolution black-and-white and color images, to animations that may be recorded to video tape or encoded into one of the computer based movie formats, such as MPEG, QuickTime, AVI, FLC, or FLI. The core software contains the capability to provide heterogeneous, distributed computing, allowing the user to customize their runtime environment to best adapt a given problem to the computer, network and other environmental factors.

91-95 Funding (\$K): 100      Dates: 1993



Technology Transfer: Presentation at 1993 Geothermal Research Council Annual Meeting

Key Documentation:

Key Personnel: L. E. Greenwade, 208-526-1276, leg@inel.gov

Lab Capabilities Applied: Computer Science, Geology, Hydrodynamics, Geothermal Reservoir Analysis



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**Category:** Oil Processing & Refining (1)

**Laboratory:** Idaho National Engineering Laboratory      **Contact:** R. E. Rice, 208-526-1992, rrr@inel.gov

**Title:** Improved Catalyst Development

**Description:** An INEL program funded by the Bureau of Mines has lead to the development of extensive capability for the preparation and testing of catalysts for use in a wide range of chemical processes. They include: new, more active and durable methane oxidation catalysts prepared from activated multi-component metal alloys for use in three types of exhaust systems; catalysts for the control of carbon monoxide, hydrocarbons, and NOx in exhaust emissions from gasoline fueled vehicles and off-gases from various chemical processes; a new series of metal alloy-based catalysts for the oxidative coupling of methane to form ethane and ethylene, and to a limited extent higher hydrocarbons; a novel and unique method of preparing steam reforming and carbon dioxide conversion catalysts that may offer a means of developing a whole new series of highly active and selective catalysts for these processes; and activated metal alloy hydrogenation/oxygenation catalysts which have been shown to offer improved impurity poisoning resistance, regeneration, and increased activity.

**91-95 Funding (\$K):** 1330      **Dates:** 1985-present



**Technology Transfer:** Several mechanisms are in place or possible, including CRADAs with industrial partners or direct licensing.

**Key Documentation:** U.S. Patent No. 5,081,083 (1991), R. B. Wright

**Key Personnel:** R. B. Wright, 208-526-0959

**Lab Capabilities Applied:** Advanced Materials and Processing, Chemical Processing



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Category: Exploration (3, 14), Development (3, 16)

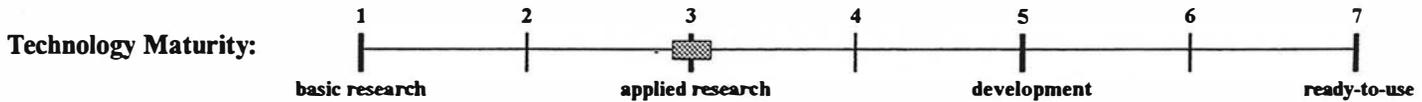
Laboratory: Idaho National Engineering Laboratory      Contact: R. E. Rice, 208-526-1992, rrr@inel.gov

Title: Large Downhole Seismic Sensor Array

**Description:** This project is intended to help industry more economically acquire high-frequency, three-component subsurface seismic data. Evolving computational techniques will then be able to process and interpret such data in ways that will greatly enhance our ability to find and extract oil and gas. The goal is to greatly reduce the costs of seismic surveys, performed in wells, by creating a new downhole information acquisition and processing system that is faster operating, less expensive to build, and easier to deploy than existing systems.

Using advanced computer-aided engineering tools a 300-channel downhole passive seismic sensing network that can be deployed into both vertical and deviated wellbores is being developed. The network will contain 100 three-component sensor modules that can quickly couple to the sidewall of the wellbore and have the coupling action detected. Fiber optics and other newer technologies will be used to develop the sensing and deployment subsystems which will interface to a custom high-speed surface data acquisition and control system. Subsurface information can then be collected in real time at the surface where it can be stored and processed. Advanced computational methods will allow portions of the recorded data, that are critical to monitoring and control, to be processed on site.

91-95 Funding (\$K): 1200      Dates: 1995



Technology Transfer: Industry partnership formed with several major companies

Key Documentation: Proposal to Advanced Computer Technology Initiative

Key Personnel: J. R. Fincke, 208-526-2031, jf1@inel.gov

Lab Capabilities Applied: Fiberoptics, Mechanical and Electrical Engineering, Geophysics, Numerical Modeling, System Design and Fabrication



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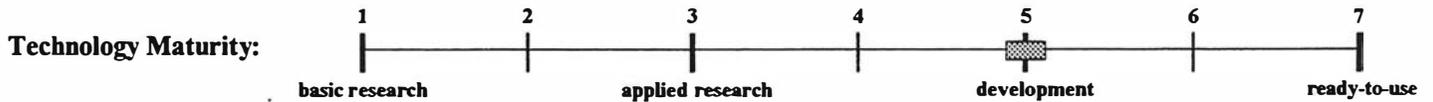
**Category:** Environmental & Regulatory (5, 14)

**Laboratory:** Idaho National Engineering Laboratory      **Contact:** R. E. Rice, 208-526-1992, rrr@inel.gov

**Title:** Above-Ground Storage Tank Leak Detection System Certification Facility

**Description:** The American Petroleum Institute (API) and their working group for Above-Ground Storage Tank Monitoring have recently initiated this program to develop and certify instrumentation that could be used to detect small leaks in ASTs. Such instrumentation, demonstrated and certified to perform within well defined levels of certainty, could be used to detect leaks at a very early stage with sufficient lead time to allow repairing or removing the tank from service before any significant environmental damage could occur. This approach would be much less expensive than modifying existing tanks to include an integral leak containment capability such as a double bottom. There is not a facility available for certification of above-ground storage tank sensors. API estimates a facility such as this would cost several million dollars. A joint DOE-API effort to develop a test and certification facility is being considered as a means of financing the facility through cost sharing.

**91-95 Funding (\$K):** 110      **Dates:** 1995



**Technology Transfer:** Facility use agreements

**Key Documentation:** Facility conceptual design, progress reports

**Key Personnel:** C. Shapiro, 208-526-8688, cs5@inel.gov  
 R. C. Hill, 208-526-8306, hil@inel.gov

**Lab Capabilities Applied:** Hydrology, Vadose Zone Monitoring & Modeling, Sensor Design, Prototype Instrument Fabrication, Laser Technology & Instrumentation, Prototype Instrument Testing, Safety Sensor System Computer Codes, Hostile Environment Sensor Systems, Engineering - General





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Category: Oil Processing & Refining (4, 21)

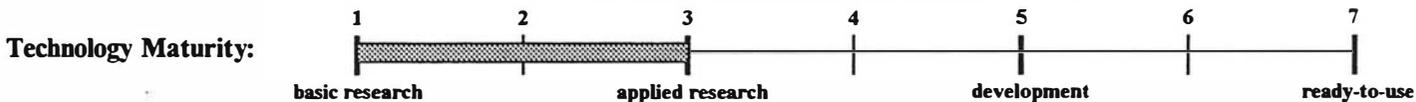
Laboratory: Idaho National Engineering Laboratory      Contact: R. E. Rice, 208-526-1992, rrr@inel.gov

Title: Plasma Upgrading of Heavy Oil and Residuum

Description: The goal of this cooperative program is to investigate and demonstrate the technical feasibility of two novel plasma technologies for upgrading heavy oil and residuum and determine the economic viability of the processes for application in the field as well as in refineries. The development of these processes for commercial use will depend on the technical merit and on engineering economics (i.e., conversion efficiency). The current effort involves a Cooperative Research & Development Agreement (CRADA) with Phillips Petroleum Company and is designed to address problems related to the progressively heavier crude oils available to U.S. refineries. INEL is addressing various process parameters including cracking of asphaltenes, hydrogenation of unsaturated products, removal of sulphur and heavy metals, and process economics and modeling.

Development of a successful upgrading technology will allow U.S. refineries to accommodate feedstock which currently has little value and cannot be processed by existing technologies.

91-95 Funding (\$K): 950      Dates: 1994-present



Technology Transfer: Present results at technical meetings and publish in appropriate journals, licensing of process

Key Documentation: Patent

Key Personnel: C. P. Thomas, 208-526-0165, cpt@inel.gov  
 P. C. Kong, 208-526-7579, pck@inel.gov

Lab Capabilities Applied: Physical Chemistry, Plasma Physics, Mechanical Engineering, Design and Fabrication



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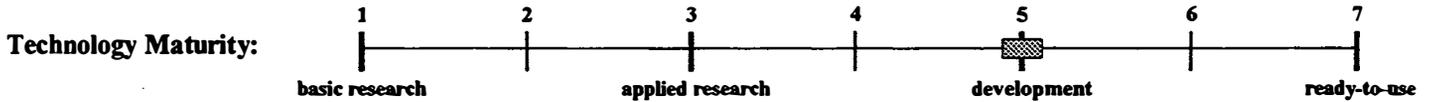
Category: Oil Processing & Refining (12, 13, 3)

Laboratory: Idaho National Engineering Laboratory      Contact: R. E. Rice, 208-526-1992, rrr@inel.gov

Title: Industrial Plant Life Extension and Integrity Evaluations

Description: Lifetime extension technologies developed to address general industry and INEL Non-destructive evaluation (NDE) needs will provide necessary assessment tools allowing the domestic refinery industry to safely extend plant life. This program has a long-term goal to apply novel NDE techniques to monitor industrial structures in two areas: 1) high temperature flaw detection and sizing and 2) NDE for toughness, embrittlement, and property deterioration. The first need is addressed by a unique noncontacting ultrasonic laser/electromagnetic acoustic transducer system for high temperature flaw detection and sizing. The deliverable will be a practical, robust engineering design and prototype of a noncontacting ultrasonic system for monitoring structures operating at production temperatures. To measure toughness, embrittlement and property deterioration requires the application of several novel NDE techniques and correlation of the NDE measurements with destructive fracture mechanics test findings. Based on this correlation, a suite of measurement and analysis techniques and procedures for the determination of property degradation in refinery structures will be made available either as systems or enhancements to existing NDE equipment.

91-95 Funding (\$K): 200      Dates: 1985-present



Technology Transfer: Will occur through an industrial consortium, licensing agreement

Key Documentation: Internal INEL reports, patents

Key Personnel: N. M. Carlson, 208-526-6302, nmc2@inel.gov  
 W. G. Reuter, 208-526-1708, wgr2@inel.gov

Lab Capabilities Applied: Fracture Mechanics, Applied Mechanics Modeling, Sensor Development, Process Control, Flexible Manufacturing, Advanced Materials Development, Metals & Non-metals, Welding Strategy, Control, and Procedures Qualification, Corrosion Testing Analysis



**Index:** 93

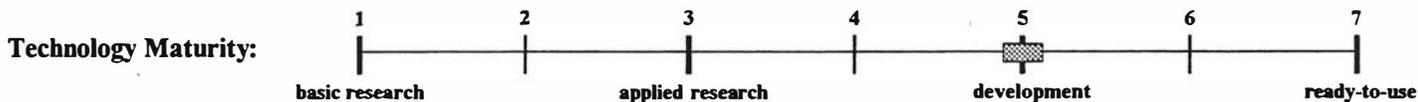
**Category:** Gas Gathering (5), Production (6), Deepwater Offshore (6)

**Laboratory:** Idaho National Engineering Laboratory      **Contact:** R. E. Rice, 208-526-1992, rrr@inel.gov

**Title:** Measurement of Component Ratio in Oil/Water/Gas Mixtures and Determination of Flow Regime

**Description:** Measurements of the individual flow rates of oil, gas, and water from individual wells in a field are required to develop reservoir management strategies for optimization of total production over the life of the field. This research examines the techniques of tomographic reconstruction of electrical impedance measurements for the determination of component fraction and velocity in pipelines. Electrical impedance imaging works by reconstructing phase distribution from measurements of impedance distributions at a pipeline cross-section. The objective is the demonstration of a rugged, inexpensive electrical sensor technique and application of reconstruction techniques to the data obtained for the determination of phase distribution and flow regime in flowing oil/water/gas mixtures. Impedance measurement techniques are not applicable to very high void fraction flows. A special flow acceleration/deceleration element is also being developed to supplement impedance techniques to extend the range of measurement.

**91-95 Funding (\$K):** 150      **Dates:** 1995



**Technology Transfer:** Licensing agreement, industry consortium

**Key Documentation:**

**Key Personnel:** J. R. Fincke, 208-526-2031, jf1@inel.gov

**Lab Capabilities Applied:** Mechanical and Electrical Engineering, Sensor Development, Computer Sciences



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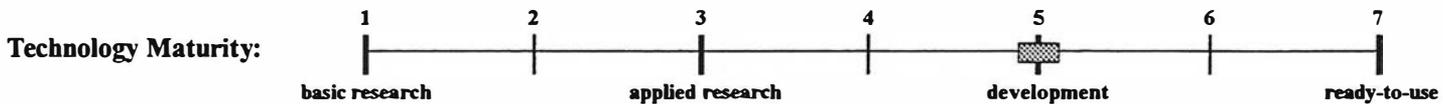
Category: Gas Gathering (5), Oil Processing & Refining (16, 17)

Laboratory: Idaho National Engineering Laboratory      Contact: R. E. Rice, 208-526-1992, rrr@inel.gov

Title: Complex Multi-Fluid Flow Analysis

**Description:** The RELAP5 code is a two-fluid multi-dimensional fluid flow code that was developed for detailed evaluations of the pressure and flow fields that can develop in fluid systems. While it was originally developed for studying the behavior of nuclear reactor coolant systems, it has since been expanded to cover a host of fluid systems. Funding from several sponsors support a \$10M annual program. Recent applications have been made to space power systems, chemical process systems, and even to the study of blood flow in the human cardiovascular system. The code is being improved on a continuing basis and is applicable to numerous fluid systems in a refinery. Approximately 10% of the developmental program has direct application to chemical and refinery process systems.

91-95 Funding (\$K): 1000      Dates: 1990-present



Technology Transfer: Software licensing, journal articles, papers

Key Documentation: Users Manuals, technical reports

Key Personnel: B. W. Dixon, 208-526-4928, bwd@inel.gov

Lab Capabilities Applied: Computational Fluid Dynamics, Process Modeling



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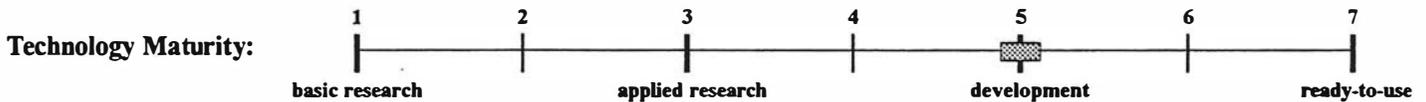
Category: Environmental & Regulatory (10, 12)

Laboratory: Idaho National Engineering Laboratory      Contact: R. E. Rice, 208-526-1992, rrr@inel.gov

Title: Removal of Organic Contaminants from Solid Materials

**Description:** The INEL has developed processes for removal of organic contamination from solids associated with the exploration, production, refining, and transport of petroleum and petroleum products and other organic contaminants. An engineering-scale pilot plant has been constructed with a design capacity of 1,300 lbs/hr for use in determining the capability of the processes to remediate soils contaminated from spills and for an environmentally friendly, cost-effective treatment of refinery solid wastes. The technology is an effective combination of solvent extraction and soil washing processes that is applicable to polar and non-polar compounds, heavy hydrocarbons, and high organic concentrations. The process has been demonstrated effective at the pilot plant level to be capable of removing 99.7% (50,000 to 144 ppm reduction) of heavy petroleum residuum from tank sludge solids at a feed rate of 10 Kg/min.

91-95 Funding (\$K): 110      Dates: 1993-1994



Technology Transfer: Publication in appropriate journals and presentation at scientific meetings, license agreement.

Key Documentation: Patent, technical reports

Key Personnel: C. P. Thomas, 208-526-0165, cpt@inel.gov

Lab Capabilities Applied: Environmental Technologies, Soil Science, Vadose Zone Monitoring, Vadose Zone Modeling, Organic Chemistry, Prototype Sensor Design, Fabrication and Testing, Engineering - ME, CE, IE, Petroleum, EE



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Category: Environmental & Regulatory (12)

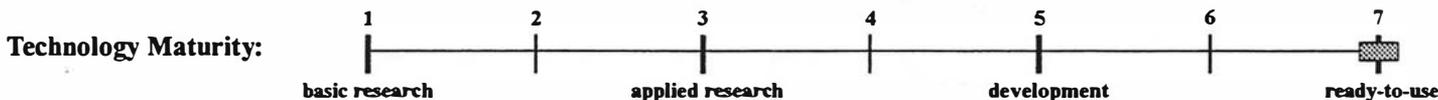
Laboratory: Idaho National Engineering Laboratory      Contact: R. E. Rice, 208-526-1992, rrr@inel.gov

Title: Development and implementation of enhanced bioremediation of hydrocarbons in the petroleum industry: production, refinery, distribution systems

Description: Microbial degradation of contaminants in soil, in groundwater, and in vapor streams is becoming an important alternative technology for meeting regulatory demands. Integrated in-situ and ex-situ treatment technologies utilizing the indigenous microbial populations of biological flora present at contaminated sites is proving to be a valuable remedial action. Several methods have been developed to assess, monitor, and predict microbial cleanup activities. The methods use actual field samples to determine the rate of degradation, factors required for optimization, and the presence of a microbial flora with degradative capabilities. These methods provide useable and pertinent information for the site manager or field engineer to use in designing a field bioremediation system.

Several BTEX and petroleum-contaminated field sites are now under bioremediation. Vapor-phase reactors for ex-situ treatment of volatiles from tanks and pump-and-treat systems have also been developed. Bioprocessing of industrial waste streams containing high loading of toluene and xylene (2000-5000 ppm) are being demonstrated. A new meso-scale apparatus has been developed to simulate the actual contaminated aquifer conditions experienced in the field. This apparatus produces data which (1) can relate lab to field rates and (2) demonstrates that biotreatment can be an effective remediation technology and reduce levels of BTEX below 1 ppb.

91-95 Funding (\$K): 300      Dates: 1993-present



Technology Transfer: Work is being done with Conoco as a sponsor through Montana State University's Biofilm Engineering Center. Other major oil companies receive updates on research. The State of Montana is using INEL on their Leaking Underground Storage Tank Program.

Key Documentation: Wolfram, J. H., L. Gawel, "Biological Degradation of BTEX Compounds by Field Water Samples to Below EPA Drinking Water Standards", SPE/EPA Exploration and Production Environmental Conference, San Antonio, TX 1993.

Cruden, D., J. H. Wolfram, R. D. Rogers, and D. T. Gibson, "Physiological Properties of a Pseudomonas Strain Which Grows with p-xylene in a Two-Phase (organic-aqueous) Medium," Appl. Environ. Microbiol. 58, 2723-2729.

Key Personnel: J. H. Wolfram, 208-526-1809, jhw2@inel.gov

Lab Capabilities Applied: Equipment (respirometer), unique microscopic techniques and the special apparatus (simulated aquifer)



Index: 97

**Category:** Environmental & Regulatory (10)

**Laboratory:** Idaho National Engineering Laboratory      **Contact:** R. E. Rice, 208-526-1992, rrr@inel.gov

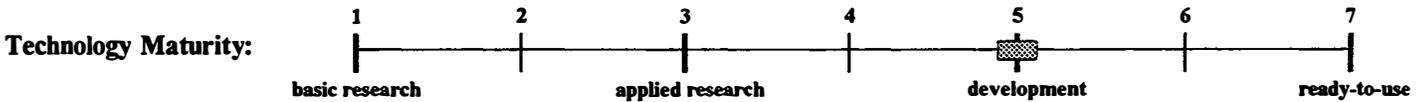
**Title:** Hydrothermal Oxidation of Toxic Materials

**Description:** Hydrothermal Oxidation (HTO) is currently being studied in bench scale and test bed sizes to determine the destruction efficiency, resolve technical challenges, determine cost data, and to better understand the characteristics of supercritical water reactions with toxic materials. From these scaled systems, future facilities will be built to provide a source of highly efficient destruction of toxic waste originating from many sources.

The toxic by-products from petroleum operations can be tested for destruction efficiency, cost effectiveness, and reliability with the INEL HTO test bed. The test bed is being constructed with the flexibility to evaluate competing chemical reactors and components as well as evaluate a wide range of toxic wastes. The test program is scheduled to start in early 1996 and extend for 5 years.

Representatives of the petroleum industry have expressed interest in conducting research on possible use of dry holes as an in-situ HTO reaction chamber.

**91-95 Funding (\$K):** 3000      **Dates:** 1995



**Technology Transfer:** Technical reports and symposium papers, licensing agreements

**Key Documentation:** Patents

**Key Personnel:** T. R. Charlton, 208-526-9324, trc@inel.gov  
 J. M. Beller, 208-526-1205, bmj@inel.gov

**Lab Capabilities Applied:** Biochemistry, Organic & Physical Chemistry, Nuclear Waste Char., Waste Processing/Reduction, Pollution Prevention, Waste Stabilization, High Temperature Waste Destruction, Remote Waste Identification & Char., Toxic & Haz. Waste Facility Design/Construct.



Index: 98

Category: Production (21)

Laboratory: Idaho National Engineering Laboratory      Contact: R. E. Rice, 208-526-1992, rrr@inel.gov

Title: Microbial Enhanced Oil Recovery and Reservoir Fundamentals

**Description:** This project consists of two tasks that include research and application studies for improved methods of enhanced oil recovery. The objectives include the development of microbial enhanced oil recovery (MEOR) systems with documented recovery mechanisms for application to reservoirs containing medium to heavy crude oils, leading to the design and implementation of industry cost-shared field demonstration project of MEOR technology, and the evaluation of reservoir wettability and its effect on oil recovery. The research is enhanced by academic and industrial collaborations with the New Mexico Institute of Mining and Technology Petroleum Recovery Research Center (NMPRRC) to study wettability (the interaction of fluids with mineral surfaces) and with Phillips Petroleum Company through a CRADA for Microbial Enhanced Oil Recovery and Biotechnology for Oil Field Applications. Cooperative research and technology transfer activities are focused on: 1) implementation of a cost-shared field demonstration of MEOR technology, 2) cooperative research with Phillips, and 3) laboratory research in direct support of field activities.

Facilities at the INEL are well equipped for the study of fluid flow through porous media (temperatures to 100 degrees C, pressures to 2,000 psi), and development of enhanced oil recovery processes and include full instrumentation and expertise for characterization of petrophysical properties including gas and liquid permeabilities and porosities. The staff is also highly experienced in modeling and field applications of enhanced oil recovery process.

91-95 Funding (\$K): 4000      Dates: 1989-1995

1	2	3	4	5	6	7
basic research	applied research		development		ready-to-use	

Technology Transfer: Publication in open literature

Key Documentation: CRADA with Phillips Petroleum Co. - MEOR and Biotechnology for Oil Field Applications  
Thomas, C. P., Bala, G. A., and Duvall, M. L., "Surfactant Based Enhanced Oil Recovery Mediated

Key Personnel: G. A. Bala, 208-526-8178, gb3@inel.gov  
C. P. Thomas, 208-526-0165, cpt@inel.gov

Lab Capabilities Applied: Petroleum Engineering, Geology, Microbiology, Biochemistry, Chemistry, Environmental Science, Reservoir Modeling, Chemical Engineering



Index: 99

Category: Environmental & Regulatory (9, 10)

Laboratory: Idaho National Engineering Laboratory      Contact: R. E. Rice, 208-526-1992, rrr@inel.gov

Title: Large-Scale Infiltration Study

**Description:** The high degree of heterogeneity present in fractured rock formations precludes utilization of small or intermediate scale observation alone for hydrologic and geochemical characterization efforts. An integrated program of large scale field experiments, along with supporting laboratory investigations, was initiated at the INEL to provide the most reliable information obtainable regarding aquifer flow and contaminant transport through the vadose zone.

An aquifer pumping test was performed which involved pumping the Snake River Plain aquifer at approximately 3000 gallons per minute for a period of six weeks. This water was piped 5,800 ft. to a 6.5 acre infiltration basin. Conservative and reactive tracers were added to the infiltrating water for assessing actinide and fission product surrogate retardation factors and dispersion parameters.

Infiltrating water was monitored with several overlapping systems, including 63 wells screened at various transmissive layers within the first 200 ft. depth, and geophysical techniques. Water and tracer migration were tracked with downhole nuclear moisture logging and gamma spectroscopy, as well as geophysically.

The wells drilled inside of the basin were completed in such a way as to prevent the vertical movement of water through the annular space.

91-95 Funding (\$K): 6000      Dates: 1993-present



Technology Transfer: Publications in open literature

Key Documentation: Patents pending

Key Personnel: K. J. Dooley, 208-526-2068, d @inel.gov

Lab Capabilities Applied: Vadose Zone Monitoring & Modeling, Rock Mechanics, Drilling & Completion, Environmental Monitoring, Hydrology, Geohydrology, Integrated Project Management, Geophysical R&D, Geophysical Logging



Index: 100

Category: Environmental & Regulatory (6, 9, 11, 14), Production (2, 16, 17, 18, 19), Development (4)

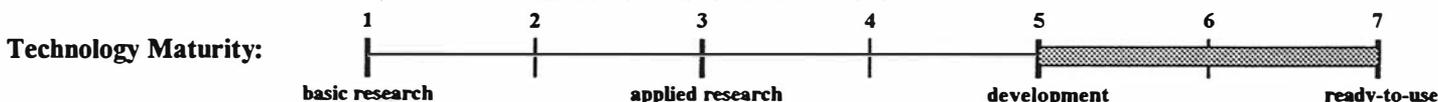
Laboratory: Idaho National Engineering Laboratory Contact: R. E. Rice, 208-526-1992, rrr@inel.gov

Title: US Air Force Installation Restoration Program

**Description:** As part of the U.S. Air Force Installation Restoration Program, two critical removal actions are being implemented at March Air Force Base, California. Construction and start-up of a Groundwater Extraction and Treatment System, completed in 1992, addressed removal and treatment of groundwater contaminated with a variety of volatile organic compounds. A pump-and-treat system utilizing liquid phase granular activated carbon was the primary treatment process. A second system now under construction addresses removal of jet fuel which leaked from an underground storage tank farm and currently reside on top of the water table beneath a former tank farm area. The primary treatment process utilized includes oil/water separation, air stripping, and vapor treatment and recovery using zeolite adsorption and condensation. Groundwater fate and transport modeling played a major role in developing the conceptual designs for these removal actions and for assessing their performance and effectiveness.

The remedial effort in the Tank Farm area presents unique challenges. The groundwater table has been steadily rising (14 ft.) for several years and has resulted in a JP-4 jet fuel plume with complex geometry in the saturated zone. This area is referred to as the smeared product zone. Conventional pump and treat technologies are ineffective in removing contaminants in this application. Chemical surfactants are being bench-scale and field-scale tested to determine the effectiveness for removal of a significant portion of the entrained jet fuel. Partitioning and non-partitioning chemical tracer tests will be utilized and verified by borehole analysis to determine jet fuel inventories before and after chemical surfactant treatment. Removal of remaining contaminants will be addressed by innovative, bioremediation efforts including pulsed oxygen delivery and biosparging.

91-95 Funding (\$K): 10000 Dates: 1990-present



**Technology Transfer:** The Department of Energy and March AFB will license some of the technologies developed. Others will be made available through non-proprietary publications at the conclusion of the remedial effort.

**Key Documentation:** March Air Force Base, Operable Unit #3, Feasibility Study Report, EGG-CEE-11473, Rev. 0; Record of Decision, March Air Force Base, Operable Unit 3, November 1994 (draft)

**Key Personnel:** L. Brown, 208-526-5510, lyb@inel.gov  
J. Sherick, 208-526-5469, nis@inel.gov

**Lab Capabilities Applied:** Hydrologic and Geologic Mapping and Interpretation, Advanced 3D modeling, Oscillatory Flow Testing for Vapor Vacuum Extraction, Removal of Non-aqueous Phase Contamination, Chemical Tracer Methods, Enhanced Bioremediation, Soil Air Permeability Evaluation



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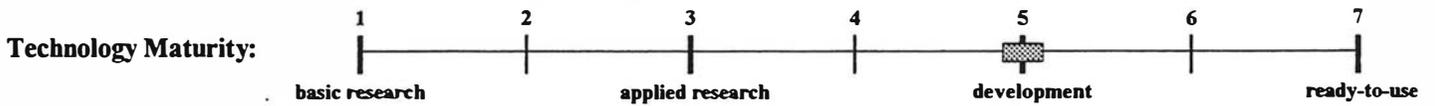
Category: Environmental & Regulatory (10)

Laboratory: Idaho National Engineering Laboratory      Contact: R. E. Rice, 208-526-1992, rrr@inel.gov

Title: Development of Biofilters for the Treatment of Hazardous Gases and Vapors

**Description:** The goal of this project is to develop and commercialize biofilters for the treatment of hazardous gases and vapors. These biofilters are being developed under agreements with two U.S. industrial partners. Target compounds of interest include nitrogen oxides, halocarbons, terpenes, alcohols, and certain hydrocarbons. The program is focusing on developing and demonstrating high efficiency biofilters that offer capital and operating cost advantages over best available competing technologies. Depending on the circumstances in question, these competitive technologies are generally carbon filtration, thermal oxidation and catalytic oxidation. Data generated to date in this biofiltration program have shown that in many instances, biofilters offer significant cost advantages over all of these conventional technologies while achieving highly effective removal of the gas or vapor in question.

91-95 Funding (\$K): 590      Dates: 1994-present



Technology Transfer: Publications in appropriate journals and presentations at scientific meetings

Key Documentation: Supporting documents for successful 1994 R&D 100 Award competition

Key Personnel: W. A. Apel, 208-526-1783, waa@inel.gov

Lab Capabilities Applied: Biotechnology, Biochemistry, Organic Chemistry



**Index:** 102

**Category:** Oil Processing & Refining (19)

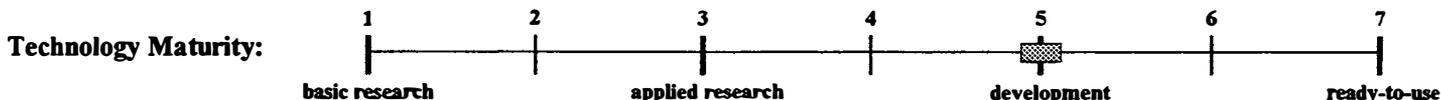
**Laboratory:** Idaho National Engineering Laboratory      **Contact:** R. E. Rice, 208-526-1992, rrr@inel.gov

**Title:** Polyphosphazene Membranes for Chemical Separations

**Description:** The goal of this project area is to investigate and determine the feasibility of using inorganic phosphazene polymer membranes to perform chemical separations in harsh environments. Union Carbide requires a separation that is difficult and costly to perform. If a membrane can be developed that will survive the process conditions, while at the same time performing the separation needed, it would save energy and significantly improve the economics of the process. During the past ten years of research on polyphosphazene membranes, the Idaho National Engineering Laboratory (INEL) has developed the integrated capabilities necessary to design a polymer system, synthesize the material, characterize it, cast films, and execute separation performance testing for the polymer in both liquid and gas separation applications.

Media and Process Technology has expertise in ceramic membrane module applications and the Idaho National Engineering Laboratory has developed polyphosphazene membranes. The current research combines these two aspects into the development of a unique membrane system. A pallet mounted, transportable membrane unit will be constructed. This will enable on-site testing of the membranes under 'real-life' conditions--including refinery related separations problems.

**91-95 Funding (\$K):** 760      **Dates:** 1994-present



**Technology Transfer:** Through industrial partnership

**Key Documentation:** 2 CRADAs (INEL/Union Carbide; INEL/Media & Process Technology)

**Key Personnel:** M. Stone, 208-526-8664, mls2@inel.gov  
E. Peterson, 208-526-1521, esp@inel.gov

**Lab Capabilities Applied:** Organic Chemistry, Organometallic Chemistry (Catalysts), Analytical Chemistry, Polymer Chemistry



**Index:** 103

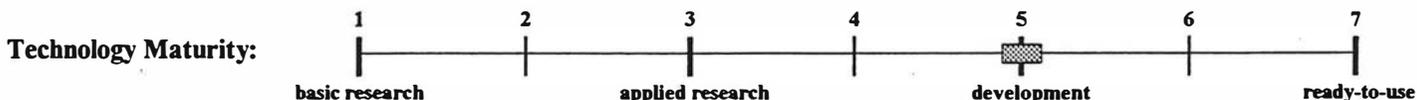
**Category:** Environmental & Regulatory (10)

**Laboratory:** Idaho National Engineering Laboratory      **Contact:** R. E. Rice, 208-526-1992, rrr@inel.gov

**Title:** Heavy Metals and Halocarbon Removal from Aqueous Waste Streams

**Description:** The goal of this project is to determine the feasibility of using inorganic phosphazene polymer membranes combined with Chromatochem, Incorporated's chelation chromatography process to remove heavy metal ions and organic chemical contaminants from harsh chemical process streams. Chromatochem, Inc. has several specific processes in mind. If a system can be developed that survives the process conditions, while at the same time performing the separations needed, significant amounts of energy can be saved. Chromatochem, Inc. has developed the chelation chromatography process during the past several years, and made it available to the medical community. Currently, Chromatochem is modifying the system to perform environmental separations. During the past ten years of research on polyphosphazene membranes, the Idaho National Engineering Laboratory (INEL) has developed the integrated capabilities necessary to design a polymer system, synthesize the material, characterize it, cast films, and execute separation performance testing for the polymer for both liquid and gas separation applications.

**91-95 Funding (\$K):** 500      **Dates:** 1994-present



**Technology Transfer:** Through partnership with Chromatochem

**Key Documentation:** CRADA between INEL and Chromatochem

**Key Personnel:** M. Stone, 208-526-8664, mls2@inel.gov  
E. Peterson, 208-526-1521, esp@inel.gov

**Lab Capabilities Applied:** Organic Chemistry, Organometallic Chemistry (Catalysts), Analytical Chemistry, Polymer Chemistry, Metal Extractions



**Index:** 104

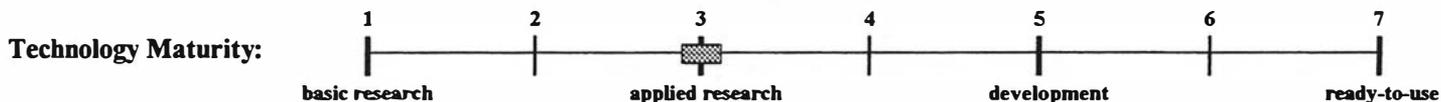
**Category:** Exploration (3, 4), Drilling & Completion (11)

**Laboratory:** Idaho National Engineering Laboratory      **Contact:** R. E. Rice, 208-526-1992, rrr@inel.gov

**Title:** Vertical Seismic Profiling While Drilling

**Description:** This project exploits a new, patented technology which uses seismic signals generated by a drill bit to produce a reverse Vertical Seismic Profile (VSP). By acquiring and processing Seismic-While-Drilling (SWD) data, the position of the drill bit relative to a seismic reflection section can be determined on-site and in real-time. This look-ahead-of-the-bit information can be used by the driller to set casing or increase mud weight prior to entering over-pressurized zones. The method does not require a pilot signal; thus it has application to many drilling environments and different bit types. There is no interruption of drilling and no associated costs for logging. The method is best implemented with an on-site computer to enhance timeliness and avoid large data-storage requirements. The objective of this project is to develop and test this field recording and processing system.

**91-95 Funding (\$K):** 300      **Dates:** 1995



**Technology Transfer:** Industry partnership formed with Utah Geophysical, et al.

**Key Documentation:** Proposal to Advanced Computer Technology Initiative, Patent # 5,012,453 (Katz, 1991)

**Key Personnel:** D. M. Weinberg, 208-526-4274

**Lab Capabilities Applied:** Geophysical Engineering, Electrical Engineering, Computer Science



Index: 105

Category: Oil Processing & Refining (15)

Laboratory: Idaho National Engineering Laboratory      Contact: R. E. Rice, 208-526-1992, rrr@inel.gov

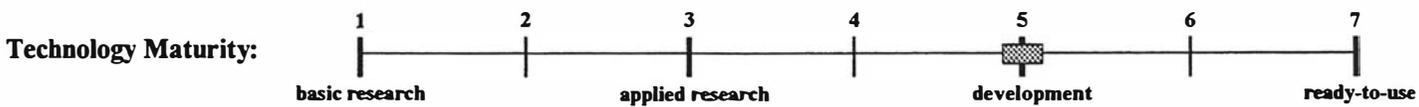
Title: Human Centered Performance Systems

**Description:** This computer program is structured to develop human performance evaluation methods and data specifically aimed at the elimination of error producing conditions and improving the performance and efficiency of a variety of high risk technologies. Data collection methods, databases, and analysis techniques have been developed and are currently being utilized by the participants. These tools include human reliability analysis techniques, human performance taxonomies and databases, data analysis techniques, and guidelines for improving human performance. These tools are directed at the reduction of incidents resulting in environmental insult, and/or economic. The system will build on previous efforts in the aviation and nuclear industries where successful programs have been developed and implemented.

Further efforts are underway to develop methods that will allow the introduction of increased automation in high technology systems safely and reliably. It is well known that most efforts to remove the human from the operating loop has resulted in increased error rates often resulting in increased accidents and failures. Typically this has been referred to as "clumsy automation". These programs are examining the contribution of risk of these new automated technologies to total risk of the system and are identifying better ways to model the contribution of risk in the design phase so that it may be reduced or eliminated. The result will be methods that can be applied by the designers of advanced systems that will reduce human error in the areas of design, as well as operation and maintenance.

Much of this work is generic and can be applied to systems of interest to the petroleum industry, such as in refineries, gas processing plants, and pipelines.

91-95 Funding (\$K): 3600      Dates: 1994-present



Technology Transfer: Technical papers and articles, symposia

Key Documentation: Technical reports

Key Personnel: H. Blackman, 208-526-0245, hsb@inel.gov

Lab Capabilities Applied: Probabilistic Risk Assessment, Human Reliability Analysis, Human Centered Automation, Incident Investigation, Human Performance Data Collection and Analysis



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Category: Gas Storage (3)

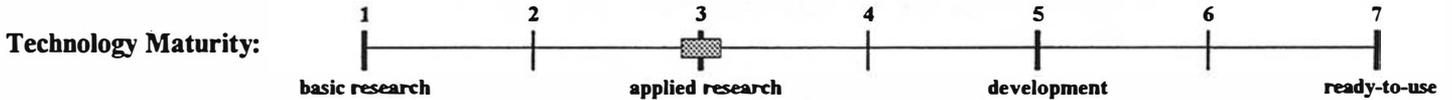
Laboratory: Lawrence Berkeley Laboratory

Contact: Paul A. Witherspoon, 510-486-5082, pawitherspoon@lbl.gov

Title: Gas Storage in Aquifers

**Description:** We are studying the dynamics of gas storage in aquifers to an accuracy never before possible. One of the key problems in aquifer storage is knowing where the gas bubble has developed as water is displaced down structure. The bubble's location is important in placing the injection and withdrawal wells to maximize gas production and to minimize water production. Field data from the Hillsboro aquifer gas storage project in Illinois have been used to develop a numerical model that includes the 3-D geometry of the anticlinal structure and proper parameters to describe the heterogeneous aquifer sand. The LBL-developed TOUGH2 code has been incorporated into the ITOUGH2 code. ITOUGH2 uses inversion algorithms enabling one to determine reservoir parameters that can be used in producing a model performance more closely conforming to field data. The dynamics of aquifer gas storage can be studied more accurately with such systems. The TOUGH2 code has also been modified to produce a detailed mesh around the points of injection and withdrawal, which makes it possible to investigate how the injection gas dries out the sand and how the dried-out region around the wellbore affects the process of water-coning during gas withdrawal.

91-95 Funding (\$K): 100      Dates: 1994-present



Technology Transfer: Technical reports

**Key Documentation:** 1) Witherspoon, P.A., Fuller, P., and Finsterle, S., 1995, "Three-Dimensional Multiphase Effects in Aquifer Gas Storage," in Proc. LBL 1995 TOUGH Users Workshop, K. Pruess, ed.  
2) Finsterle, S.A., 1993, ITOUGH2 User's Guide, Lawrence Berkeley Laboratory Report LBL-34581, Berkeley, CA.

**Key Personnel:** Paul A. Witherspoon, 510-486-5082, pawitherspoon@lbl.gov  
Stefan A. Finsterle, 510-486-5205, safinster@lbl.gov  
Karsten Pruess, 510-486-6732, pruess@csa2.lbl.gov

**Lab Capabilities Applied:** Reservoir Engineering, Numerical Modeling, Finite Element Analysis, Inverse Theory, 3-D Visualization



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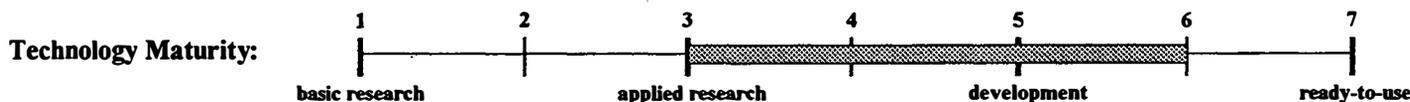
**Category:** Development (10, 14, 29, 30)

**Laboratory:** Lawrence Berkeley Laboratory      **Contact:** Ernest L. Majer, 510-486-6709, elmajer@lbl.gov

**Title:** LBL/Industry Fractured Reservoir Performance Definition Project

**Description:** The goal of this work is to demonstrate state-of-the-art technology in fluid-flow modeling and geophysical imaging as the basis for an interdisciplinary approach for predicting the behavior of heterogeneous, fractured gas reservoirs. The product of this work will be improved interpretational and predictive methods to be used by the petroleum industry to enhance gas recovery from existing and new reservoirs. This effort will also provide feedback for refining geophysical methods. The work is being carried out in two phases. The first phase consists of experiments conducted at Conoco's Newkirk borehole test facility to map fracture characteristics. These experiments employ detailed high-resolution, vertical seismic profiling and seismic-crosshole and single-well imaging. The resulting data, along with geologic and core data, are combined with hydrologic data and inverted to define the flow properties of a fractured reservoir rock. The second phase is to take the developed technology and apply it to a gas reservoir at the production scale.

**91-95 Funding (\$K):** 1300      **Dates:** 1992-present



**Technology Transfer:** Technical reports, demonstrations

**Key Documentation:**  
 1) Peterson, J.E., Majer, E.L., Daley, T.M., Queen, J., D'ontro, P., and Rizer, W., "Fracture Detection Using Crosswell and Single Well Surveys," Geophysics, in press.  
 2) Datta Gupta, A., Vasco, D.W., and Long, J.C.S., "Detailed Characterization of a Fractured Limestone Formation Using Stochastic Inverse Approach," SPE/DOE 27744, pp. 71-86.

**Key Personnel:** Ernest L. Majer, 510-486-6709, elmajer@lbl.gov  
 Jane C.S. Long, 510-486-6697, jcslong@lbl.gov

**Lab Capabilities Applied:** High Resolution Seismic Imaging, Crosshole Imaging, Single-Hole Imaging, Hydrologic Inversions



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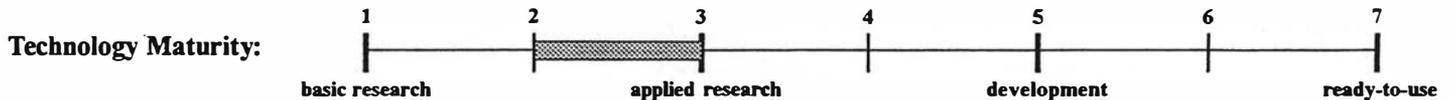
Category: Development (9, 3, 8, 10)

Laboratory: Lawrence Berkeley Laboratory      Contact: L. R. Myer, 510-486-6456, lrmyer@lbl.gov

Title: Influence of Clay and Clay Fluid Interaction on Seismic Wave Attenuation in Reservoir Rocks

**Description:** In order to understand the effects of clays on the attenuation of seismic waves in gas-reservoir rocks, compressional and shear waves were propagated across thin layers pressed between optically smooth silica disks and through silica beads coated with clay. Na-montmorillonite was tested in the presence of water, ethyl alcohol, and decane of various quantities. Kaolinite was also tested using water. Results showed that if a single continuous clay layer absorbed liquid in the interlamellar space between platelets, the interface was effectively decoupled so that most of the energy in an incident shear wave was reflected. The grain contact geometry in the bead samples gave rise to pumping losses for both compressional and shear waves in addition to viscous losses. In parallel with the laboratory measurements, a theoretical model was developed. Maxwell and Kelvin rheologic models incorporated into seismic-displacement discontinuity theory resulted in two bounding theoretical models. The experimental observations were modeled, yielding excellent agreement with the Maxwell model for the simple clay-layer tests and the Kelvin model for the bead tests.

91-95 Funding (\$K): 400      Dates: 1990-1993



Technology Transfer: Peer-reviewed papers, conference presentations and proceedings, industry review meetings

**Key Documentation:** 1) Suarez-Rivera, R., Cook, N.G.W., and Myer, L.R., "Study on the Transmissions of Shear Waves across Thin Liquid Films and Thin Clay Layers," Proceedings of 33rd U.S. Rock Mechanics Symposium, J.R. Tillerson and W. Wawersik, eds., Balkema, pp. 937-946 (1992).  
2) Ita, S., Cook, N.G.W., and Myer, L.R., "The Effect of Clay-Fluid Interaction on Ultrasonic Seismic Wave Propagation," in Rock Mechanics Models and Measurements, Challenges from Industry, P. Nelson and S. Laubach, eds., Proceedings of 1st North American Rock Mechanics Symposium, pp. 783-790, 1994.

**Key Personnel:** K. Nihei, 510-486-5349, ktneihei@lbl.gov  
L. Myer, 510-486-6456, lrmyer@lbl.gov  
N. Cook, 510-486-6602

**Lab Capabilities Applied:** Laboratory Rock Mechanics--Seismic Wave Propagation, Numerical Simulation



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Category: Production (23, 18)

Laboratory: Lawrence Berkeley Laboratory

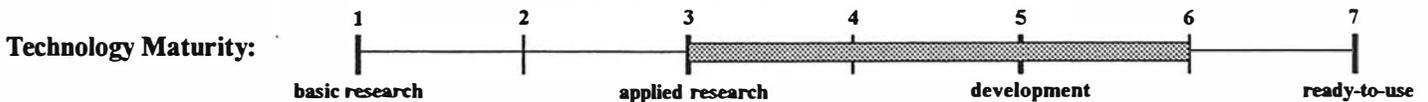
Contact: Tad W. Patzek, 510-643-5834, patzek@patzek.berkeley.edu

Title: Feasibility of Steam Drive in Diatomite

**Description:** The diatomaceous oil fields of California contain an estimated 10 billion barrels of original-oil-in-place (OOIP). For reference, this figure is roughly comparable to the OOIP in Prudhoe Bay, Alaska. Production from the diatomite is frustrated by exceptionally low rock permeability and a chemically unstable rock matrix. Although diatomite is very porous (25% to 65%), diatomaceous rocks characteristically have relatively large pore bodies connected to throats that are only 0.1 to 1 micron in diameter, as compared to 10 to 100 microns for sandstone. These narrow throats make diatomite almost impermeable (0.1 to 10 mD). To compensate for low permeability, wells in the diatomite are hydrofractured. Yet, even after hydrofracturing, waterflood on 1-1/4- and 5/8-acre patterns has suffered from low injectivity, poor sweep, and unwanted hydrofracture extensions. However, steamflooding on 5/8-acre spacing is a very attractive recovery technique. It succeeds because oil recovery occurs by both thermal expansion of oil through heat conduction and direct displacement of oil by steam and hot water entering oil-filled pore space.

Our goal is to help the oil industry bring steam drive online as a commercially viable oil-recovery process for diatomaceous oil fields. Currently, there are four components to the project: (1) interpreting steam-drive results from field pilot projects, (2) development of new reservoir simulation tools to understand and predict steam-drive recovery processes and fractured-rock dynamics, (3) integration of data-visualization tools with (1) and (2) to aid interpretation and communication of results, and (4) analysis of the geochemistry (e.g., rates of rock dissolution) of diatomite subjected to steam. The latter component is being done by Lawrence Livermore National Laboratory.

91-95 Funding (\$K): 400      Dates: 1994 - Present



Technology Transfer: Joint LBL-industry interpretation of field results, SPE papers, SPE and other technical conferences, public domain software

Key Documentation: 1) Kovscek, A. R., Johnston, R. M., and Patzek, T. W., SPE 29622, "Evaluation of Rock/Fracture Interactions During Steam Injection Through Vertical Hydrofractures," SPE Western Regional Meeting, Bakersfield, CA, March 8-10, 1995.  
2) Ilderton, D. C., Patzek, T. W., Rector, J. W., and Vinegar, H. J., SPE 28383, "Passive Imaging of Hydrofractures in the South Belridge Diatomite," SPE Ann. Tech. Conf. and Exhibition, New Orleans, LA, Sept. 1994.

Key Personnel: T. W. Patzek, 510-643-5834, patzek@patzek.berkeley.edu  
A. R. Kovscek, 510-486-5926, kovscek@garnet.berkeley.edu  
F. Piao, 510-486-7446, fanpiao@michael.berkeley.edu

Lab Capabilities Applied: Petroleum Engineering, Reservoir Engineering, Reservoir Simulation, Chemical Engineering, Numerical Methods.



Index: 110

Category: Development (9, 5, 6, 13)

Laboratory: Lawrence Berkeley Laboratory      Contact: L. R. Myer, 510-486-6456, lrmyer@lbl.gov

Title: Effects of Heterogeneity on the Mechanical Properties of Rock

**Description:** This research will develop a new fundamental understanding of the role of heterogeneity on the mechanical properties of rock. Results are directly applicable to reservoir compaction and wellbore-failure studies. At LBL, work focuses on two areas: fundamental processes of deformation and failure, and the relationships between microstructure and static and dynamic moduli of rock. Building on work carried out in a previous study on micromechanics of rocks supported by the Department of Energy, Office of Basic Energy Sciences, a boundary-element-method computer code is being used to investigate the deformation and failure of rock as simulated by an assemblage of grains. A numerical study to evaluate the effects of grain size, strength, and spatial distribution is nearly complete. In order to replicate realistic grain-failure patterns, it was necessary to include in the model dilatation forces associated with grain failure. This approach emphasizes the importance of mechanisms such as frictional sliding on the failure process. Work also continued on the discrete-element simulator LDDA, which will permit modeling of large kinematics as well as elastic displacements. A baseline version of the code is nearly complete. Emphasis in FY 95 and FY 96 will be on implementing algorithms for realistic constitutive behavior of element contacts and for fracturing of elements.

91-95 Funding (\$K): 300      Dates: 1993-present

1	2	3	4	5	6	7
basic research		applied research		development		ready-to-use

Technology Transfer: Peer-reviewed papers, conference presentations and proceedings

**Key Documentation:** 1) Nihei, K.T., Myer, L.R., Kemeny, J.M., Liu, Z., and Cook, N.G.W., 1994, "Effects of Heterogeneity and Friction on the Deformation and Strength of Rock," in Fracture and Damage in Quasibrittle Structures, Bazant, Bittman, Jirased and Mazars, eds., E&FN Spon., Condon, pp. 479-494.  
2) Zhong, L., Myer, L.R., and Cook, N.G.W., 1994. "Numerical Simulation of the Effects of Heterogeneities on Macro-Behavior of Granular Materials," in Computer Methods and Advances in Geomechanics, Proceedings of the Eighth International Conference of the Association for Computer Methods and Advances in Geomechanics, Sirivardane and Zaman, eds., Balkema, pp. 611-616.

**Key Personnel:** K. Nihei, 510-486-5349, ktnihei@lbl.gov  
L. Myer, 510-486-6456, lrmyer@lbl.gov  
N. Cook, 510-486-6602

**Lab Capabilities Applied:** Numerical Simulation-Boundary Element, and Combined Discrete and Finite Element Codes, Laboratory Rock Mechanics, Deformation and Strength



Index: 111

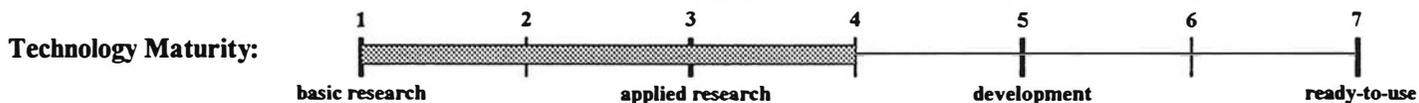
Category: Environmental & Regulatory (10)

Laboratory: Lawrence Berkeley Laboratory      Contact: Alexis T. Bell, 510-642-1536, bell@cchem.berkeley.edu

Title: Low Temperature Catalysts for the Oxidation of Methane

**Description:** We are developing catalysts for the low-temperature combustion of methane and other low-molecular-weight alkanes. Such catalysts are needed for the light-off of natural-gas catalytic combustors, the removal of trace levels of methane from natural burning processes and engines, and the control of hydrocarbon emissions from automobiles. While many catalysts for these purposes have been evaluated, most require temperatures > 500 C to achieve complete combustion of alkanes. In this project, we are seeking catalysts for the efficient oxidation of alkanes at temperatures < 250 C. Reducible metal oxides promoted by metal particles of gold or palladium are candidates for study. Since methane is the most refractory alkane, we will give primary emphasis to understanding the relationships between catalyst composition, structure, and activity for complete oxidation of methane. This project was initiated with LBL internal research funds on the basis of peer-reviewed competitive proposals. New proposals have been submitted to other funding sources.

91-95 Funding (\$K): 125      Dates: 1995-present



Technology Transfer: Conference papers, journal papers

Key Documentation: Contact key personnel for information

Key Personnel: Alexis T. Bell, 510-642-1536, bell@cchem.berkeley.edu

Lab Capabilities Applied: Chemical Engineering, Catalysis, Combustion



Index: 112

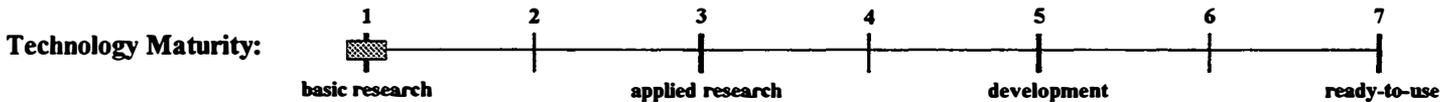
Category: Development (9, 13)

Laboratory: Lawrence Berkeley Laboratory      Contact: L. R. Myer, 510-486-6456, lrmyer@lbl.gov

Title: Laboratory and Theoretical Analysis of Transport Paths in Single Natural Fractures

Description: This research will produce new data on and greater understanding of the fracture void space and its control on single- and two-phase flow. The topological characteristics may provide the key to sealing relationships. Results of this program have application to industrial problems at several scales. At the pore scale, algorithms developed in this study form the basis for a new technology to derive flow properties from images of the pore space of drill cuttings. At the reservoir scale, results will lead to new architectures for simulation of flow in extremely heterogeneous systems.

91-95 Funding (\$K): 300      Dates: 1993-present



Technology Transfer: Peer-reviewed papers, conference presentations and proceedings

Key Documentation: 1) Yang, G., Cook, N.G.W., and Myer, L.R., 1994, "Analysis of Preferential Flow Paths Using Graph Theory," Int. J. Rock Mech. Min. Sci. & Geomech. Abstr., 30(7), 1423-1429.  
 2) Yang, G., Cook, N.G.W., and Myer, L.R., 1994, "Application of Graph Theory to Network Models of Porous or Fractured Media Flow," in Computer Methods and Advances in Geomechanics, Proc. IACMAG 8th Conf., Siriwardane and Zaman, eds., Balkema, pp. 1299-1304.

Key Personnel: K. Nihei, 510-486-5349, ktneihei@lbl.gov  
 L. Myer, 510-486-6456, lrmyer@lbl.gov  
 N. Cook, 510-486-6602  
 G. Yang, 510-642-5213

Lab Capabilities Applied: Numerical Simulation, Rock Mechanics Laboratory-Fluid Flow Measurements, Laboratory Pore Scale Visualization



Index: 113

Category: Development (3, 9, 10, 12, 14)

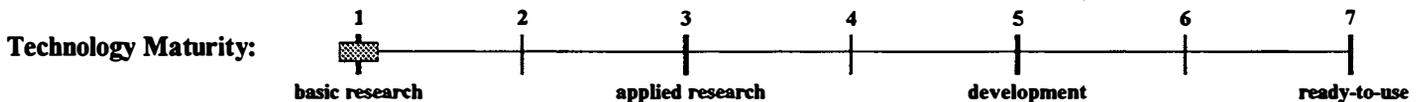
Laboratory: Lawrence Berkeley Laboratory

Contact: L. R. Myer, 510-486-6456, lrmyer@lbl.gov

Title: Energy Partitioning of Seismic Waves in Fractured Rock

**Description:** The objectives of this program are to develop a new understanding of: (1) the partitioning of energy between body waves, guided waves, and scattered waves; (2) techniques for exciting these waves; (3) the effects on these waves of spatial variation in properties; and (4) the effects of finite-length fractures. Results of this study are directly applicable to the characterization of fractured reservoirs by seismic methods. We are performing laboratory measurements and numerical calculations to study wave propagation at oblique angles of incidence to single and multiple fractures. Building on work conducted in a previous study funded by the U.S. Department of Energy, Office of Basic Energy Sciences, we have developed a boundary integral equation (BIE) numerical model to calculate the response of point sources in a three-dimensional medium containing fractures represented by displacement discontinuities. This program investigated the complete wavefield resulting from a point source located on and at a distance from a single fracture. Results show that a single fracture traps energy in the form of interface waves traveling at velocities close to both compressional and shear body waves. The wave amplitudes are a function of fracture stiffness and source characteristics. In FY 95 and FY 96, the program is emphasizing the study of the scattered wavefield and the influence of discontinuities on the resonant behavior of rock structures.

91-95 Funding (\$K): 300      Dates: 1993-present



Technology Transfer: Papers in refereed journals, conference presentations

**Key Documentation:** 1) Gu, B., Cook, N.G.W., Nihei, K.T., and Myer, L.R., 1994, "Modeling Elastic Wave Propagation in a Medium with Non-welded Interfaces Using the Boundary Integral Equation Method," in Computer Methods and Advances in Geomechanics, Proc. IACMAG 8th Conf., Siriwardane and Zaman, eds., Balkema.  
2) Nihei, K.T., Myer, L.R., and Cook, N.G.W., 1994, "Effects of Non-welded Interfaces on Guided SH-waves," Geophys. Res. Lett. v. 21, No. 9, pp. 745-748.

**Key Personnel:** K. Nihei, 510-486-5349, ktnihei@lbl.gov  
L. Myer, 510-486-6456, lrmyer@lbl.gov  
N. Cook, 510-486-6602

**Lab Capabilities Applied:** Numerical Modeling-Boundary Integral Equation Codes, Rock Mechanics Laboratory (Seismic Wave Propagation)



Index: 114

Category: Development (3)

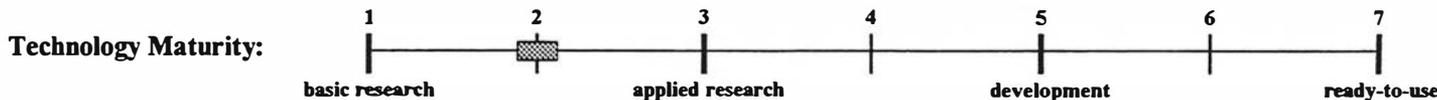
Laboratory: Lawrence Berkeley Laboratory

Contact: L. R. Myer, 510-486-6456, lrmyer@lbl.gov

Title: Application of Guided Waves to the Detection and Characterization of Continuous Flow Units and Bounding Surfaces

Description: Gas reservoir production is controlled by the architecture of flow units, fractures, sealing elements, and bounding surfaces that result from deposition and diagenesis. Differences between the elastic properties of these units and surfaces will allow many of them to support the propagation of guided waves. Techniques using guided waves to delineate flow units and sealing and bounding surfaces offer major advantages over conventional cross-well, vertical seismic profiling and surface seismic techniques. In contrast to body waves used in conventional seismic methods, the energy in guided waves is trapped adjacent to the unit or surface of interest and can propagate over large distances. The primary objective of this research is to develop relationships between the properties of layers and surfaces and the propagation velocities and particle displacements of the various modes of guided waves that can be expected in gas reservoirs. These relationships are necessary to infer the locations and continuity of layers and interfaces and to extract information such as thickness, elastic moduli, density, and interface stiffnesses from seismic surveys in a more effective manner than is currently possible with present seismic methods.

91-95 Funding (\$K): 500      Dates: 1993-present



Technology Transfer: Peer reviewed papers, conference presentations and proceedings, industry review meetings

Key Documentation: (None Provided)

Key Personnel: K. Nihei, 510-486-5349, ktneihei@lbl.gov  
L. Myer, 510-486-6456, lrmyer@lbl.gov  
N. Cook, 510-486-6602

Lab Capabilities Applied: Numerical Simulation, Laboratory Rock Mechanics--Seismic Wave Propagation



Index: 115

Category: Exploration (14, 1)

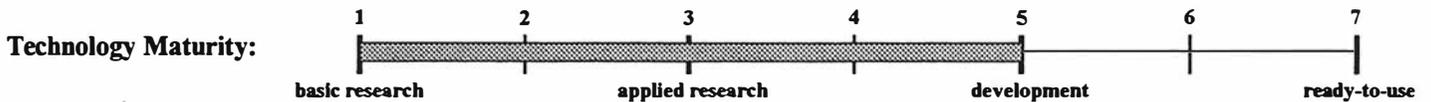
Laboratory: Lawrence Berkeley Laboratory

Contact: H.F. Morrison, 510-642-3157, hfmenggeo@garnet.berkeley.edu

Title: Subsalt Imaging with Marine Magnetotellurics

**Description:** This is a new project (effective 3/95) to develop and test the full capability of performing marine magnetotelluric (MT) surveys in the Gulf of Mexico for the exploration and delineation of hydrocarbon reservoirs beneath salt structures. The project also includes the development of methods for quantitative joint interpretations of MT, gravity, and seismic data for these structures. The project is made up of two highly integrated parts. The first is the development of efficient, commercially realizable MT systems for deployment in deep water. In a previous feasibility study, we joined with Scripps to develop and field-test a prototype. With support from industry partners, Scripps now proposes to build eight such systems that can be deployed by any marine contractor for routine survey operations. The second part is the utilization of the MT survey data, in conjunction with gravity and seismic survey data provided by the sponsor companies, for joint inversion to an accurate geological/petrophysical image of the subsurface.

91-95 Funding (\$K): 350      Dates: 1995 - Present



**Technology Transfer:** Public distribution of field results and inversion codes, collaboration with several companies including Amoco, BP, Chevron, Exxon, Geotools Corp., Louisiana Land and Exploration, NWG Associates, Texaco, Unocal

**Key Documentation:** 1) deGroot-Hedlin, C., Constable, S., 1990, "Occam's Inversion to Generate Smooth, Two-Dimensional Models from Magnetotelluric Data," *Geophysics*, v. 55, pp. 1613-1624.  
 2) Webb, S.C., Constable, S.C., Cox, C.S., and Deaton, T., 1985, "A Seafloor Electric Field Instrument," *J. Geomagn. Geoelectr.*, v. 37, pp. 1115-1130.

**Key Personnel:** H.F. Morrison, 510-642-3157, hfmenggeo@garnet.berkeley.edu  
 G.M. Hoversten, 510-642-3804, mhovers@violet.berkeley.edu  
 S.C. Constable, 619-534-2409, steve\_constable@gppqm.ugsd.edu

**Lab Capabilities Applied:** Petroleum Exploration, Electromagnetic Modeling, Joint Inversion of Geophysical Data



**Index:** 116

**Category:** Development (10, 14, 17)

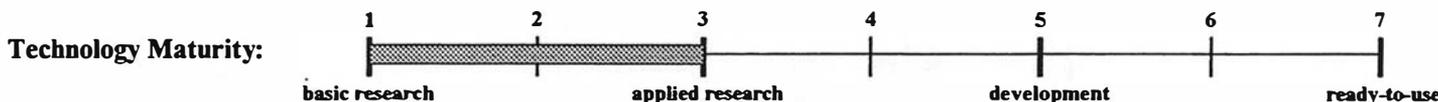
**Laboratory:** Lawrence Berkeley Laboratory

**Contact:** Alex Becker, 510-643-9182,  
alex@violet.berkeley.edu

**Title:** Surface-to-Borehole Electromagnetic Surveying (Vertical Electromagnetic Profiling)

**Description:** Formation electrical resistivity is indicative of formation porosity; thus measuring formation resistivity can provide essential information complementing that from conventional seismic tools. This project covers all aspects of an attempt to map formation resistivities by using an array of surface and borehole tools. Aspects of this project include experiment design, equipment design and fabrication, data acquisition, and data interpretation. A small-scale field test of the new technology was successfully carried out in 1994 at the University of California's Richmond Field Station. The survey technique, with measurements at frequencies up to 10 kHz, appears to be a promising tool for reservoir characterization. The work was funded by a six-member oil-industry consortium.

**91-95 Funding (\$K):** 120      **Dates:** 1993-1994



**Technology Transfer:** Documentation made available to the consortium, but further transfer is pending

**Key Documentation:** Contact Alex Becker for information

**Key Personnel:** Alex Becker, 510-643-9182, alex@violet.berkeley.edu  
 H. Frank Morrison, 510-642-3157, hfm@geo.berkeley.edu  
 K. H. Lee, 510-486-7468, khlee@lbl.gov

**Lab Capabilities Applied:** Geophysical Instrumentation, Geophysical Field Surveys, Electromagnetic Theory, Numerical Modeling.



Index: 117

Category: Development (10, 14, 29, 30)

Laboratory: Lawrence Berkeley Laboratory

Contact: Thomas V. McEvelly, 510-486-7347, tvmccevilly@lbl.gov

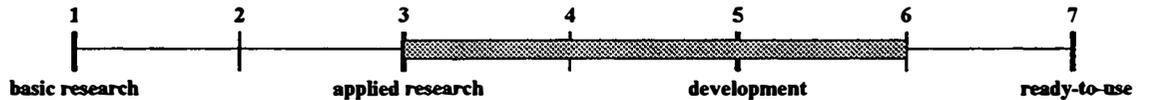
Title: Geophysical Measurements Facility

**Description:** The Geophysical Measurements Facility (GMF) was established at LBL to minimize the costs associated with collecting field data and to maintain equipment in a field-ready state. Many projects that involve field measurements often spend a large proportion of the funds refurbishing, renting, or buying equipment. By sharing equipment, and properly maintaining the existing instrumentation, the overall field costs should be minimized. GMF is available to serve all agencies and laboratories participating in DOE programs, not just LBL. For example, Sandia has placed a portable drill rig at GMF. The list of equipment at GMF is too long to detail here but in general includes a variety of equipment for seismic- and electrical-measurement methods. The seismic equipment includes microearthquake digital recording systems, seismic vibrators, cross-hole and single-hole imaging systems, a VSP recording and processing system, and acoustic emission systems. The electrical equipment includes controlled-source EM, DC-resistivity, and SQUID magnetometers. GMF also has a large variety of general field and test equipment such as meters and scopes. In addition, the facility houses state-of-the-art well-test systems and sampling facilities for groundwater analysis as well as a borehole test facility. Among the most recent additions are two complete well-logging vehicles (donated by Dresser-Atlas). Recently GMF moved into new quarters with expanded shop and fabrication capabilities and space for large-scale block testing.

91-95 Funding (\$K): 400

Dates: 1988-present.

Technology Maturity:



Technology Transfer: Technical reports, demonstrations

Key Documentation: (None Provided)

Key Personnel: T.V. McEvelly, 510-486-7347, tvmccevilly@lbl.gov  
L.R. Myer, 510-486-6456, lrmyer@lbl.gov  
E.L. Majer, 510-486-6709, elmajer@lbl.gov

Lab Capabilities Applied: Engineering Design, Instrument Maintenance and Fabrication



Index: 118

Category: Production (16)

Laboratory: Lawrence Berkeley Laboratory

Contact: C.J. Radke, 510-642-5204,  
radke@cchem.berkeley.edu

Title: Mechanisms of Mobility Control with Foams

**Description:** Improving oil recovery from existing fields is a crucial problem, as most domestic reservoirs are nearing depletion with standard production techniques. Because of the extreme heterogeneity of almost all reservoirs, mobility control in any improved production technique is paramount. Unfortunately, the critical need to maintain mobility control is not well-practiced. Current IOR processes (including steam flooding, hydrocarbon injection, carbon dioxide and nitrogen flooding, alkaline flooding, and surfactant flooding) demand much improved mobility control, both in the localized treatment of injection or production wells and in deep penetration attempts.

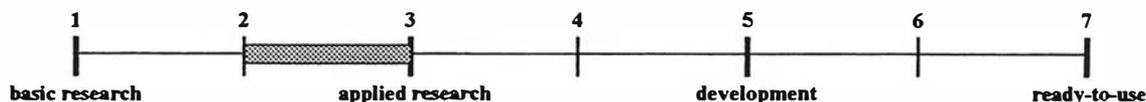
This work explores the use of gas-aqueous surfactant dispersions (also called generically "foams") as a general mobility-control agent both for single-injection or production-well treatments and for establishing global sweep improvement, all for a range of IOR processes. Initially, considerable effort was directed toward a fundamental understanding of how foams are generated, how they are stabilized, and how they flow in porous media. The program now is directed toward applying those fundamental and mechanistic findings to modeling foam blockage and displacement processes and to devising appropriate surfactant screening procedures for designing effective chemical packages. We have recently incorporated a conservation equation for the number density of foam bubbles into an implicit, three-dimensional, compositional, and thermal-reservoir simulator and created a fully functional, mechanistic foam simulator. Because foam mobility is a strong function of bubble texture, the bubble population balance is necessary to make accurate predictions of foam flow behavior. The program currently has five research elements: (1) foam simulator development, (2) long-core foam displacement experiments, (3) foam displacement in the presence of oil, (4) measurements of thin film forces, and (5) dynamic tension and surface rheology studies.

91-95 Funding (\$K):

1500

Dates: 1991-present

Technology Maturity:



Technology Transfer:

Technical publications, DOE reports, industrial affiliates, technical meetings, seminars, workshops

Key Documentation:

- 1) Aronson, A.S., Bergeron, V., Fagan, M.E., and Radke, C.J., 1994, "The Influence of Disjoining Pressure on Foam Stability and Flow in Porous Media," *Colloids and Surfaces A: Physicochemical Eng. Aspects*, v. 83, pp. 109-120.
- 2) Kovscek, A.R., and Radke, C.J., 1994, "Fundamentals of Foam Transport in Porous Media," in *Foams: Fundamentals and Applications in the Petroleum Industry*, Advances in Chemistry Series 242, Laurier L. Schramm, ed., Chapter 3, pp. 113-163.

Key Personnel:

C. J. Radke, 510-642-5204, radke@cchem.berkeley.edu  
T. W. Patzek, 510-643-5834, patzek@patzek.berkeley.eduLab Capabilities  
Applied:

Petroleum and Chemical Engineering, Reservoir Engineering, Reservoir Simulation, Fluid Dynamics, Capillarity, Colloid and Surface Chemistry, Dispersed Phase Flow, Numerical Analysis, Field Application



Index: 119

Category: Environmental & Regulatory (10)

Laboratory: Lawrence Berkeley Laboratory

Contact: Joseph Jaklevic, 510-486-5647, jmjaklevic@lbl.gov

Title: Airborne Emissions Monitoring and Analysis

Description: The EPA is currently considering new air-quality standards for air toxics. A key issue in assessing control costs is determining the level of control appropriate to the oil-refining industry. LBL has strong experimental research capabilities focused on automated instrumentation for large-scale environmental monitoring and analysis. The Engineering Division of LBL has designed and implemented an atmospheric aerosol sampling-and-analysis network based on size-segregated particle sampling, followed by nondestructive analysis using a variety of methods. Specific developments include an automatic dichotomous aerosol sampler, a system for x-ray fluorescence analysis of particles collected on membrane filters, and a sensitive beta-gauge for total-mass monitoring. These instruments were subsequently adapted for use by the U.S. Environmental Protection Agency for inorganic-pollutant monitoring. Related activities include the development of sophisticated chemical-analysis techniques such as x-ray powder diffraction, synchrotron-based fluorescence analysis, and extended x-ray absorption fine-structure analysis.

91-95 Funding (\$K): 200      Dates: 1975-1991



Technology Transfer: Technical reports, demonstrations

Key Documentation: Jaklevic, J.M. and Giauque, R.D., 1992, "Energy-Dispersive X-Ray Fluorescence Analysis Using X-Ray Tube Excitation," in Handbook on X-Ray Spectroscopy: Methods and Techniques, Van Grieken and Makowicz, eds., Marcel Dekker, p. 151.

Key Personnel: Joseph Jaklevic, 510-486-5647, jmjaklevic@lbl.gov

Lab Capabilities Applied: Semiconductor Detector Research, Low-Noise Electronics, Computer Systems Engineering, Chemical Analysis Techniques



**Index:** 120

**Category:** Development (1, 6, 9, 10, 11, 12)

**Laboratory:** Lawrence Berkeley Laboratory      **Contact:** Jane C.S. Long, 510-486-6697, [jcslong@lbl.gov](mailto:jcslong@lbl.gov)

**Title:** Characterization of Fractured Reservoirs

**Description:** Efficient production from fractured reservoirs has long been a problem. Because the fracture network can be highly heterogeneous, some wells may be connected by fracture flow paths and other wells not. In addition, faults may serve both as hydraulic connections and barriers to flow. These conditions are problematic for accessing pockets of oil and for efficient-drive secondary recovery schemes.

LBL has developed a suite of technologies for characterizing fracture and fault systems. These include geomechanically based models for fracture growth, geophysical methods for fracture detection, and inverse methods for the analysis of hydraulic effective-fracture-network identification. These latter methods use well test, tracer test, or possibly production data to define the connectivity of the fracture system conditioned on the geomechanical and geophysical data. These methods have been applied to the Conoco Borehole Test Facility in Oklahoma in cooperation with Conoco, Phillips, and Amoco. In addition, the methods are being developed and used for a variety of applications outside of the petroleum industry.

**91-95 Funding (\$K):** 3000      **Dates:** 1991-1995

**Technology Maturity:**

1	2	3	4	5	6	7
basic research	applied research		development		ready-to-use	

**Technology Transfer:** Please contact Jane C.S. Long for information about report.

**Key Documentation:** Available from key personnel.

**Key Personnel:** Jane C.S. Long, 510-486-6697, [jcslong@lbl.gov](mailto:jcslong@lbl.gov)  
 Christine Doughty, 510-486-6453, [cadoughty@lbl.gov](mailto:cadoughty@lbl.gov)  
 Ernie Majer, 510-486-6709, [elmajer@lbl.gov](mailto:elmajer@lbl.gov)  
 John Peterson, 510-486-6709, [barstow@ccs.lbl.gov](mailto:barstow@ccs.lbl.gov)  
 Don Vasco, 510-486-6709, [vasco@ccs.lbl.gov](mailto:vasco@ccs.lbl.gov)

**Lab Capabilities Applied:** Petroleum Engineering, Reservoir Engineering, Applied Mathematics, Numerical Simulation, Inverse Analysis, Field Testing, Subsurface Imaging



Index: 121

Category: Development (9)

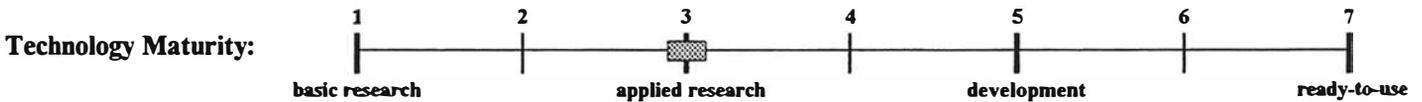
Laboratory: Lawrence Berkeley Laboratory      Contact: L. R. Myer, 510-486-6456, lrmyer@lbl.gov

Title: Analysis and Reduction of Well Failures in Diatomite Reservoirs

**Description:** Subsurface compaction in California's diatomite reservoirs continues to result in costly well failures. The purpose of this project is to improve our understanding of the geomechanical processes and to develop tools and operating strategies to mitigate future well damage. The cooperative research program includes the following tasks. Task 1 consists of analyzing existing field data, including stimulation and reservoir pressure records, production and injection histories, subsidence data, lithologic and structural data, and well-failure data. Well-by-well production and injection data, subsidence and geologic data, and well-failure records are displayed by means of a 3-D graphics visualization system. The displays will be the basis for establishing relationships between the reservoir behavior and observed well failures and for elucidating the mechanisms and spatial distribution of the well failures. Task 2 consists of laboratory measurements of time-dependent mechanical properties (creep) under reservoir conditions. Experiments identify the influence of aqueous solutions introduced by water flooding and which are known to accelerate the deformation of siliceous and clay-bearing rocks. Task 3 involves the evaluation of available geomechanical computer codes developed both commercially and at national laboratories to model reservoir and overburden response leading to well failure.

Note: This work is a joint project between Lawrence Berkeley Laboratory and Sandia National Laboratories

91-95 Funding (\$K): 350      Dates: 1994-present



Technology Transfer: Industry/laboratory working groups, SPE papers, refereed journal articles

Key Documentation: (None Provided)

Key Personnel: Janet Jacobsen, 510-486-4450, jsjacobsen@lbl.gov  
 Jahan Noorishad, 510-486-4905, j\_noorishad@lbl.gov  
 Joanne Fredrich, 505-844-2096  
 Wolfgang Wawersik, 505-844-4342

Lab Capabilities Applied: Numerical Geomechanics Simulators, Rock Mechanics Laboratory Apparatus, Graphics Visualization Systems



Index: 122

Category: Oil Processing &amp; Refining (9)

Laboratory: Lawrence Berkeley Laboratory

Contact: Enrique Iglesia, 510-642-9673,  
iglesia@cchem.berkeley.edu

Title: Solid Superacid Catalysts for Isomerization and Alkylation

**Description:** The goal of this program is to discover and advance mesoporous inorganic solids as catalysts for two important reactions in the manufacture of fuels: the alkylation of isobutane with light olefins and the isomerization of normal paraffins to isoparaffins. Both processes lead to highly branched fuel components with high octane. Two types of inorganic solids are currently under study: (1) tungsten oxide clusters and films on zirconia supports and (2) heteropolyacid Keggin clusters supported on silica. The initial stages of the program involve the use of novel synthesis techniques for the generation of high acid-site densities within mesoporous support structures and the chemical and physical characterization of surface acid sites within these solids. The program also includes detailed studies of the mechanism of alkylation and isomerization reactions, with specific emphasis on the control of undesirable side reactions such as cracking and polymerization, which lead to loss of selectivity and catalyst deactivation. Poor selectivity and rapid deactivation currently prevent the use of inorganic solid acids as replacements for liquid acid and halogenated solid catalysts.

91-95 Funding (\$K): 230

Dates: 1994-present

1

2

3

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7

Technology Maturity:

basic research

applied research

development

ready-to-use

**Technology Transfer:** Technical collaborations with Exxon Research and Engineering Co. Presentations at AIChE and ACS annual meetings.

**Key Documentation:** 1) Iglesia, E., Barton, D., Soled, S.L., Miseo, S., Baumgartner, J.E., and Gates, W.E., 1995, Proc. 14th North American Meeting of the Catalysis Society.  
2) Iglesia, E., Soled, S.L., and Kramer, G., 1993, Journal of Catalysis, v. 144, p. 238.

**Key Personnel:** Enrique Iglesia, 510-642-9673, iglesia@cchem.berkeley.edu  
David G. Barton, 510-642-9673  
Stuart L. Soled (Exxon Research and Engineering), 908-730-2577

**Lab Capabilities Applied:** Heterogeneous Catalysis, Surface Science, Reaction-Reactor Engineering and Design, Materials Sciences



Index: 123

Category: Production

Laboratory: Lawrence Berkeley Laboratory

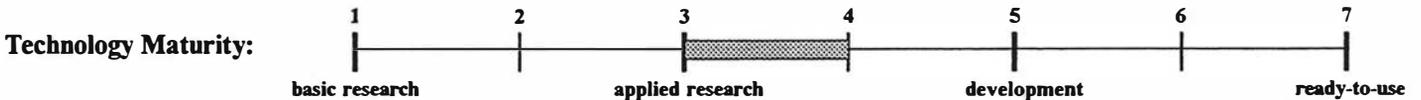
Contact: Tad W. Patzek, 510-643-5834, patzek@patzek.berkeley.edu

Title: Optimal Fluid Injection and Producibility in Fractured, Low-Permeability Reservoirs

**Description:** An optimal injection policy minimizes formation damage while producing maximum oil for the amount of fluid injected. Fluid injection into low-permeability reservoirs, such as diatomite or chalks, either for pressure maintenance or oil displacement, is problematic. Injection rates must be held in check to prevent reservoir damage from overpressuring, which may induce unwanted fractures or extend existing fractures; however, rates must be high enough to make recovery economical. Reservoir engineers currently develop injection policy from past experience, from their knowledge of the state of reservoir stress as a function of depth and depletion, from reservoir performance history, and, usually, from predictions of future performance based on reservoir simulation. Although an oil field is a complex system, injectors are usually controlled individually without feedback among neighboring injectors.

The result of this project will be a unique, computer-assisted operations (CAO) tool to promote oil recovery from fractured, low-permeability reservoirs undergoing a secondary or tertiary fluid injection process. The tool functions by making "expert" decisions on how to optimize fluid injection and maintain oil production, while limiting reservoir damage and well failures, hence maximizing profit. Features of this tool will include: (1) real-time, well-by-well monitoring of the progress of injected fluid, along with the evolution of reservoir permeability; (2) neural networks for compiling individual well responses to water, steam, or carbon dioxide injection; (3) reservoir simulation based upon trends recognized by the neural network for making long-term injection policy decisions; and (4) project-wide coupling of well-head controllers that recognize the oil field as a complex coupled system.

91-95 Funding (\$K): 250      Dates: 1995 - Present



Technology Transfer: SPE papers, SPE and other technical conferences, public domain software, joint LBL-industry injection policy development

Key Documentation: Contact T. W. Patzek for information.

Key Personnel: T. W. Patzek, 510-643-5834, patzek@patzek.berkeley.edu  
 A. R. Kovscek, 510-486-5926, kovscek@garnet.berkeley.edu  
 M. Nikraves, 510-486-5926, nikraves@michael.berkeley.edu

Lab Capabilities Applied: Petroleum Engineering, Reservoir Engineering, Reservoir Simulation, Chemical Engineering, Numerical Methods, Control Theory



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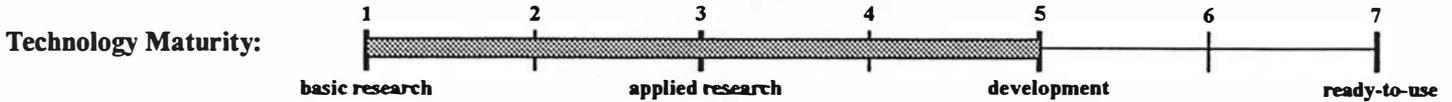
Category: Environmental & Regulatory (5, 6)

Laboratory: Lawrence Berkeley Laboratory      Contact: Ki Ha Lee, 510-486-7468, khlee@lbl.gov

Title: Design, Construction, and Application of a Very-Early-Time Electromagnetic (VETEM) System for Detailed Mapping of the Shallow Subsurface

**Description:** Commercially available electromagnetic (EM) instruments and interpretational software are not well suited to meeting requirements for the following tasks: (1) detection of objects such as drums and boxes buried at shallow depths; (2) description and characterization of subsurface geology and hydrology, including such properties as porosity, permeability, and water saturation; and (3) identification and tracing of pollutants including hydrocarbon spills. Using currently available state-of-the-art EM induction methods, we cannot investigate structures at shallow depths (less than 5 m). At the other end of the spectrum, ground-penetrating radar (GPR) systems typically investigate only the top meter or so when clay minerals are present in the soil. Hence, there is a gap in our detection capability between the lower limit of GPR and the upper limit of EM induction techniques. Furthermore, interpretational software for current EM systems neglects dielectric properties, an excellent signature associated with an oil spill. The objective of this research is to develop a survey methodology, both hardware and software, that fills the gap between GPR and traditional EM induction. In terms of frequency, this will be between 100 kHz and about 30 MHz. This is a joint project with participants from the Idaho National Engineering Laboratory, U.S. Geological Survey, Lawrence Berkeley Laboratory, Sandia National Laboratories, University of Utah, University of Arizona, and University of California at Berkeley. LBL's task includes: (1) development of 1-D and 3-D forward and inverse solutions with frequencies up to 1 GHz, (2) coordination with the technology transfer groups, and (3) system analysis to guide instrument design.

91-95 Funding (\$K): 305      Dates: 1993-present



Technology Transfer: An industry review panel consisting of Zonge Engineering, Geonics, EMI, Newmont, Sensors & Software, and EPA is guiding the direction of research activity through regular meetings. Members of this group will receive the technology.

Key Documentation: None Provided

Key Personnel: Ki Ha Lee, 510-486-7468, khlee@lbl.gov  
 Ganquan Xie, 510-486-7134, g\_xie@lbl.gov  
 H.F. Morrison, 510-642-3157, hfmenggeo@garnet.berkeley.edu  
 Alex Becker, 510-643-9182

Lab Capabilities Applied: Numerical Modeling--Inversion and Interpretation, System Design and Analysis



**Index:** 125

**Category:** Environmental & Regulatory (9, 2, 6, 9, 15)

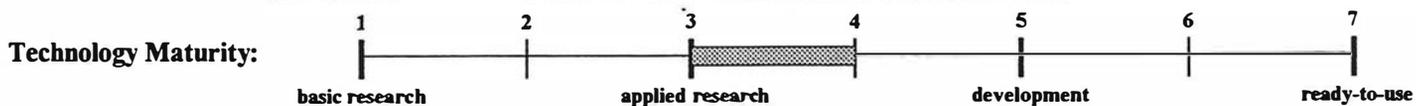
**Laboratory:** Lawrence Berkeley Laboratory

**Contact:** J. C. S. Long, 510-486-6697,  
jcslong@lbl.gov

**Title:** Analog Site for Characterization of Fractured Rock

**Description:** Many petroleum resources are located in fractured rock, and characterization of fractured sites in order to predict transport of contaminants for environmental remediation activities can be problematic. The locations of fractures is often a mystery, while their effect on flow can be dramatic. Thus, the three key issues that influence remediation of these sites are: (1) finding the fractures that control fluid flow and transport, (2) analyzing flow and transport in the fracture system, and (3) predicting and controlling induced changes to the fracture system. This project is designed to identify reliable tools and methodologies for characterizing the fractures that control flow and transport in specific geologic settings. Characterization tools will be used to predict the outcome of flow and transport experiments in fractured basalts in the vadose zone, in order to assess the utility of these tools for characterizing important hydrologic features in similar contaminated sites. The goals of the project are: (1) to gain an understanding of infiltration into fractured rock, specifically to determine which components of the medium control flow, which physical processes are dominant, and how these interact; (2) to learn how to make relevant measurements in such systems, specifically what to measure, how to design and deploy instrumentation, and how to perturb the system; and (3) to learn how to predict the behavior of the system by building a model of the system, parameterizing the model with data, using the model to predict behavior, and then checking that prediction against further experimental data.

**91-95 Funding (\$K):** 634      **Dates:** 1994-Present



**Technology Transfer:** Seminars, scientific papers and presentations, tech-transfer workshops and training sessions planned

**Key Documentation:** Contact Jane Long for a list of publications and training information.

**Key Personnel:** Jane C. S. Long, 510-486-6697, jcslong@lbl.gov  
Peter Zawislanski, 510-486-4157, ptzawislanski@lbl.gov

**Lab Capabilities Applied:** Vadose Zone Hydrology, Reservoir Engineering, Applied Mathematics, Numerical Simulation, Inverse Analysis, Field Testing



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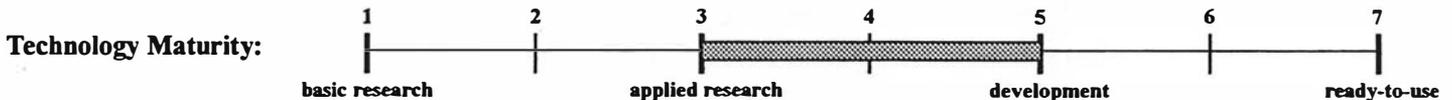
Category: Environmental & Regulatory (4, 8, 9, 12, 14)

Laboratory: Lawrence Berkeley Laboratory      Contact: Sally M. Benson, 510-486-5875, smbenson@lbl.gov

Title: Site Remediation Analysis and Decision Support

**Description:** The goal of the SELECT project is to design and develop a distributed, object-oriented computer architecture to integrate, analyze, and present environmental information. This information would help managers select cost-effective environmental-remediation strategies that maximize the reduction of health risks while minimizing costs. The architecture incorporates state-of-the-art scientific advances in site characterization, subsurface and atmospheric transport processes, exposure pathway analysis, health-hazard assessment, and cost analysis of remediation options. We have developed an initial PC version of the SELECT software that includes animated 3-D visualization of contaminant transport and graphical displays of exposure, health-risk, and remediation costs. The core of SELECT is the numerical model T2VOC for subsurface contaminant transport. Developed at LBL with DOE support, this code is used to calculate the multiphase transport of volatile organic compounds. Other models in SELECT include CAL TOX and a version of STAR. CAL TOX was developed for Cal/EPA by UC Davis and Lawrence Livermore National Laboratory. It models human exposure to pollutants in soil and water. STAR is used to model advective transport of VOCs into buildings. Health-risk assessments are based on potency values from the LBL, U.S. EPA, and Cal/EPA databases. The SELECT risk module plots dose versus time for inhalation, oral, and dermal contact, and compares hypothetical cancer hazards from various background sources to the remediation actions chosen, including no action.

91-95 Funding (\$K): 800      Dates: 1994-present



Technology Transfer: Demonstrations, conference papers

Key Documentation: Oldenburg, C., Benson, S., Pruess, K., Daisey, J., Brown, N., Gold, L., and Macfarlane, J., 1995, "The SELECT Environmental Remedy Tool: A Platform for Multiphase Transport Modeling," submitted to 1995 ASME/AIChE National Heat Transfer Conference, Portland, OR, Aug. 5-9, 1995.

Key Personnel: Sally Benson, 510-486-5875, smbenson@lbl.gov  
 Nancy Brown, 510-486-4241, njbrown@lbl.gov  
 Joan Daisey, 510-486-7491, jmdaisey@lbl.gov  
 Lois Gold, 510-486-7080, lsgold@lbl.gov  
 Curt Oldenburg, 510-486-7419, cmoldenburg@lbl.gov

Lab Capabilities Applied: Numerical Modeling, Hydrogeology, Atmospheric Science, Computer Science, Toxicology, Health Risk Assessment, Environmental Remediation Technology



Index: 127

Category: Oil Processing &amp; Refining (9, 11)

Laboratory: Lawrence Berkeley Laboratory

Contact: Gabor A. Somorjai, 510-486-4831,  
somorjai@garnet.berkeley.edu

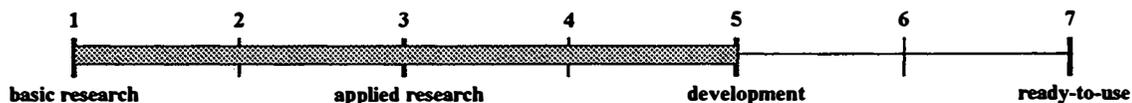
Title: Development of Solid Acid Catalysts for Gasoline Alkylation

**Description:** The goal of this project is to develop economically and environmentally superior gasoline alkylation catalysts. There are significant incentives to replacing with solid acids the sulfuric and hydrofluoric acids now used in large-scale processes. This change would alleviate current cost and disposal issues. LBL has the facilities and capabilities to obtain fundamental information on the operation mechanisms of solid-acid catalysts so as to ensure their success. LBL is currently in discussions with Catalytica, Inc., to enter into a CRADA. Under this agreement, LBL would prepare model catalysts and thin oxide films, modify them with promoters, and characterize them by means of surface science techniques. The catalysts would then be tested under industrial conditions in our unique reaction chamber and further characterized after the reactions.

91-95 Funding (\$K): 840

Dates: 1995 - Present

Technology Maturity:



Technology Transfer: A CRADA application will be developed pending discussions with Catalytica.

Key Documentation: Contact the key personnel for information

Key Personnel: Gabor Somorjai, 510-486-4831, somorjai@garnet.berkeley.edu

Lab Capabilities Applied: Chemical Engineering, Catalysis, Surface Science



Index: 128

Category: Oil Processing &amp; Refining (9, 11)

Laboratory: Lawrence Berkeley Laboratory

Contact: Gabor A. Somorjai, 510-486-4831,  
somorjai@garnet.berkeley.edu

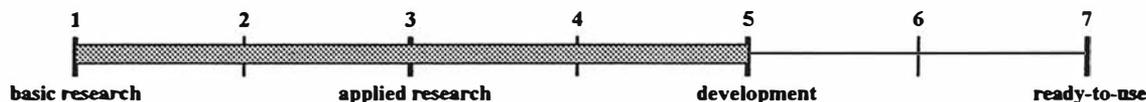
Title: Development of Poison Resistant, Low Deactivation Rate, Platinum-Based Bimetallic Catalysts

**Description:** Pt-Re, Pt-Ir, and Pt-Sn bimetallic catalysts are utilized to produce high-octane gasoline from naphthas. We are exploring new methods for producing catalysts with uniform particle size in the 1-10 nm range and with controlled distances between particles in the same spatial range. Our goal is to develop catalysts with superior thermal and chemical stability using electron-beam lithography and chemical-vapor deposition technologies. By having careful control of particle size and distribution, we hope to change the selectivity (for example, from dehydrocyclization to isomerization). Alumina and silica will be used as supports, and controlled acidity will be one of the variables. These catalysts will be tested under industrial conditions in our unique reaction chamber and can be fully characterized by surface science techniques.

91-95 Funding (\$K): 300

Dates: 1995 - Present

Technology Maturity:



Technology Transfer: A CRADA application will be developed pending current discussions with industrial partners.

Key Documentation: Contact the key personnel for information

Key Personnel: Gabor Somorjai, 510-486-4831, somorjai@garnet.berkeley.edu

Lab Capabilities Applied: Chemical Engineering, Catalysis, Surface Science



Index: 129

Category: Oil Processing &amp; Refining (7, 9, 23)

Laboratory: Lawrence Berkeley Laboratory

Contact: Dale L. Perry, 510-486-4819

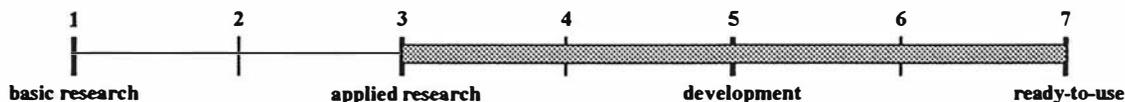
Title: Synthesis and Characterization of Heterogeneous Catalysts for the Petroleum Industry

**Description:** We are designing, synthesizing, and characterizing novel heterogeneous catalysts for applications in the petroleum industry, such as the synthesis of ethane and ethylene from methane-oxygen mixtures. In addition, we are planning studies of new acid catalysts that can replace acid systems containing hydrofluoric acid in order to reduce the risk of accidents and minimize the introduction of hydrofluoric acid into the environment. These catalysts will vary in composition, surface area and morphology, acidity, and form (e.g., powder, wafer, or film) so as to be available for a wide array of applied and fundamental uses. The technical approach will be to take advantage of LBL's expertise in preparing novel solid-state catalysts and determining their material, chemical, and catalytic properties. We will use a wide variety of experimental techniques that include the Advanced Light Source, a state-of-the-art synchrotron facility at LBL. This unique facility will allow us to monitor the heterogeneity of different metals (both intentional and contaminant) in the catalysts at the femtogram level and also to study their catalytic properties in greater detail than has ever been possible. The participating industrial partner will specify the properties of the catalysts and test their catalytic activity (e.g., yield and selectivity) for chosen reactions of interest to the petroleum industry. The end result of this collaboration will be a new class of solid-state catalysts that are safer for industrial use and make possible the minimization of previously used chemicals that are dangerous both to humans and to the environment.

91-95 Funding (\$K): 475

Dates: 1990-present

Technology Maturity:



Technology Transfer: Literature publications, international meetings, patent pending

**Key Documentation:** 1) Perry, D. L., et al., 1993, J. Mater. Res., v. 8, p. 2400.  
2) Perry, D. L., 1994, J. Mater Res., v. 9, p. 2993.

Key Personnel: Dale L. Perry, 510-486-4819

**Lab Capabilities Applied:** Advanced Light Source, X-Ray and Infrared Instrumentation, Chemical Engineering, Catalysis, Spectroscopy, Surface Science, Materials Science



Index: 130

Category: Oil Processing &amp; Refining (2, 1, 4)

Laboratory: Lawrence Berkeley Laboratory

Contact: Enrique Iglesia, 510-642-9673,  
iglesia@cchem.berkeley.edu

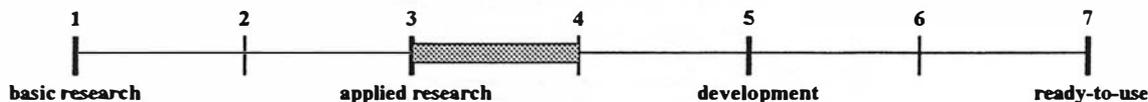
Title: Catalytic Membranes for Paraffin Activation and Hydrogen Transport

**Description:** The goal of this program is to develop catalytic membranes based on thin films of perovskite oxide structures for the activation of methane and other light paraffins. One side of the high-temperature inorganic membrane catalyzes the dehydrogenation of the paraffin to methyl radicals (which dimerize to give ethane) or to the corresponding olefins; the resulting hydrogen atoms transfer across the membrane. Hydrogen is recovered as H<sub>2</sub>, used in a hydrogenation reaction, or burned with air on the opposite side of the membrane. This program involves: (1) synthesis and characterization of thin films of proton-conducting metal oxides via vapor deposition, controlled hydrolysis, and sol-gel techniques; and (2) characterization of the catalytic and hydrogen-transport properties of the formed materials. Concurrent reaction-separation devices such as catalytic membranes are likely to become critical components in the introduction of hydrogen-rich light paraffin components into refinery feedstocks and in the recovery and management of hydrogen in future refinery operations.

91-95 Funding (\$K): 425

Dates: 1991 - Present

Technology Maturity:



Technology Transfer: Technical papers

**Key Documentation:** 1) Iglesia, E., Heinemann, H., and Perry, D.L., 1993, Proc. DOE Contractors Meeting, Morgantown, WV.  
2) Iglesia, E. and Perry, D.L., 1995, Proc. DOE Contractors Meeting, Baton Rouge, LA.  
3) Reyes, S.C., Kelkar, C.P., and Iglesia, E., 1993, Catal. Lett., v. 19, p. 167.

**Key Personnel:** Enrique Iglesia, 510-642-9673, iglesia@cchem.berkeley.edu  
Heinz Heinemann, 510-486-5976  
Richard W. Borry, 510-642-9673

**Lab Capabilities Applied:** Heterogeneous Catalysis, Surface Science, Reaction-Reactor Engineering and Design, Materials Sciences



Index: 131

Category: Environmental &amp; Regulatory (10)

Laboratory: Lawrence Berkeley Laboratory

Contact: Peter Zawislanski, 510-486-4157,  
ptzawislanski@lbl.gov

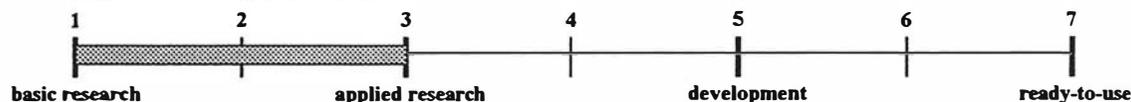
Title: Fractionation and Cycling of Selenium in the Biogeochemical System of Suisun and San Pablo Bays

**Description:** In the late 1980s, elevated concentrations of selenium in ducks and clams of the San Francisco Bay were discovered. Natural inputs of selenium into the Bay are exceeded by discharges from oil refineries. Although adverse effects have not been observed, there is concern that selenium will accumulate in the food web. Suspended and bottom sediments are important links in the food web through which selenium is redistributed and often concentrated. Task I of this project aims to define methodology for fractionation of selenium on Bay sediments. Fractionation allows for the determination of how an element is associated with the solid phase, e.g., as an organic coating, an adsorbed phase, inorganic precipitate, and so on. Subsequently, the more critical question of how selenium is redistributed to and from sediments needs to be addressed. It can take many chemical forms; some of these are soluble, and consequently available to the ecosystem, but also more mobile and readily flushed from the system. The elemental form is less bio-available but can persist in the sediment for long periods of time. Task II deals with measuring the amount of selenium occurring as each chemical species (i.e., determining the speciation) and developing a framework for understanding and predicting chemical reactions from one form to another. This will be accomplished through a series of field and laboratory experiments. The definition of sediments as a sink or source of selenium is necessary to assess the possible short-term and long-term exposures of biological organisms.

91-95 Funding (\$K): 800

Dates: 1994 - Present

Technology Maturity:



**Technology Transfer:** Periodic internal reports, reports to funding agencies, articles in refereed journals, methodologies shared with industry and other research groups

**Key Documentation:** 1) Field Work Proposal to DOE/Fossil Energy.  
2) Detail Workplan to the Regional Water Quality Control Board.

**Key Personnel:** Peter Zawislanski, 510-486-4157, ptzawislanski@lbl.gov  
Sally Benson, 510-486-5875, smbenson@lbl.gov  
Scott Mountford, 510-486-6772  
Angus McGrath, 510-486-4157, aemcgrath@lbl.gov  
Thomas Johnson, 510-486-4975, tmjohnson@lbl.gov  
Susan Anderson, 510-486-4

**Lab Capabilities Applied:** Selenium Chemistry, Analytical Chemistry, Field Sampling Design, Laboratory Experimentation Design, Stable Isotope Geochemistry, Aquatic Ecotoxicology



Index: 132

Category: Development (10)

Laboratory: Lawrence Berkeley Laboratory      Contact: Ki Ha Lee, 510-486-7468, khlee@lbl.gov

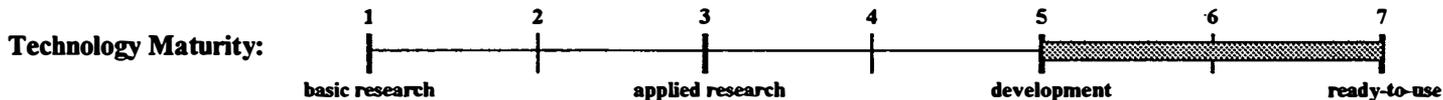
Title: Multifrequency Electromagnetic (EM) Imaging for Reservoir Characterization

**Description:** The electrical conductivity of sedimentary rocks is controlled by their porosity, hydraulic permeability, temperature, saturation, and pore fluid conductivity. These rock parameters play important roles in the development and production of hydrocarbon resources. For these reasons, resistivity well logs have long been used by geologists and reservoir engineers in the petroleum industry to map variations in pore fluid, to distinguish between rock types, and to determine completion intervals in wells. Reservoir simulation and process monitoring rely heavily on the physical characteristics of the reservoir model. At present, numerical codes use point measurements of porosity, permeability, and fluid saturation and extrapolate these data throughout a three-dimensional (3-D) grid. The knowledge of a high-resolution geophysical parameter such as electrical conductivity would aid this extrapolation and improve the reservoir-simulation effort.

We have developed a 3-D inversion scheme for imaging electrical conductivity using the integral equation method and the standard least-squares approach. The code has been tested successfully with the crosshole EM data Mike Wilt of Lawrence Livermore National Laboratory collected at Lost Hills' steam injection experiment (Wilt et al., 1994). The objective of the EM experiment was to see if we could monitor the subsurface process by observing changes in electrical conductivity caused by steam injection. By analyzing the difference in electrical conductivity before and after the injection, we were able to describe the development of a major steam chest in the vicinity of the injection point.

This development is coupled to a cooperative project, "Subsurface EM Measurement," involving Lawrence Berkeley Laboratory and private industry. Current participants are Texaco, Schlumberger, Atlas Wireline Service, OYO, and Noranda.

91-95 Funding (\$K): 785      Dates: 1990-1994



Technology Transfer: Publication of results, 3-D inversion code available

Key Documentation: Wilt, M., Torres-Verdin, C., and Lee, K.H., 1994, "Crosshole EM Imaging for Monitoring of Steam Flooding at Lost Hills," presented as a poster session at the 1994 SEG D&P Forum, Economic Impact of Geophysical and Geostatistical Reservoir Characterization, Big Sky, Montana, July 17-22, 1994.

Key Personnel: Ki Ha Lee, 510-486-7468, khlee@lbl.gov  
 Ganquan Xie, 510-486-7134, g\_xie@lbl.gov  
 H.F. Morrison, 510-642-3157, hfmenggeo@garnet.berkeley.edu  
 Alex Becker, 510-643-9182

Lab Capabilities Applied: Numerical Modeling--Inversion and Interpretation, System Design and Analysis



**Index:** 133

**Category:** Production

**Laboratory:** Lawrence Berkeley Laboratory      **Contact:** Emilio U. Antunez, 510-486-5866, emilio@jard.lbl.gov

**Title:** Subsidence, Analysis, and Control

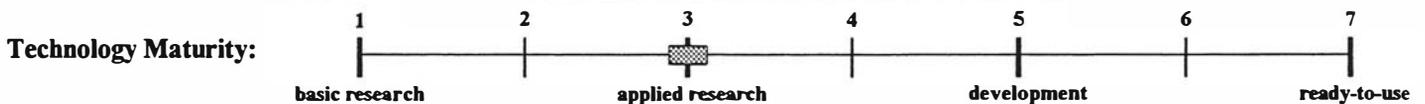
**Description:** Massive fluid extraction from clastic subsurface oil reservoirs causes pore volume deformation in response to changes in reservoir fluid pressure. Compaction, the vertical component of this type of rock deformation, may cause drastic changes in surface elevation (subsidence) and may activate stresses that potentially could damage man-made facilities (e.g., surface installations and sheared well casings). Subsidence may be preventable or controllable if the mechanisms causing the problem are fully understood and remedial actions are taken. In some oil fields, compaction may enhance the production of fluids, but eventually it also may cause wellbore failures and damage to surface installations. These problems are costly, even in unpopulated areas.

On the basis of our existing compaction-subsidence simulators, LBL, in collaboration with industry, is developing advanced simulators that could help analyze the subsidence-causing mechanisms in oil fields. The use of these codes would help industry in the implementation of production/injection scenarios: (1) to estimate the additional oil recovery due to compaction, (2) to develop subsidence-mitigation strategies, and (3) to minimize stress perturbations.

Wilmington Oil Field data will be used to test the simulators. This field has a long history of oil production; has experienced a significant amount of subsidence; has one of the most complete public domain databases of reservoir properties, production data, and injection data; and has documented incidents on several parts of the field where subsidence has been caused by different mechanisms. These data would provide enough input to test the new subsidence codes.

These new simulators would be applicable to any reservoir where compaction and subsidence are a problem (oil, geothermal, or groundwater reservoirs).

**91-95 Funding (\$K):** 200      **Dates:** 1995 - Present



**Technology Transfer:** Conference papers, computer codes available through the Energy Sciences and Technology Software Center, training on the use of the codes, seminars.

**Key Documentation:**

**Key Personnel:** Emilio U. Antunez, 510-486-5866, emilio@jard.lbl.gov  
 Karsten Pruess, 510-486-6732, pruess@csa2.lbl.gov  
 Marcelo Lippmann, 510-486-5035, marc@csa.lbl.gov  
 Jahan Noorishad, 510-486-4905, shiva@csa.lbl.gov

**Lab Capabilities Applied:** Petroleum Engineering, Reservoir Engineering, Rock Mechanics, Simulation, Physics, Computer Facilities, Visualization



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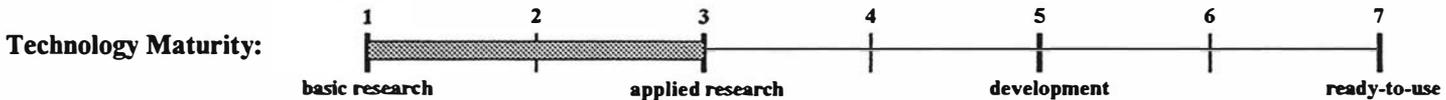
Category: Exploration (1, 7), Development (4, 8)

Laboratory: Lawrence Berkeley Laboratory      Contact: Don DePaolo, 510-643-5064, djdepaolo@lbl.gov

Title: Integrated Isotopic Studies of Fluid Flow Processes and Time Scales in Sedimentary Basins

**Description:** Our efforts in the area of fossil energy supply are concerned with establishing the geological characteristics of sedimentary basins that affect fluid transport and, consequently, hydrocarbon migration; e.g., fluid sources and sinks, rates and types of diagenetic reactions, amount and duration of paleo-fluid flow, and permeability changes during basin evolution. This information provides a valuable background for exploration and the development of advanced extraction and monitoring technologies. The degree to which the isotopic composition of elements dissolved in fluids is modified by the permeable rock medium depends on several parameters: the ratio of fluid velocity to water-rock reaction rate, the ratio of the effective porosity to the rock/fluid element concentration ratio, and the influence of external fluid sources. Hydrocarbon transport depends upon the same parameters. Therefore, by measuring the spatial and temporal variations in isotopic composition of multiple elements in fluids and their rock media, it should be possible to "image" the subsurface reservoir in terms of these parameters. We have emphasized: (1) the use of noble gas isotopes and their concentrations in fluids from sedimentary basins to identify fluid sources and to understand large-scale fluid migration; (2) the use of Sr isotopes as a means of stratigraphic correlation to understand geologic structure, the evolution of permeability, and the types of fluids that have inhabited the pore space during post-depositional history; and (3) the use of a combined approach (Nd, Sr, O, K-Ar) to understand the relationships between sediment provenance, sedimentation rates, post-depositional fluid migration and diagenetic reactions, and hydrocarbon accumulation.

91-95 Funding (\$K): 500      Dates: 1990-present



Technology Transfer: Publications in open literature, contract work, collaboration

**Key Documentation:** 1) DePaolo, D.J., and Finger, K.L., 1991, "High-Resolution Strontium-Isotope Stratigraphy and Biostratigraphy of the Miocene Monterey Formation, Central California," Geol. Soc. Bull., v. 103, pp. 112-124.  
 2) Hiyagon, H., and Kennedy, B.M., "Noble Gases in CH<sub>4</sub>-Rich Gas Fields, Alberta, Canada," Geochim. Cosmochim. Acta., v. 56, pp. 1569-1589 (1992).

**Key Personnel:** D.J. DePaolo, 510-643-5064, djdepaolo@lbl.gov  
 B.M. Kennedy, 510-486-6451, bmkenedy@lbl.gov  
 M. Conrad, 510-486-6141, msconrad@lbl.gov  
 K. Nishiizumi, 510-643-9361

Lab Capabilities Applied: Isotope Geochemistry, Mass Spectrometry, Fluid Flow Modeling, Basin Modeling



Index: 135

Category: Development (25, 30, 31, 33)

Laboratory: Lawrence Berkeley Laboratory

Contact: Wes Bethel, 510-486-7353, ewbethel@lbl.gov

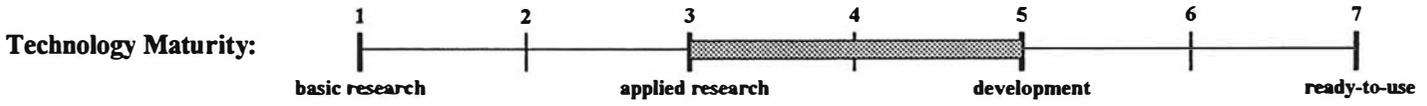
Title: Advanced Flux Visualization and Virtual Reality for Reservoir Engineering

**Description:** Building upon a prototype virtual reality/visualization system developed at LBL, a team of reservoir engineers and computer-visualization specialists will investigate alternate techniques for visualizing fluid fluxes calculated in the simulation of a petroleum reservoir. For large reservoir simulations, current techniques result in hard-to-interpret images. The techniques that will be investigated for this project include: (1) using alternate geometric icons, (2) combining an iconic representation of fluid flow with visualization of component concentration, (3) use of direct volume rendering, (4) data decimation, and (5) use of a scalar value to represent a multi-component flux as a form of data reduction. The initial prototypes of the algorithms will be built in a modular visualization environment and later ported to production software.

The team will also test and evaluate several low-cost, virtual-reality input/output devices to interface with the visualization environment. In a reservoir simulation, these devices would be used not only to specify 3-D input (e.g., well location and perforation), but also to position data probes to obtain output at a specified location in the numerical grid and to place particles for particle tracking as part of advection or streamline calculations.

This project will result in better tools for flux visualization and demonstrate how virtual reality devices can be used to create advanced user interfaces for reservoir simulators.

91-95 Funding (\$K): 200      Dates: 1995 - Present



Technology Transfer: A CRADA is in preparation.

Key Documentation: Contact key personnel for information

Key Personnel: Wes Bethel, 510-486-7353, ewbethel@lbl.gov  
 Janet Jacobsen, 510-486-4450, jsjacobsen@lbl.gov  
 Nancy Johnston, 510-486-5093, nejohnton@lbl.gov

Lab Capabilities Applied: Reservoir Simulation, Numerical Modeling, 3-D Visualization, Code Development



Index: 136

Category: Development (10, 15)

Laboratory: Lawrence Berkeley Laboratory Contact: Ki Ha Lee, 510-486-7468, khlee@lbl.gov

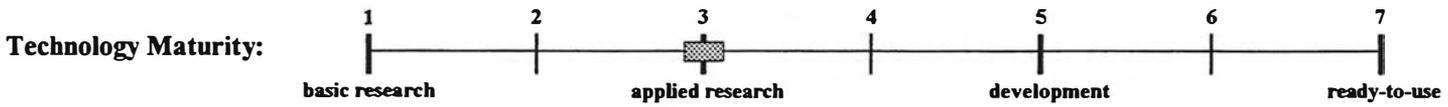
Title: Electromagnetic (EM) Imaging through Steel-Well Casing

**Description:** The ability to utilize crosshole low-frequency EM imaging is of great interest for reservoir characterization and process monitoring. One of the most important problems facing the use of subsurface EM imaging in an oil-field environment is steel-cased wells. EM fields propagate through a metal casing, but their amplitude is greatly attenuated and phase-shifted because of the electrical conductivity and magnetic permeability of the steel casing.

Numerical studies as well as laboratory measurements of EM fields inside an infinitely long metal pipe in a homogeneous whole space have been presented by Augustin et al. (1989) and Wu and Habashy (1994). These studies used coaxial loop sources outside the pipe. Uchida et al. (1991) have extended the technique to simulate the crosshole configuration, in which the source is placed inside a cased well and measurements are made in a second uncased borehole. In reality, the physics is more complicated than the ideal cases previously studied. A casing string is made up of a number of segments, and, within each segment and at connecting collars, the properties vary. Furthermore, the host medium is not homogeneous but may be reasonably well represented by either a layered earth or a cylindrically symmetric one about the borehole axis. To understand the way this realistic model affects fields inside and outside the casing, we are developing and conducting numerical modeling studies coupled with field experiments to verify the numerical model analysis and future application of the EM imaging technique.

This development is coupled to a cooperative project, "Subsurface EM Measurement," involving Lawrence Berkeley Laboratory and private industry. Current participants are Texaco, Schlumberger, Atlas Wireline Service, OYO, and Noranda.

91-95 Funding (\$K): 200 Dates: 1994-present



**Technology Transfer:** Talks at SPE and SEG conferences, peer-reviewed journal papers, Energy Science and Technology Software Center (for code distribution)

**Key Documentation:**

- 1) Augustin, A.M., Kennedy, W.D., Morrison, H.F., and Lee, K.H., 1989, "A Theoretical Study of Surface-to-Borehole Electromagnetic Logging in Cased Holes," *Geophysics*, v.54, pp. 90-99.
- 2) Uchida, T., Lee, K.H., and Wilt, M., 1991, "Effect of Steel Casing on Crosshole EM Measurements," Expanded Abstracts, 442-445, 61st SEG Annual International Meeting & Exposition, Houston, Texas.
- 3) Wu, X., and Habashy, T.M., 1994, "Influence of Steel Casings on Electromagnetic Signals," *Geophysics*, v. 59, pp. 378-390.

**Key Personnel:** Ki Ha Lee, 510-486-7468, khlee@lbl.gov Ganquan Xie, 510-486-7134, g\_xie@lbl.gov  
 H.F. Morrison, 510-642-3157, hfmengeo@garnet.berkeley.edu Alex Becker, 510-643-9182

**Lab Capabilities Applied:** Numerical Modeling--Inversion and Interpretation, System Design and Analysis



Index: 137

Category: Development (10, 14, 29, 30)

Laboratory: Lawrence Berkeley Laboratory      Contact: Ernest L. Majer, 510-486-6709, elmajer@lbl.gov

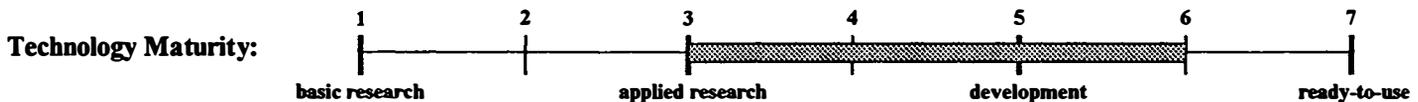
Title: High-frequency Seismic-Acoustic Imaging

**Description:** LBL has designed, fabricated, and implemented a high-resolution piezoelectric system for crosshole imaging in a variety of geologic environments. Distances between holes has ranged from a few meters to hundreds of meters, with resolution varying from a few cm at the shorter ranges to a meter at the widest hole separations. The source can be used in dry and water-filled holes (diameters as small as 5 cm) and operates in pulse and sweep modes. Pulse widths as small as 10 microseconds are used at a repetition rate of 10 to 50 Hz. In the sweep mode, frequencies may be varied from 200 to 15,000 Hz, but 500 to 5,000 Hz is typical. The 12-channel data recording system, expandable to 48 channels, performs a 16-bit A/D conversion at 400,000 samples/second.

The system includes in-field data processing and tomographic display and can handle an arbitrary 3-D well geometry. Concurrently, LBL has been developing a variety of numerical inverse techniques for producing velocity and wave-attenuation tomograms.

The system has been used to image fracture zones in crystalline rocks and to characterize small-scale heterogeneities in oil-bearing sediments. It is now being used to track fluid movement during steam and water floods in the South Belridge field, a diatomite reservoir in California. The system has been upgraded to withstand temperatures to 200 C.

91-95 Funding (\$K): 1000      Dates: 1989-present



Technology Transfer: Technical reports, demonstrations

**Key Documentation:** 1) Vasco, D.W., Majer, E.L., and Johnson, L.R., 1993, "Ensemble Inference in Geophysical Inverse Problems," Geophys J. Intern., v. 115, pp. 711-728.  
2) Vasco, D.W. and Majer, E.L., 1993, "Wave Path Travel-Time Tomography," Geophys. J. Intern., v. 115, pp. 1055-1069.

**Key Personnel:** Ernest L. Majer, 510-486-6709, elmajer@lbl.gov  
John Peterson, 510-486-4267, jepeterson@lbl.gov  
Donald W. Vasco, 510-486-5206, dwvasco@lbl.gov

**Lab Capabilities Applied:** Numerical Modeling, Inverse Theory, High-voltage Instrumentation, Data Acquisition/Signal Processing



**Index:** 138

**Category:** Development (10, 14, 29, 30)

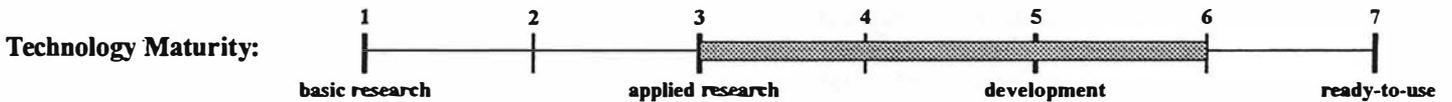
**Laboratory:** Lawrence Berkeley Laboratory

**Contact:** Ernest L. Majer, 510-486-6709, [elmajer@lbl.gov](mailto:elmajer@lbl.gov)

**Title:** Subsurface Imaging for Characterizing the Effects of Natural Heterogeneity on Transport Properties

**Description:** The goal of this work, funded by the U.S. Department of Energy's (DOE's) Subsurface Science Program, is to use subsurface imaging to identify the fundamental scales of physical-parameter variation that control transport behavior relative to predicting subsurface microbial behavior. With this information, it may be possible to relate physical and chemical parameters (i.e., those parameters that geoscientists have experience measuring in situ) to microbial properties. The approach uses controlled meter-scale field sites and supplementary laboratory and intermediate-scale information to characterize those physical properties that affect fluid flow and chemical transport and that can be imaged with in situ methods. The work will be tightly integrated with chemical and microbial characterization and process-definition efforts in the DOE's Subsurface Heterogeneity and Bacterial Transport Subprograms. Field work is under way to define and characterize the natural subsurface physical heterogeneity at DOE sites where information has been gathered on the microbial and chemical properties.

**91-95 Funding (\$K):** 1420      **Dates:** 1991-present



**Technology Transfer:** This work has served as a basis for the application of subsurface high-resolution imaging for defining transport properties at DOE-contaminated sites.

**Key Documentation:** Vasco, D.W., Majer, E.L., and Johnson, L.R., 1993, "Ensemble Inference in Geophysical Inverse Problems," *Geophys. J. Intern.* 115, 711-128.

**Key Personnel:** Ernest L. Majer, 510-486-6709, [elmajer@lbl.gov](mailto:elmajer@lbl.gov)  
Donald W. Vasco, 510-486-5206, [dwvasco@lbl.gov](mailto:dwvasco@lbl.gov)

**Lab Capabilities Applied:** High-Resolution Cross-Hole Imaging, Laboratory Analysis of Core, Hydrologic Analysis



Index: 139

Category: Gas Processing

Laboratory: Lawrence Berkeley Laboratory

Contact: Robert G. Bergman, 510-642-2156,  
rgberg@violet.berkeley.eduTitle: Transition Metal-Catalyzed Conversion of CO, NO, H<sub>2</sub>, and Organic Molecules to Fuels and Petrochemicals

**Description:** The purpose of this project is to develop new methods for using transition metals to activate carbon-hydrogen (C-H) bonds in alkanes and other organic molecules. This work has important fundamental and practical implications. The discovery that metals can activate alkane C-H bonds has opened up a new area of chemistry, and we have made substantial progress in understanding how these alkane activation reactions work. Activation of C-H bonds in alkanes would have major impact in the areas of chemical synthesis and transportable fuels. Alkanes are a major constituent of petroleum, but they are utilized only rarely in chemical synthesis because their inherent reactivity is so low. Metal activation of alkane C-H bonds is the first step in converting alkanes into functionalized organic molecules. This conversion will allow alkanes to be used as feedstocks for a wide range of industrially important organic chemicals. Abundant quantities of the smallest alkane, methane, are often produced with crude oil. At remote locations, methane is simply burned ("flared") because it is too dangerous and expensive to liquefy and transport to sites where it is needed as a fuel. Using alkane C-H activation reactions to oxygenate methane would convert it to methanol, a much more easily transportable fuel, and thus utilize a precious carbon resource.

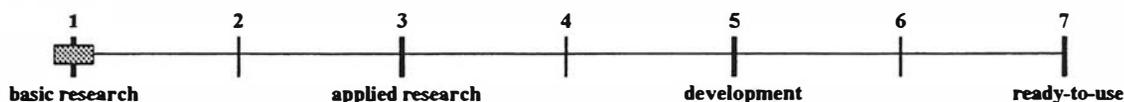
91-95 Funding (\$K):

260

Dates:

1994 - Present

Technology Maturity:



Technology Transfer:

Publications in the open literature, papers delivered at universities and national meetings

Key Documentation:

1) Bengali, A.A., Arndtsen, B.A., Burger, P.M., Schultz, R.H., Weiller, B.H., Kyle, K.R., Moore, C.B., Bergman, R.G., 1995, "Activation of Carbon-Hydrogen Bonds in Alkanes and Other Organic Molecules by Ir(I), Rh(I), and Ir(III) Complexes," *Pure and Applied Chemistry* 1995, v. 67, pp. 281-288.

2) Bergman, R.G., 1992, "Activation of Carbon-Hydrogen Bonds in Alkanes and Other Organic Molecules Using Organotransition Metal Complexes," in *Homogeneous Transition Metal Catalyzed Reactions*, Moser, W.R., and Slocum, D.W. Eds.; Am. Chem. Soc., Washington, D.C., pp. 211-220.

Key Personnel:

Robert G. Bergman, 510-642-2156, rgberg@violet.berkeley.edu

Lab Capabilities  
Applied:

Basic Research Techniques, Nuclear Magnetic Resonance Spectrometry, Mass Spectrometry, X-Ray Diffraction.



Index: 140

Category: Environmental & Regulatory (8, 14)

Laboratory: Lawrence Berkeley Laboratory

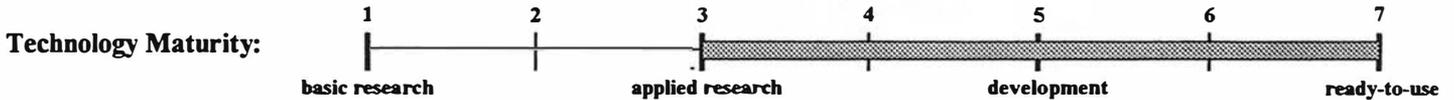
Contact: Nancy Brown, 510-486-4241, nsbrown@lbl.gov

Title: Airborne Emissions and Air Quality

**Description:** The EPA is currently considering new air-quality standards for air toxics. A key issue in assessing control costs is determining the level of control appropriate to the oil-refining industry. LBL has strong theoretical, modeling, and experimental research efforts and capabilities focused on the production and destruction of emissions at the source, and their transport and fate in the atmosphere. Computationally, LBL has the capability to apply its emission-inventory models to provide better estimates of the petroleum industry's contributions to the air-toxics inventory. These models are used to predict meteorology and photochemistry in urban areas and over larger regions. Existing codes include meteorological, photochemical, and emissions-inventory models. Since the chemistry requires the bulk of the computational effort, LBL would like to port the photochemical code to a high-performance computing environment, such as workstation clusters, in order to make it more accessible to users. Other improvements planned include descriptions of the gas-phase chemistry, addition of gas-to-particle conversion chemistry, and addition of aqueous-phase chemistry to model toxic behavior.

91-95 Funding (\$K): 500

Dates: 1978-present



Technology Transfer: Technical reports, demonstrations

**Key Documentation:** 1) Koszykowski, M.L., Armstrong, R.E., Cline, R.E., Jr., Macfarlane, J.F., Chen, J.Y., and Brown, N.J., 1993, "ACME--The Advanced Combustion Modeling Environment," in Computing at the Leading Edge: Research in the Energy Sciences, U.S. Government Printing Office 1993-785-007, pp. 61-69.  
 2) Macfarlane, J.F., Armstrong, R.C., Cline, R.E., Dai, F., Chen, J.Y., Brown, N.J., and Koszykowski, M.L., 1993, "Application of Parallel Object-Oriented Environment and Toolkit (POET) to Combustion Problems," Hawaii International Conference on System Sciences, 1993.

Key Personnel: Nancy Brown, 510-486-4241, nsbrown@lbl.gov

Lab Capabilities Applied: Numerical Modeling, Photochemistry, High Performance Computing, Meteorology, Atmospheric Science



Index: 141

Category: Development (1, 6, 10, 14, 12)

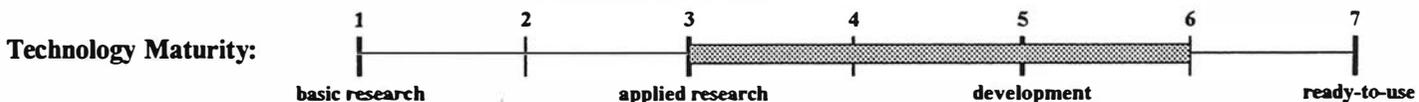
Laboratory: Lawrence Berkeley Laboratory      Contact: C. Doughty, 510-486-6453, cadoughty@lbl.gov

Title: Definition of Reservoir Heterogeneities

**Description:** An important problem facing petroleum producers is recovery of oil and gas from heterogeneous or partially depleted compartmentalized reservoirs. The success of such recovery programs depends on the successful interpolation and extrapolation of in-situ point measurements made from the surface and wells to the volumetric properties affecting the production of the resource. Often the difficulties in producing oil and gas from such environments arise from a lack of understanding of the details of the subsurface and the inability to effectively use the available hydrologic, geophysical, and rock-property data in reservoir simulators. Although individual technologies such as logging, surface and cross-well geophysics, and well-testing methods provide large amounts of data about the subsurface, there is a crucial need to properly integrate and interpret these data for use in predictive models.

LBL personnel work cooperatively with British Petroleum (BP) and the University of Oklahoma (OU), to design integrated geophysical and hydrologic investigative procedures and analysis techniques using data from the Gypsy site, a borehole test facility located in a fluvial depositional environment. Research focuses on integrating well-test interference analysis with cross-well seismic imaging and geologic information. Through the quantification of channel-sand distributions and heterogeneities, we hope to advance the techniques of reservoir-performance definition for fluvial depositional environments.

91-95 Funding (\$K): 799      Dates: 1992-1994



**Technology Transfer:** SIAM and AGU presentations, papers in "Geophysics" and "Water Resources Research," meetings with industry research partners.

**Key Documentation:** 1) Vasco, D. W., Peterson, J. E., Jr., and Majer, E. L., 1994, "Beyond Ray Tomography: Ensemble Interference and Cluster Analysis," submitted to Geophysics.  
2) Doughty, C., Long, J.C.S., Hestir, K., and Benson, S.M., 1994, Hydrologic Characterization of Heterogeneous Geologic Media with an Inverse Method Based on Iterated Function Systems, Water Resour. Res., 30 (6), 1721-1745.

**Key Personnel:** Christine Doughty, 510-486-6453, cadoughty@lbl.gov  
Don Vasco, 510-486-5206, vasco@ccs.lbl.gov  
John Peterson, 510-486-4267, barstow@ccs.lbl.gov  
Tom Daley, 510-486-7316, tom@ccs.lbl.gov  
Jane Long, 510-486-6697, jcslong@lbl.gov  
Ernie Majer, 510-486-670

**Lab Capabilities Applied:** Petroleum Engineering, Reservoir Engineering, Applied Mathematics, Numerical Simulation, Inverse Analysis, Field Testing, Subsurface Imaging



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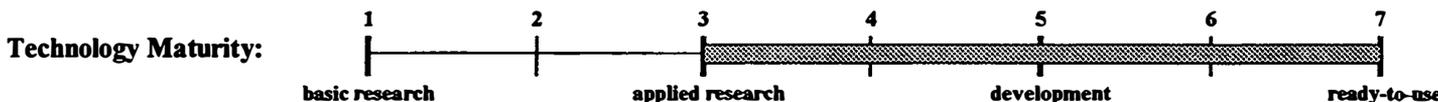
Category: Development (25, 30, 31) Exploration (14, 16, 10)

Laboratory: Lawrence Berkeley Laboratory Contact: Marcelo Lippmann, 510-486-5035  
mjlippman@lbl.gov

Title: Geothermal Reservoir Engineering

Description: The Geothermal Group has maintained an active project focused on the characterization of geothermal reservoirs since the mid-1970s. We have taken a multidisciplinary approach to developing numerical modeling and field methods for: (1) defining reservoir heterogeneities, (2) determining reservoir properties and the hydrogeological/geochemical characteristics of the system, and (3) evaluating the energy content and predicting hot water and steam production in response to production/injection activities. Teams of geologists, geochemists, geophysicists, and reservoir engineers have worked collaboratively on a number of different systems, collecting and analyzing field data and conducting basic scientific investigations related to the prediction and modeling of subsurface conditions and processes. The team, working with LBL engineers, has also developed, built, and used a wide array of new geophysical and well-testing/sampling equipment when none was commercially available. Much of the technology is directly applicable to the oil and gas industry and has led to a number of past and current projects with the Gas Research Institute and individual petroleum companies. Examples of technologies produced include: (1) the MULKOM/TOUGH family of reservoir-simulation codes for the transport of multiphase fluids, chemical species, and heat; (2) borehole instrumentation such as a high-temperature, high-pressure flow-through fluid sampler; and (3) geophysical tools such as the Automatic Seismic Processor (ASP).

91-95 Funding (\$K): 2000 Dates: 1974-present



Technology Transfer: Geothermal Resources Council Transactions, International TOUGH Users workshops, papers in technical journals, Proc. Stanford Workshops on Geothermal Reservoir Engineering, LBL reports.

Key Documentation: The LBL contact for information regarding publication lists. More than 70 papers were published in the 1991-1995 period.

Key Personnel: Karsten Pruess, 510-486-6732, k\_pruess@lbl.gov  
Marcelo Lippmann, 510-486-5035, mjlippmann@lbl.gov  
Ernest Majer, 510-486-6709, elm@ccs.lbl.gov

Lab Capabilities Applied: Petroleum Engineering, Reservoir Engineering, Mechanical Engineering, Scientific Instrumentation, Geophysical Engineering, Geochemistry, Isotope Geochemistry



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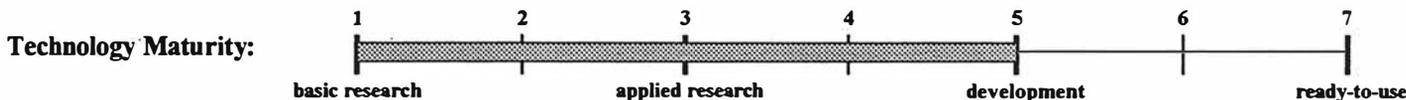
Category: Environmental & Regulatory (10, 12)

Laboratory: Lawrence Berkeley Laboratory      Contact: Donald Lucas, 510-486-7002, lucas@ux5.lbl.gov

Title: Control and Measurement of Toxic and Hazardous Compounds

Description: We are developing new diagnostic methods for the measurement of toxic or hazardous species that occur in combustion. We have used excimer-laser fragmentation fluorescence spectroscopy (ELFFS) to measure chlorinated hydrocarbons and metal species in near real time at ppb levels. In-situ Fourier transform infrared spectroscopy has also been developed to study a wide range of chemical compounds at high temperatures and in the presence of large concentrations of water and carbon dioxide. We are also studying the use of high temperatures to enhance or destroy particular chemical species. The work is focused on chlorinated hydrocarbons and the alteration of their reaction pathways using additives such as hydrocarbons. Reaction-mechanism data are being developed on the basis of laboratory-scale experiments.

91-95 Funding (\$K): 1000      Dates: 1991-present



Technology Transfer: A CRADA has been signed with ThermoMatrix, Inc., San Jose, CA

Key Documentation: Contact the key personnel for information

Key Personnel: Donald Lucas, 510-486-7002, lucas@ux5.lbl.gov  
 Kathy Koshland, 510-642-8769

Lab Capabilities Applied: Laser Spectroscopy, Instrumentation, Combustion Engineering



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Category: Deepwater Offshore (9, 16), Environmental & Regulatory (8), Production (22)

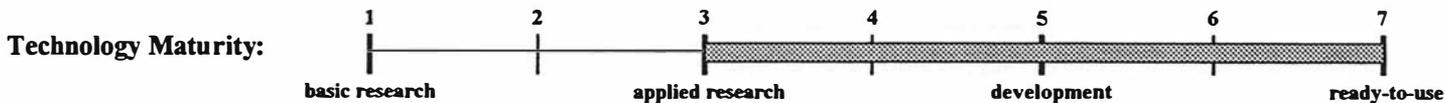
Laboratory: Lawrence Livermore National Laboratory      Contact: Rose McCallen, Ph.D (510) 422-4633 or 423-0958, mccallen1@llnl.gov

Title: Large-Eddy Simulation of Separating Turbulent Flow Using the Finite Element Method

**Description:** The goal of this research is to accurately simulate the temporally and spatially varying flow in and around three-dimensional objects where flow separation is important because of its influence on net characteristics such as drag and heat transfer. Simulation of turbulent boundary layer separation is probably the most difficult problem in computational fluid dynamics. Large-eddy simulation (LES) coupled with the finite element method (FEM) was selected because LES provides a high degree of accuracy with a minimum of empiricism and FEM accurately treats complex geometries of practical interest. This research effort focuses on the investigation of LES/FEM methods and wall modeling (i.e., approximations at walls to reduce discretization requirements) for separating flows with complex geometry - an area currently being ignored by the flow simulation community.

The resulting computational tool can be used to predict the temporally- and spatially-varying flow around offshore platforms and risers, atmospheric and land-water flow for pollutant dispersion, aerodynamic flow around ground or air vehicles, and flow in ducts or pipes. A focus area has been the modeling of flow around buildings to predict the dispersion of pollutants from stacks. We are actively seeking industrial collaborators from the environmental organizations (e.g., U.S. Environmental Protection Agency), car and trucking industry (e.g., Ford, Navistar, and the American Trucking Association Federation), oil and gas industry (e.g., PMB Engineering), and others with complex engineering flow simulation needs.

91-95 Funding (\$K): 500      Dates: 1993 - Present



**Technology Transfer:** Collaboraton with a university (UC Davis), journal publications, conference proceedings, external and internal presentations, proposals for applying research to industrial and government applications.

**Key Documentation:** McCallen, R., Gresho, P., Leone, J., and Kollmann, W., 1994, "Large-Eddy Simulation using the Finite Element Method," ASME Fluids Engineering Summer Meeting, Lake Tahoe, NV, June 19-23, 1994.  
McCallen, R., 1993, "Large-Eddy Simulation of Turbulent Flow using the Finite Element Method", Ph.D. Thesis, University of California, Davis.

**Key Personnel:** Mark Christon, (510) 422-8847, christon1@llnl.gov; Barbara Kornblum (510) 423-8172, kornblum1@llnl.gov

**Lab Capabilities Applied:** Fluid dynamics is a core competency at LLNL, with 230 publications per year, and LLNL is a world leader in FEM. We are using existing LLNL codes and developing a massively parallel capability using LLNL's parallel computers.



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**Category:** Environmental & Regulatory (9), Development (25),

**Laboratory:** Lawrence Livermore National Laboratory      **Contact:** Steven F. Ashby (510)423-2462, sfashby@llnl.gov

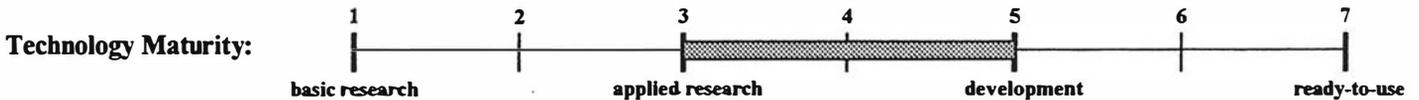
**Title:** High-Performance Computing Strategies for Subsurface Flow and Chemical Migration

**Description:** LLNL and IT are developing a sophisticated simulator that will make possible rapid, accurate, and highly resolved simulations of groundwater flow and chemical transport in three-dimensional, heterogeneous porous media. To enable such detailed simulations, we are employing state-of-the-art numerical methods and the power of massively parallel processing. For example, we are now able to solve problems with more than one million spatial zones in just a few seconds using an efficient multigrid algorithm on the CRAY T3D.

This simulator will yield a more realistic picture of chemical transport and transformation processes than is presently available. Simulations will be used to help waste management experts evaluate more reliably the efficacy of various remediation procedures, ranging from small underground storage tank cleanups to major Superfund projects. The simulator also will allow industry to manage cleanup efforts in the most cost-effective manner, saving tens of millions of dollars per year.

The same technology can be applied to oil reservoir simulation, and the underlying numerical methods (especially the parallel linear solvers) have widespread utility within the petroleum industry.

**91-95 Funding (\$K):** 2100      **Dates:** 1993 - Present



**Technology Transfer:** The computational technology will be promulgated via journal publications, conference presentatons, and technical exchanges. LLNL and IT will market the software with the help of a third party.

**Key Documentation:** S. F. Ashby and J. C. Meza, High Performance Computing Strategies for Subsurface Flow and Chemical Migration, LLNL technical report UCRL-PROP-112600, January 1993. This is the TTI proposal that resulted in the CRADA between LLNL and IT.

S. F. Ashby, R. D. Falgout, S. G. Smith, and A. F. B. Tompson, Modeling Groundwater Flow on MPPs, in Proceedings of the Scalable Parallel Libraries Conference, held at Mississippi State University, October 6-8, 1993, IEEE Computer Society Press. This paper describes the code and presents some preliminary results.

**Key Personnel:** Andrew Tompson, (510) 422-6348, afbt@llnl.gov; Robert Falgout, (510) 422-4377, rfalgout@llnl.gov; Chuck Baldwin, (510) 423-0670, baldwin5@llnl.gov; William Bost, (510) 423-2873, wjbosl@llnl.gov; Steven Smith (510) 423-8958, smith84@llnl.gov

**Lab Capabilities Applied:** Mathematical modeling and numerical methods  
 High performance computing (especially parallel processing)  
 Hydrology and geostatistics  
 Scientific visualization



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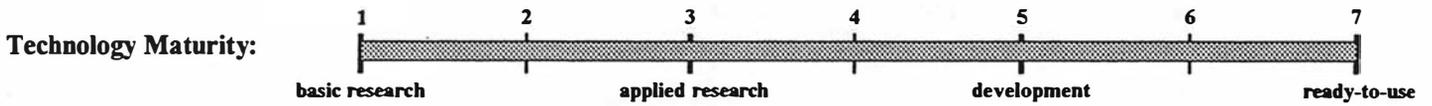
Category: Environmental & Regulatory (7, 10, 8, 14)

Laboratory: Lawrence Livermore National Laboratory      Contact: Dr. Charles K. Westbrook (510) 422-4108, charlie@physics.llnl.gov

Title: Chemical Kinetics of Refinery Toxic Emissions and the Clean Air Act

Description: This project develops chemical reaction mechanisms to describe production and emission of toxic combustion byproducts from industrial burners, especially those used by petroleum refineries using natural gas, refinery fuel gas and related feeds. Specific goals are prediction of air toxics which are subject to Clean Air Act regulations, particularly including formaldehyde, 1,3-butadiene, benzene, toluene, methanol and other products of incomplete combustion. Detailed chemical kinetic reaction mechanisms are combined with complex 3D fluid mechanics models, including effects of turbulence and radiation.

91-95 Funding (\$K): 2000      Dates: 1993 - Present



Technology Transfer: Publications in open lieterature, collaboratons with CRADA partners.

Key Documentation: "Numerical Modeling Capabilities for the Simulation of Toxic By-Products Formation in Combustion Processes", W.J. Pitz, C.K. Westbrook, A.E. Lutz, R.J. Kee, S. Senkan, and J.G. Seebold, Combustion Science and Technology 101, 1-6 (1994)

Key Personnel: William Pitz (510) 422-7730, pitz@llnl.gov

Lab Capabilities Applied: Chemical reaction modeling, CFD, computer simulations



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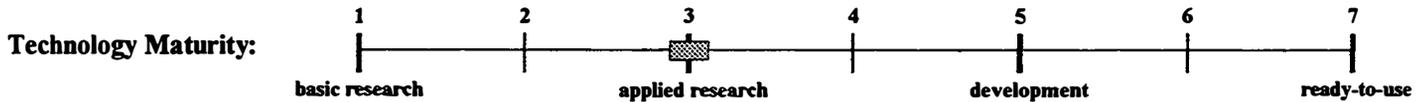
Category: Production (23, 24)

Laboratory: Lawrence Livermore National Laboratory      Contact: Carol J. Bruton (510) 423-1936, bruton1@llnl.gov

Title: Chemistry of Diatomite Dissolution and Silica Precipitation during Steam Flooding

Description: Shell is currently operating steam drive pilots in the South Belridge Diatomite. The giant diatomaceous oil fields in California hold more than 10 billion barrels of light oil-in-place. However, the extremely reactive nature of diatomite results in massive dissolution and re-precipitation during steam flooding which alter the hydrologic and mechanical properties of the reservoir. We are using laboratory experiments and geochemical modeling to determine the physical and chemical conditions that control silica redistribution and other reactions during the steam flooding of diatomites. Quantification of these controls will enable us to design steam flooding strategies that minimize adverse effects on diatomite reservoirs. Derived chemical models will be incorporated into numerical reservoir models to determine the impact of diatomite dissolution/silica re-precipitation on oil production.

91-95 Funding (\$K): 100      Dates: 1994-Present



Technology Transfer: Staff exchange, publications in open literature, oral presentations at scientific meetings

Key Documentation: Proposal submitted to Oil Recovery Technology Project, Natural Gas and Oil Technology Partnership; Monthly activity reports submitted the NTOTP Newsletter.

Key Personnel: Carrick Eggleston, (510) 422-0745, eggleston1@llnl.gov

Lab Capabilities Applied: Experimental rock fluid interaction apparatus; X-ray diffracton, scanning electron and electron microprobe, ICP-mass and other types of spectrometry, surface area analyzer. EQ3/6 geochemical modeling computer code packages.



Index: 148

Category: Exploration (1, 7)

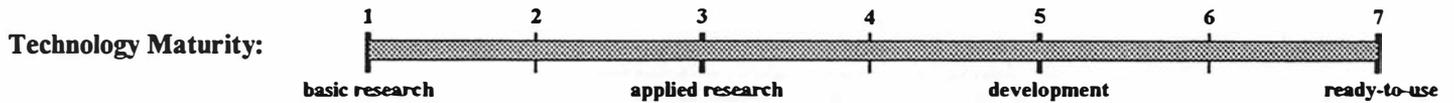
Laboratory: Lawrence Livermore National Laboratory      Contact: Alan K. Burnham (510) 422-7304, burnham1@llnl.gov

Title: Petroleum Geochemistry and Basin Modeling Project

**Description:** LLNL has been a world leader in developing and testing maturation models for basin modeling. This project has been jointly funded by the DOE (ER and FE) and up to 16 oil companies. Components of the project include measuring oil and gas generation kinetics by a variety of experimental techniques, developing algorithms and computer programs to analyze kinetic data, developing models of varying complexity for oil and gas generation and vitrinite reflectance, and developing algorithms for expulsion, compaction, and pore pressure. Accomplishments of the project include:

- (1) the commercial distribution of a kinetics analysis code (KINETICS), which is one of the most widely used codes in the world for determining petroleum generation kinetics. It was recently upgraded to include a nucleation kinetic model for proper analysis of well-preserved algal kerogens.
- (2) a demonstration that open-system kinetics predict well the timing of generation of an expelled oil phase in hydrous pyrolysis, and the disappearance of oil potential during geologic maturation.
- (3) development of one of the most widely used models for vitrinite reflectance, EASY%Ro (Sweeney et al, AAPG Bull, 74, 1559-1570 (1990)).
- (4) development of a research code, PMOD, that was used by us and several oil companies to develop compositional models of oil generation, maturation, and expulsion. We used it to model the occurrence of pore pressure and oil in the Maracaibo and Williston basins (e.g., Sweeney et al., Org Geochem, 16, 189-196 (1990); Burnham et al., Annex XII Final Report, DOE/BC/92001051, 1992), including variations in oil composition. Much of this technology is available commercially through BasinMod (from Platte River Associates), the most widely used 1D basin modeling program in the world.
- (5) use of a new isotopic labeling methods to better characterize the fundamental cracking kinetics of oil, with the goal of better defining the deadline for oil in the subsurface (Burnham et al., Energy & Fuels, 9, 190-191).
- (6) application of advanced 3D finite element codes to model faulting.

91-95 Funding (\$K): 1800      Dates: 1991-present



**Technology Transfer:** Annual briefings to industrial sponsors, reports and peer-reviewed journal publications, talks at professional meetings, licensing of software, technical collaboration

**Key Documentation:** Braun, R.L., Burnham, A.K., PMOD: a flexible model of oil and gas generation, cracking, and expulsion, Advances in Organic Geochemistry, 1991, Org. Geochem. 19, pp. 161-172, 1992. Braun, R.L., Burnham, A.K., Reynolds, J.G., Clarkson, J.E., Pyrolysis Kinetics for Lacustrine and Marine Source Rocks by Programmed Micropyrolysis, Energy & Fuels, 5, pp. 192-204, 1991.

**Key Personnel:** Alan K. Burnham, (510)422-7304, burnham1@llnl.gov; Robert L. Braun, (510)422-6650, braun2@llnl.gov; Jerry J. Sweeney, (510)422-4917, sweeney3@llnl.gov; John G. Reynolds, (510)422-6028, reynolds3@llnl.gov

**Lab Capabilities Applied:** Pyrolysis, Chemical analysis (e.g., GC-MS-MS), Kinetic analysis, Scientific computing, Modeling



Index: 149

Category: Environmental & Regulatory (7), Oil Processing & Refining (1)

Laboratory: Lawrence Livermore National Laboratory      Contact: Lucy M. Hair (510) 423-7823, hair1@llnl.gov

Title: Increased Efficiency and Pollution Reduction in Engine Systems

**Description:** The unifying theme for these three industrial collaborations is their application to increased efficiency and reduced pollutant emissions in engine systems.

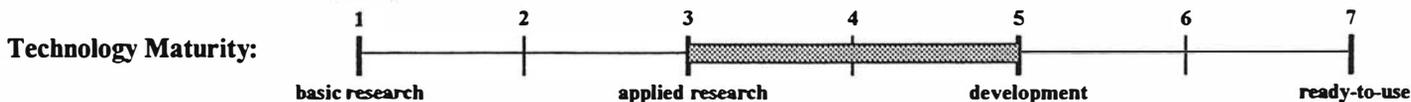
The USCAR/LEP project involves the development of catalysts and catalytic converter systems, based on LLNL aerogel technology, for the reduction of nitrogen oxide emissions from lean burn or diesel engines. Suitable NOx reduction catalysts are the enabling technology for lean-burn engines in order to meet new Clean Air Act standards, effective in 2004 nationwide and 1996 in California. Implementation of the lean-burn engines is expected to result in a significant decrease in fuel usage (increase of 4 mpg), skilled jobs growth, lessened dependence on foreign oil imports and addition of new R&D tools to the catalyst industry.

For Catalytica, Inc., new aerogel catalyst supports are being developed specifically to withstand the high temperatures experienced in a gas-turbine engine. Here, the concept is to aid combustion of the fuel catalytically to maintain gas temperatures no higher than 1300\_C, resulting in little to no nitrogen oxide species. As for the USCAR/LEP project, this work is driven by increasingly stringent environmental regulations.

The work with Ethyl Corp. involves characterization and interpretation of the pathways of MMT, a Mn-containing gasoline additive that reduces knock in gasoline engines. This is a controversial additive; it may provide energy savings by a significant reduction in quantities of crude oil used in refining processes. In addition, it is effective at far lower concentrations (1/32 g per gallon as compared to several wt%) than current oxygenated additives mandated by law, which have the undesirable side effect of increasing nitrogen oxide emissions. However, there is research suggesting that MMT may cause deterioration in the long-term operation of the catalytic converter, and concerns about the possible health effects of manganese emissions from the tail-pipe.

The industries involved contribute expertise and research on their technologies. USCAR/LEP provides needed background on the systems and tests catalysts under realistic conditions. Catalytica, Inc. has a similar role but also characterizes and impregnates the catalyst supports with their own catalytic agents. Ethyl Corp. is working hand in hand with LLNL, providing information, helping to develop experiments and performing engineering tests on MMT.

91-95 Funding (\$K): 3000      Dates: 1993 - 1995



Technology Transfer: Quarterly technical reviews with vugraph documentation.

Key Documentation: LLNL CRADA TC-315-92C  
 LLNL CRADA TSB-841-94

Key Personnel: Paul Coronado (510) 422-0155, coronado2@llnl.gov; Wigbert J. Siekhaus (510) 422-6884, siekhaus1@llnl.gov; Carlos Colmenares (510) 422-6352, colmenares1@llnl.gov

Lab Capabilities Applied: Process of developing catalysts exploits LLNL synthesis methodology developed for weapons app., high-level characterization tools - SLAC, STM & HRTEM & molecular/quantum chemistry modeling methods for understanding catalysis/gas-surface interactions



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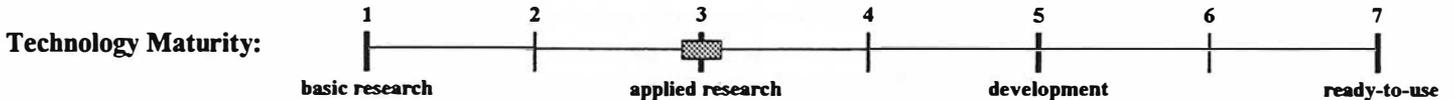
Category: Environmental & Regulatory (15)

Laboratory: Lawrence Livermore National Laboratory      Contact: Howard L. Hall (510) 422-7446, HLHall@LLNL.gov

Title: Naturally Occurring Radioactive Materials (NORM) Analysis for Oil and Gas Operations

**Description:** Naturally occurring radium isotopes can be both transported and concentrated by routine fossil fuel production activities. This has lately become of increasing interest to regulatory agencies, and places the traditionally non-nuclear oil and gas industry in the position of dealing with issues regarding the protection of the public from radiation. Radium is of special concern since it may be water-soluble in the subsurface environment, yet coprecipitate with calcium, barium, and magnesium during process steps. This study focuses on determining the capabilities of existing methods and vendors to quantify accurately radium concentrations of regulatory concern, and validating the measured data upon which regulatory decisions will be based. The study is divided into five tasks: 1) Literature review of analytical methods, 2) Methods selection and review, 3) Sampling and analysis plan for subsequent round robin, 4) Interlaboratory round robin comparison of several vendor laboratories, and 5) Report preparation with manuscript suitable for publication in the reviewed literature. The Radiation Analytical Sciences program (RAS) has been performing high-sensitivity measurements of radioactive materials in environmental samples for over twenty years. RAS not only analyzes over 20,000 environmental samples per year, but has also developed (within the LLNL Isotope Sciences Division) world-class research and development skills and personnel. The only role of the industrial participants is funding and participatory management oversight. The outcome of this project will be the development of one or more reliable methods of analysis for low concentrations of radium isotopes, and validation of the capabilities of several commercial laboratories to utilize them in the analysis of environmental samples.

91-95 Funding (\$K): 600      Dates: 1994 - Present



Technology Transfer: publications in open literature, publications in sponsor reports.

Key Documentation: Naturally Occurring Radioactive Material (NORM) Analysis for Oil and Gas Operations - Task 1 Summary (to be published by A I/GRI and as a UCRL, in progress).

Key Personnel: Steve Kreek (510) 423-2594, kreek1@llnl.gov; Bryan Bandong (510) 423-0855, bandong1@llnl.gov; Everett Guthrie (510) 423-3666, guthrie1@llnl.gov

Lab Capabilities Applied: Quantitative measurement capability for radionuclides



Index: 151

**Category:** Gas Storage (2), Environmental & Regulatory (5)

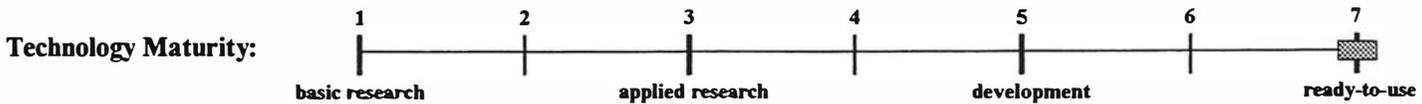
**Laboratory:** Lawrence Livermore National Laboratory      **Contact:** Mark Accatino (510) 422-7196, accatino1@LLNL.GOV

**Title:** Quantitative Gas Leak Detection / Pressure Safety Training

**Description:** The LLNL High Pressure Laboratory has the capability to pressurize large and small test vessels or systems inside of a vacuum chamber for leak-checking requirements which demand a quantitative leak-rate measurement. A calibrated Helium Mass Spectrometer Leak Detector is used to measure the quantitative helium leak rate of the test object, for comparison to standard calibrated leak rates. This capability was developed for several LLNL and DOE programs which required measured leak rates for components / systems to a very high accuracy and resolution, as opposed to the traditional qualitative leak-checking techniques using a probe. This technology might be of interest to the natural gas and/or petroleum industry as a means for ensuring that various pressure-system components are leak-tight to a specified traceable standard. The deliverable provided by this technology is a reliable, NIST-traceable and documented method of supplying a quantitative leak rate for pressure vessels and system components.

DOE has selected the LLNL Pressure Safety Training Program for use at all of its facilities. This DOE Pressure Safety Program which was established in 1989 and which provides training for DOE and DOE contractors, can also be provided to private industry on a Work-for-Others contract basis. The training program consists of four courses: one for the orientation of all employees; the second and third for pressure assemblers, operators and users of intermediate and high pressure equipment; and the fourth for Engineers, Designers, Safety Personnel and those individuals who are responsible for documentation of pressure vessels and systems. The DOE Pressure Training Manual, developed at LLNL, is used as a guide to help establish and provide a safety program which can be detailed specifically to the individual contractor requirements. To date, over 148 classes have been presented to over 8000 attendees. A week-long hands-on training program can also be provided, with personalized training for individuals who have some shop experience but who need more familiarity with high-pressure hardware, installation, servicing and pressure-testing. This training could benefit the natural gas and petroleum industries in their pursuit of improved safety performance related to the processing and refining of oil, and also to gas processing, storage and production.

**91-95 Funding (\$K):** 1100      **Dates:** 1991 - Present



**Technology Transfer:** Brochures which describe the facility, home page on mosaic, directory of Federal Laboratory Resources, and the DOE Guide to Research Facilities.

**Key Documentation:** Ronald R. Sandberg, Safety Analysis Report for the Model UC-609 B(U) DOE Shipping Package LLNL, May 1993, UCRL-ID-111494 , Section 8.1  
DOE Pressure Safety Draft Manual, December 1993

**Key Personnel:** Chuck Borzileri, (510) 422-6076, borzileri1@llnl.gov

**Lab Capabilities Applied:** LLNL High Pressure Laboratory Facility test cells, pressure-related equipment and LLNL High Pressure Laboratory / Hazards Control Department manpower.



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Category: Development (23)

Laboratory: Lawrence Livermore National Laboratory

Contact: Thomas J. Wolery, (510) 422-5789, wolery1@llnl.gov

Title: EQ3/6, Software for Modeling Rock/Water Interactions

**Description:** Interactions in rock/water systems involving radionuclides, heavy metals, organic anions, and the common components of groundwaters and brines lie at the heart of many problems involved in nuclear waste disposal, waste stream fluid disposal, scaling and fouling of production and injection wells, environmental assessment, and environmental remediation. Our approach is to develop geochemical modeling tools (EQ3/6 software) to provide analysis and simulation of the complex, invariably linked, fundamental processes involved. This supports analysis and prediction of processes such as mineral dissolution and precipitation, oxidation-reduction, degassing, and ion exchange.

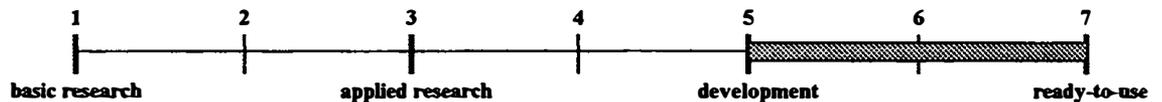
This project is currently mainly focused on problems related to the disposal of high-level nuclear waste in a potential repository at Yucca Mountain, Nevada. The scope of application of EQ3/6 on this project is very broad (site characterization, waste form dissolution, effects of heating on the rock/water system, and the geochemical behavior of leached waste components). Many of the capabilities developed for nuclear waste disposal applications are readily applicable to other problems in the petroleum industry (e.g., mineral precipitation in the subsurface due to fluid mixing or changes in temperature and pressure). For example, EQ3/6 has recently been used in a study of a process for the disposal of coalbed brines.

Unix-based and PC versions of EQ3/6 are licensed by the LLNL Industrial Partnerships and Commercialization Office. CRADAs may be arranged to meet special needs by industry.

91-95 Funding (\$K): 1500

Dates: 1984-present

Technology Maturity:



**Technology Transfer:** User manuals, Occasional short courses, Seminars, Review papers, Applications papers, INTERNET Home pages, Licensing (contact: Cookie West, LLNL Industrial Partnerships and Commercialization Office, 510-423-8030, west3@llnl.gov)

**Key Documentation:** 1) Wolery, T. J., Jackson, K. J., Bourcier, W.L., Bruton, C.J., Viani, B.E., Knauss, K.G., and Delany, J.M., "The EQ3/6 software package for geochemical modeling: Current Status," In Melchior, D.C., and Bassett, R.L., eds., Chemical Modeling in Aqueous Systems II, American Chemical Society Symposium Series, 416, American Chemical Society, Washington, DC, p. 104-116  
2) Brandt, H., Bourcier, W.L., and Jackson, K.J., "Integrated Process for Coalbed Brine Disposal," International Petroleum Environmental Conference, Houston, TX, March 2-4, 1994.

**Key Personnel:** James W. (Jim) Johnson, 510-423-7352, jwjohnson@llnl.gov  
Kenneth J. (Ken) Jackson, 510-422-6053, jackson8@llnl.gov

**Lab Capabilities Applied:** Geochemistry, Geochemical Modeling, Nuclear Waste Disposal, Waste Brine Disposal, Environmental Assessment, Environmental Remediation



Index: 153

Category: Oil Processing & Refining (2)

Laboratory: Lawrence Livermore National Laboratory

Contact: Jeffery Richardson (510) 423-5187, richardson6@llnl.gov

Title: Production Of Hydrogen From Municipal Solid Waste

**Description:** The overall goal of this project is to assess the economics and demonstrate the technical feasibility of converting municipal solid waste (MSW), and potentially other biomass resources, to hydrogen through high temperature gasification. Approximately 200 million tons of MSW are produced annually in the United States, and the vast majority is deposited in landfills. Environmental concern over air pollution and the ash by-product has limited incineration as a disposal method and concern over water pollution makes siting of future landfills difficult and expensive. MSW is predominantly composed of carbon, hydrogen and oxygen, and as such is a potential energy source. Thus, development of the technology necessary for gasification of MSW to hydrogen has the potential to address a number of economic, environmental, societal and resource issues. The project has six major focused objectives: 1) laboratory demonstration of hydrothermal processing of increasingly more realistic representations of MSW; 2) laboratory demonstration of slurry pumping and gasification of hydrothermally processed MSW components; 3) evaluation of the economics of conversion of MSW to hydrogen, including determination of threshold tipping fees, processing and ash disposal costs, solids content and slurry heating value, and possible addition of supplemental fuels to increase the overall slurry heating value beyond that obtainable using solely MSW; 4) pilot scale process modeling and demonstration of hydrothermal processing of MSW and MSW components; 5) pilot scale gasification of MSW components; 6) technical and economic evaluation of potential end-use commercial insertions of hydrogen into the economy (e.g., blending with natural gas, premium fuel for fuel cells, feedstock for chemicals production or oil upgrading). Initial work will focus on the use of a Texaco slurry fed gasifier.

91-95 Funding (\$K): 850      Dates: 1995 - Present



**Technology Transfer:** Publications in open literature, presentations at national meetings, presentations at program reviews, direct contact with interested industrial partners.

**Key Documentation:** Pasternak et al, MSW to Hydrogen, Lawrence Livermore National Laboratory, Livermore Calif., UCRL-JC-116421 (1994)  
C.B. Thorsness, Process Modeling of Hydrogen Production from Municipal Solid Waste, Lawrence Livermore National Laboratory, Livermore Calif., UCRL-ID-119231 (1994)

**Key Personnel:** H. Wallman (510) 423-1522, hwallman@llnl.gov, C.B. Thorsness (510) 422-8124, thorsness1@llnl.gov

**Lab Capabilities Applied:** Coal gasification experience, hydrous pyrolysis experience, related fossil fuel processing experience.



**Index:** 154

**Category:** Development (8, 9)

**Laboratory:** Lawrence Livermore National Laboratory      **Contact:** Stephen C. Blair, (510) 422-6467, blair@s55.es.llnl.gov

**Title:** Analysis of Wellbore Stability, Seal Integrity, and Rock Fracture in the Subsurface Using Statistical Models.

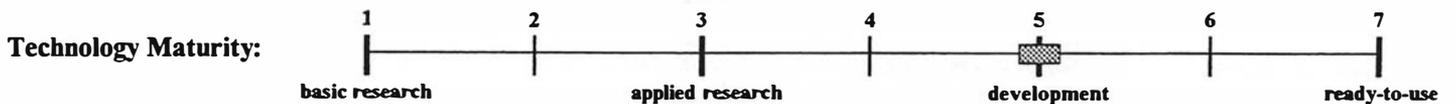
**Description:** Researchers at LLNL have developed a statistical model for rock fracture in compression that simulates the progressive fracture of clastic rocks common in the oil field. This model provides for incorporation of local heterogeneity in composition and structure inherent in the rock formation. The model could be applied to analyze well bores, seals and hydrofracturing operations variety of subsurface environments. LLNL also has an experienced geoscience staff and a high-performance computing capability, both of which are needed to supplement and balance the experts provided by industry.

Industry involvement includes collaborators who will provide expertise in well bore stability or seal stability problems in a variety of environments; funding for visiting scientists from industry to work with LLNL staff on fracture simulation; and in-kind support including case histories of well bore or seal failures!

Well bore stability problems are frequently encountered in the exploration and development of oil fields. Collapse of a well bore because of sanding or well-bore breakout can dramatically increase drilling and completion costs and may cause a well to be abandoned. Instability of a well bore is often due to progressive or time-dependent fracture of the rock formation and is not easily simulated using the numerical models that are currently available.

Objectives associated with well bore stability studies are to improve our understanding of the rock fracture processes that cause well-bore instability and to develop (1) a computational tool that will provide improved estimates of the minimum drilling fluid density required to maintain stability of high-angle or horizontal wells and (2) the ability to anticipate and avoid excessive sand production from petroleum wells.

**91-95 Funding (\$K):** 600      **Dates:** 1993 - Present



**Technology Transfer:** Publications in the open literature, staff exchanges, release of computer code.

**Key Documentation:** Blair, S.C. "Analysis of Compressive Fracture in Rock Using Statistical Techniques", Ph.D. Thesis, U.C. Berkeley, 1994.  
 Daveler, S.A. and S.C. Blair, "Fracrock User's Manual" UCRL MA119099, LLNL, 1994.

**Key Personnel:** Stephanie Daveler, (510) 423-2249, daveler2@llnl.gov

**Lab Capabilities Applied:** Fracture Mechanics of Rock, Statistical Modeling, Rock Physics



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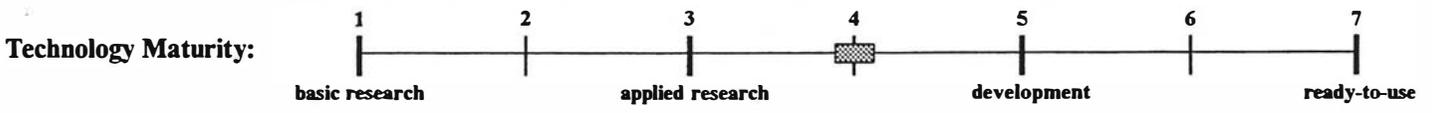
Category: Production (3), Oil Processing & Refining (12)

Laboratory: Lawrence Livermore National Laboratory Contact: Robert S. Glass (510) 423-7140, glass3@llnl.gov

Title: Corrosion Sensors

Description: The economic costs of corrosion in the U. S. alone is estimated to be between \$8 billion and \$126 billion per year. A realistic figure of \$30 billion per year has been suggested as the savings if early detection of corrosion and appropriate corrosion prevention measures were taken. The development of sensors which could provide information related to environmental compatibility and provide an early warning of potential catastrophic failure of materials and structures would find enormous application. Such applications include monitoring the structural integrity of bridges, aircraft, ground transportation, pipelines, boilers, etc. The rates and modes of corrosion attack on a given material are related to environmental conditions, such as the pH and the concentration of chloride ion. Microbiologically-influenced corrosion may also contribute, in some cases even predominate. Since corrosion is an electrochemical process, tied to environmental factors, corrosion sensors based upon electrochemical measurement methods have considerable merit. We are developing electrochemical microsensors consisting of an array of electrodes (sensors) which can simultaneously monitor corrosion parameters of chosen structural materials (e.g., corrosion potential and rate) and the particular environmental (chemical) factors which accelerate corrosion. The sensors are fabricated in the LLNL Micro Technology Center using state-of-the-art microfabrication methods. Our methods are appropriate for mass fabrication of sensors. The immediate current application involves the development of microsensors for monitoring corrosion in aging military aircraft.

91-95 Funding (\$K): 200 Dates: 1994 - Present



Technology Transfer: Presentations to companies through Technology Transfer Office, Laboratory Capabilities document

Key Documentation: R.S. Glass, W.L. Clarke, Jr., and D.R. Ciarlo, "Corrosion Sensor, " U.S. Patent No. 5,306,414 (April 1994)

Key Personnel: Dino R. Ciarlo (510) 422-8872, ciarlol@llnl.gov; Daniel M. Makowiecki (510) 422-5794, no e-mail

Lab Capabilities Applied: Microfabrication; thin film deposition; sensors; electrochemical measurements



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Category: Environmental & Regulatory (2, 10)

Laboratory: Lawrence Livermore National Laboratory      Contact: Robert S. Glass (510) 423-7140, glass3@llnl.gov

Title: Portable Electrochemical Sensor for Environmental Monitoring and Process Control

**Description:** The increasing emphasis on environmental issues, waste reduction, and improved efficiency for industrial processes has mandated the development of new chemical sensors for field or in-plant use. Specifically, sensors are needed to gauge the effectiveness of remediation efforts for sites which have become contaminated, to effect waste minimization, and to detect the presence of toxic, hazardous, or otherwise regulated chemicals in waste effluents, drinking water, and other environmental systems. In this regard, electrochemical sensors are particularly useful for the measurement of inorganic species in aqueous systems. However, the commercial instrumentation currently available has been designed primarily for laboratory research or analysis. Most instruments are bulky, or in other ways are not easily adaptable for field work. Portable systems are needed for field use where real time analyses are necessary.

In our work, we have developed a complete, portable electrochemical system capable of operating in-the-field for "on command" measurement of the analyte(s) of interest. The system is very compact, weighing only 0.76 kg. It comes equipped with an optional battery pack for stand-alone operation. The multichannel device is capable of monitoring up to eight elements of a sensor electrode array. The disposable sensor array could be configured to monitor for species such as Cl<sup>-</sup>, Pb<sup>2+</sup>, Cd<sup>2+</sup>, Cu<sup>2+</sup>, CN<sup>-</sup>, Ag<sup>+</sup>, pH, etc. In addition to stand-alone operation, the system can be interfaced with a notebook computer, or it can communicate with a remotely placed host computer over an RS232 serial line. A distributed monitoring system, with units placed at various sites throughout a manufacturing plant, or environmental system, is one potential application.

91-95 Funding (\$K): 1000      Dates: 1989 - 1993

Technology Maturity:      1                      2                      3                      4                      5                      6                      7

   basic research                      applied research                      development                      ready-to-use

Technology Transfer: Publications in open literature, presentations at national conferences, widely disseminated laboratory technology capability materials, in-house presentations to companies through technology transfer.

Key Documentation: R. S. Glass, S. P. Perone, and D. R. Ciarlo, "Application of Information Theory to Electroanalytical Measurements Using a Disposable Multielement Microelectrode Array Sensor," Anal. Chem., 62 (18), 1914 (1990).  
R. S. Glass and D. R. Ciarlo, "Electrochemical Sensor/Detector System and Method," U. S. Patent No. 5, 296, 125 (March, 1994).

Key Personnel: G. Bryan Balazs (510) 423-5403, balazs1@llnl.gov; Dino R. Ciarlo (510) 422-8872, ciarlo1@llnl.gov

Lab Capabilities Applied: Microfabrication, thin film deposition, sensors, electrochemical measurements.



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Category: Environmental & Regulatory (12, 6, 9, 2)

Laboratory: Lawrence Livermore National Laboratory      Contact: Richard B. Knapp (510) 423-3328, knapp@llnl.gov

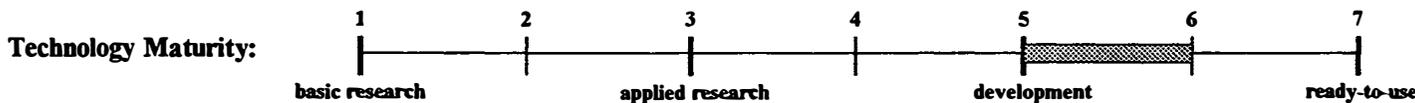
Title: In Situ Microbial Filters

**Description:** The in situ microbial filter concept is to inject TCE-degrading microbes into the subsurface without nutrients. Naturally occurring microbes are grown in surface bioreactors, separated from their growth medium, resuspended in groundwater from the site, and then injected into the subsurface. *Methylosinus trichosporium* OB3b, a methanotroph is currently employed. This process does not use nutrients in the subsurface and is called a resting-state approach; it avoids many of the problems associated with nutrient injection. The use of resting-state microbes means that filter performance will diminish with time, requiring replenishment of the filter by reinoculation; reinoculation frequency controls economic viability.

A key element of the concept is the subsurface filter implementation. A portion of the injected microbes attaches to the soil and forms a fixed-bed biofilter. The actual geometry of the biofilter depends on the injection pattern, but in general a thin region is formed which extends across the expanding contaminant plume. The attached microbes degrade TCE to harmless compounds as it is transported through the biofilter region by the flowing groundwater. An advantage of the resting-state biofilter approach is that it can be engineered so that contaminated groundwater will enter the biofilter but exit clean.

The microbial filter concept can be generalized, even though the current focus is on intercepting chlorinated ethene plumes. It is possible to inoculate and eliminate contaminant source regions and to bioremediate many classes of contaminants, especially when suites of microbial species are considered.

91-95 Funding (\$K): 8280      Dates: 1990 - Present



**Technology Transfer:** Multiple papers in the open literature and internal LLNL reports, several presentations at national meetings for professional societies and environmental theme conferences, cooperative agreement established and proposal submitted with industry partner

**Key Documentation:** Taylor, R. T., A. G. Duba, W. B. Durham, M. L. Hanna, K. J. Jackson, M. C. Jovanovich, R. B. Knapp, J. P. Knezovich, N. N. Shah, D. R. Shonnard, and A. M. Wijesinghe (1993) In situ bioremediation of trichloroethylene-contaminated water by a resting cell methanotrophic microbial filter. *Hydrological Sciences J.* 38, pp. 323-342.  
 Wijesinghe, A. M., R. B. Knapp, R. T. Taylor, and L. M. Carman (1992) Preliminary Feasibility and Cost Analysis of the In Situ Microbial Filter Concept. UCRL-ID-111021, Lawrence Livermore National Laboratory, Livermore, CA 47 pp

**Key Personnel:** Alfred G. Duba, 510-422-7306, alduba@llnl.gov  
 Kenneth J. Jackson, 510-422-6053, ken@s46.es.llnl.gov  
 Marina C. Jovanovich, 510-422-2144, jovanovich1@llnl.gov  
 Richard B. Knapp, 510-423-3328, knapprb@llnl.gov  
 Robert T. Taylor, 510-422-5652

**Lab Capabilities Applied:** Unique hydrologic code for modeling multiphase flow and microbial degradation/contaminant transport, environmental microbiology lab, large-scale bioreactor facility, environmental analytical chemistry lab, experimental test bed design and construction.



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Category: DEVELOPMENT (10)

Laboratory: Lawrence Livermore National Laboratory      Contact: Michael Wilt (510) 422-3152, Wilt2@llnl.gov

Title: Electromagnetic methods for reservoir characterization and process monitoring

**Description:** This research is to develop and apply electromagnetic geophysical methods to oil reservoir characterization. We are using electromagnetic (EM) methods to extend the borehole resistivity logs into the region between wells to increase the understanding of reservoir structure and formation properties. We are also applying these techniques to monitor Enhanced Oil Recovery (EOR) operations. We provide an image of a steam front as it propagates from injection to production wells through oil-bearing strata. Together with collaborators we have designed and constructed a field system and have carried successful field surveys at the South Belridge and Lost Hills#3 oil fields in central California, the Devine test facility in Texas and the U.C Richmond field site in California. In 1993 we began multi-year cooperative research agreement (CRADA) work with Schlumberger-Doll Research on development of a commercial crosshole EM system. We are also working closely with Mobil and Shell on multi-year EOR monitoring projects at Lost Hills Unit #3 and the South Belridge site. Since 1990 we have worked with 8 to 12 energy and service companies who have joined a research consortium through LBL/LLNL.

91-95 Funding (\$K): 5500      Dates: 1990 - Present

1	2	3	4	5	6	7
basic research	applied research		development		ready-to-use	

**Technology Transfer:** Publications - more than 10 within the past several years, CRADA with Schlumberger-Doll Research (SDR) and staff exchanges with SDR, collaborative work with Mobil, Shell, Texaco and others, contribution to LBL/LLNL research consortium.

**Key Documentation:** Multifrequency Crossborehole Electromagnetic(EM) Imaging System  
 CRADA 361-2 between LLNL and Schlumberger-Doll Research.  
 M. Wilt, K. Lee, H.F. Morrison, A. Becker, H.W. Tseng, C.T. Verdin, D. Alumbaugh, "Crosshole electromagnetic tomography: A new technology for oil field characterization", The Leading Edge, p. 173, March (1995).

**Key Personnel:** Clifford Schenkel (510) 422-1641, schenkell@llnl.gov; John Carbino (510) 422-1342, carbinol@llnl.gov; Michael Buettner (510) 422-7888, buttner1@llnl.gov

**Lab Capabilities Applied:** geophysical and remote sensing expertise and tools



Index: 159

Category: Environmental & Regulatory (7)

Laboratory: Lawrence Livermore National Laboratory      Contact: Dean Lee (510) 422-8867, lee15@llnl.gov

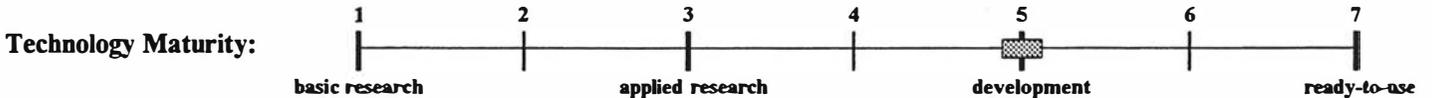
Title: Advanced Infrared Imaging Sensors

**Description:** LIFTIRS Project. The LIFTIRS Project is developing an imaging fourier transform infrared spectrometer for the purposed of remote detection, identification and quantification of chemical processes. This instrument is a multispectral imaging system in the infrared region. The instrument is being developed to look for particulates and gases in the atmosphere and other phenomena that results in temperature differences. This type of sensor can be used to detect the type of pollutants being generated by factories and other systems that generate gases. Multispectral imaging systems can also be used to detect subtle changes in plant life. The health of the forests can be monitored effectively by comparing images of the forest at various wavelengths at different times of the year. Drought and disease can be detected.

LIDAR Project. The MARL (Mobile Atmospheric Research Lab) has been working on developing an active instrument to detect and study particulates in the atmosphere. This instrument is to detect and study particulates in the atmosphere. This instrument uses the back scattered light from the laser to measure the amount of particulates in the air. This type of instrument can be used to measure the pollution levels for different parts of the forests.

Infrared and visible camera systems. A variety of specialized imaging systems have been developed and field by LLNL. Infrared cameras are useful in wide area surveillance for forest fires and other events. Visible cameras can be used to do long term surveillance of selected areas in the forests.

91-95 Funding (\$K): 4180      Dates: 1989 - Present



Technology Transfer: Publications in open lieterature and collaborative experiments.

Key Documentation: Charles L. Bennett, Michael Carter, David Fields, John Hernandez, "Imaging Fourier Transform Spectrometer", SPIE Conference Article, Vol. 1937 of SPIE Proceedings 14-15 April 1993 Orlando Florida.  
Charles L. Bennett, "Imaging Fourier Transform Spectrometer", LDRD 1995 Proposal.

Key Personnel: Dave Fields (510) 423-4945, fields2@llnl.gov; Tom Biesiada (510) 422-9258, biesiada1@llnl.gov

Lab Capabilities Applied: Optical design, image processing, mechanical design, electrical design, systems design.



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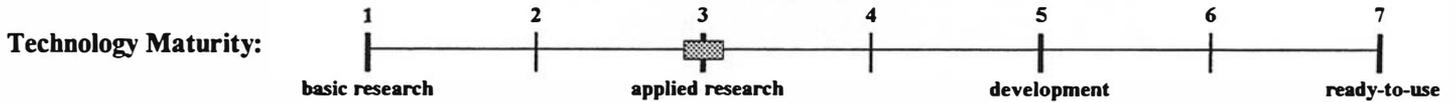
Category: Drilling & Completion (5)

Laboratory: Lawrence Livermore National Laboratory      Contact: S. Christian Simonson (510) 422-6569, c/o jensen@llnl.gov

Title: Design, Testing, and Improved Manufacturing of Well Perforation Devices

**Description:** Advanced shaped charge technology will be adapted to the design of a well bore perforator with improved performance. By the use of improved shaped charge designs, the characteristics of the perforating jet will be better matched to the desired hole configuration, and undesired side effects such as collateral damage will be reduced. The design approach includes numerical simulation techniques based on current material models and coupled with extensively diagnosed experiments. The emphasis in this program will be on achieving improved well perforation performance while conforming to petroleum industry manufacturing practices. The potential gain in performance represents a major opportunity for important benefits to oil and gas well productivity.

91-95 Funding (\$K): 200      Dates: 1993 - Present



Technology Transfer: Protected WSA information reports and information meetings.

Key Documentation: Weapons Support Agreement TC-463-93.

Key Personnel: Dennis W. Baum (510) 423-2236, baum1@llnl.gov

Lab Capabilities Applied: Uses complex continuum mechanics simulations running on large-scale computers, coupled with extensive experimental radiographic, optical, and electronic diagnostics of explosive charge performance.



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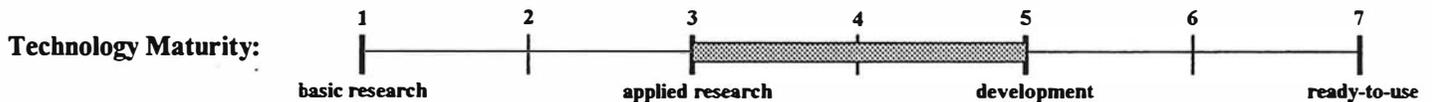
**Category:** Deepwater Offshore (16), Oil Processing & Refining (12)

**Laboratory:** Lawrence Livermore National Laboratory      **Contact:** Diane J. Chinn (510) 423-5134, chinn3@llnl.gov

**Title:** Integrity Testing of Offshore Structures

**Description:** Monitoring critical connections on an existing offshore structure can help extend its useful lifetime. This research, guided by a group of owners, fabricators and inspectors of offshore drilling structures, performed experimental and analytical work on a hybrid inspection/monitoring method for welded steel connections. In addition to steel offshore structural joints, the method developed, long-distance ultrasonic testing, can be applied to embedded pipelines and other steel infrastructure components.

**91-95 Funding (\$K):** 1000      **Dates:** 1988 - 1993



**Technology Transfer:** Publications in open literature, supervisory user's group, university contact.

**Key Documentation:** Chinn, D. J., Revealing Hidden Defects: A Hybrid Evaluation Strategy for Steel Structures, Dissertation: Delft University of Technology, ISBN 90-6275-892-4, 1993.  
Chinn, D. J., Dieterman, H. A. "Defect imaging using long-distance ultrasonic testing." In: Review of Progress in Quantitative Nondestructive Evaluation, 1991.

**Key Personnel:** Graham Thomas (510) 422-7325, thomas26@llnl.gov

**Lab Capabilities Applied:** Research performed by LLNL employee as part of Ph.D. dissertation work.



Index: 162

Category: Oil Processing &amp; Refining (22, 23, 24, 25, 27)

Laboratory: Lawrence Livermore National Laboratory

Contact: Dr. Charles K. Westbrook (510) 422-4108, charlie@physics.llnl.gov

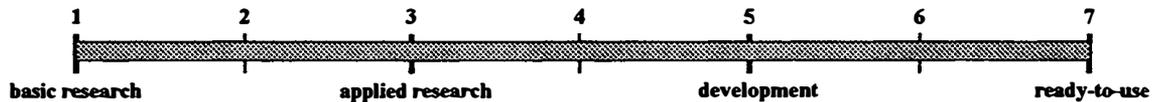
Title: Computational Modeling of Hydrocarbon Chemical Kinetics

**Description:** This project involves development, testing and application to practical systems, of very detailed chemical kinetic models for hydrocarbon pyrolysis and oxidation. Fuels as complex as octane and toluene can be modeled using chemical mechanisms with hundreds of distinct chemical species and thousands of elementary chemical reactions. The resulting models are then used to predict rates of pyrolysis, oxidation and production of intermediate and final products. Applications already demonstrated include prediction of octane quality for arbitrary hydrocarbon fuel mixtures, performance and mechanism of activity for oxygenated antiknock additives, formation of toxic intermediate species, emissions of oxides of nitrogen, performance of synthetic fuels including alcohols and other oxygenates, oxidative coupling of methane to liquid fuels, ignition properties of fuels, fuel safety, and oil stability over geological timescales.

91-95 Funding (\$K): 1000

Dates: 1991 - Present

Technology Maturity:



Technology Transfer: Publications in open literature, collaborations with CRADA partners

**Key Documentation:** C.K. Westbrook, W. J. Pitz, and W.R. Leppard, "Autoignition Chemistry of Paraffinic Fuels and Pro-Knock and Anti-Knock Additives," Society of Automotive Engineers paper SAE-912314 (1991)  
R.G. Mallinson, R.L. Braun, C.K. Westbrook, A.K. Burnham, I&EC Research 31, 37-45 (1992)

Key Personnel: William Pitz (510) 422-7730, pitz@llnl.gov

**Lab Capabilities Applied:** Computational modeling, combustion chemistry, CFD



**Index:** 163

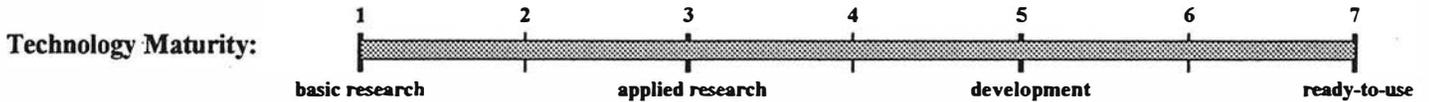
**Category:** Development (8, 19, 23), Production (3, 4, 6, 17, 19), Oil Processing & Refining (1, 7, 25)

**Laboratory:** Lawrence Livermore National Laboratory      **Contact:** Dr. James Belak (510) 422-6061, belak1@llnl.gov

**Title:** Atomic Scale Electrochemical Modeling

**Description:** This project involves molecular dynamics (MD) modeling of complex fluids and fluid-surface interactions in which the interactions are dominated by long-ranged Coulomb forces. Applications include: the structure of complex electrolytic fluids, including water, ions, and floppy molecules (e.g., surfactants) near solid surfaces (metals and silicates); adsorption/desorption processes during corrosion; interaction between clay platelets; transport of complex fluids through clay and other porous media; and formation of molecular aggregates (scale) within the complex fluid.

**91-95 Funding (\$K):** 800      **Dates:** 1993 - present



**Technology Transfer:** Publications in open literature, collaborations with CRADA partners

**Key Documentation:** Materials Research Society (MRS) Bulletin XVIII, May 1993.  
 Materials by Computer Design, Energy and Technology Review, LLNL report UCRL-52000-94-8/9, 1994.

**Key Personnel:** Christian Mailhot, (510) 422-5873, mailhot1@llnl.gov, David B. Boercker, (510) 422-4187, boercker1@llnl.gov

**Lab Capabilities Applied:** Computational modeling, combustion chemistry, molecular dynamics



Index: 164

Category: Environmental & Regulatory (7)

Laboratory: Lawrence Livermore National Laboratory      Contact: Bernie Merritt (510) 422-4479, merritt2@llnl.gov

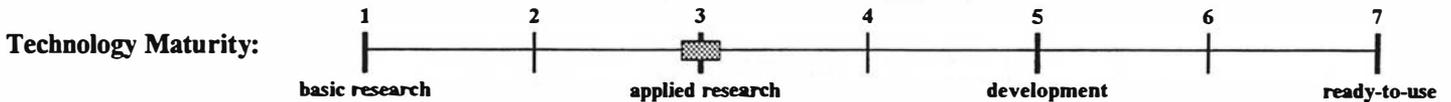
Title: Plasma Processing of Diesel Engine Exhaust

**Description:** The goal is an exhaust-gas treatment process for the reduction of NO<sub>x</sub> and hydrocarbons from diesel engines using electrical discharges or electron beams to accomplish the chemistry. The diesel-engine NO<sub>x</sub> problem is similar to the furnace and boiler NO<sub>x</sub> emission problem with the added constraint that ammonia-like additives are impractical for a mobile source. Lean-burning gasoline engines are an additional area of application because the standard three-way catalyst is rendered ineffective by the presence of oxygen. The electrical discharge approach to hydrocarbon oxidation is relatively straight forward because the oxidative radicals O and OH are easily formed. The electrical approach to NO<sub>x</sub> reduction that relies on the N radical is more difficult in a flue gas environment containing oxygen and water.

The approach is both experimental and computational involving modeling of electron/molecule interaction, chemical kinetics and simple fluid mechanics. A laboratory apparatus has been assembled for blending and metering a simulated exhaust gas, feeding the gas mixture through an electric discharge reactor, and feeding a sample of the effluent gas to a series of analyzers (chemiluminescent NO<sub>x</sub>, FTIR, GC/MS, O<sub>2</sub> cell). Several types of electrical discharge reactors are available including barrier discharge, coronal discharge, and E beam reactors. A one-cylinder diesel engine is available for testing real diesel exhaust gas.

The objective of the laboratory work is to determine the energy efficiency of both hydrocarbon oxidation and NO<sub>x</sub> reduction and to model the pertinent physical and chemical phenomena. Cummins Engine Corporation will test candidate systems in diesel-engine test cells using standard test cycles.

91-95 Funding (\$K): 3000      Dates: 1993 - Present



**Technology Transfer:** We expect to enter into a license agreement upon completion of the project. We are in the process of publishing five related papers in the open literature this year.

**Key Documentation:** CRADA T-336-92-1-C, Headquarters No: 93-MULT-123-C1-1, "Pulsed Plasma Processing of Diesel Engine Exhaust"

**Key Personnel:** M.C. Hsiao (510) 422-6455, hsiall@llnl.gov; B.M. Penetrante (510) 423-9745, penetrante@inventor2.llnl.gov; G.E. Voglin (510) 422-8865, no e-mail address; P.H. Wallman (510) 423-1522, hwallman@llnl.gov

**Lab Capabilities Applied:** Pulsed Power - magnetically-compressed, solid-state modulators  
 Chemical Engineering and Kinetics - advanced diagnostics and experimental program  
 Physics - modeling of radical generation and coupling to chemical kinetics



Index: 165

Category: Arctic Region Activities (1, 2, 5, 7)

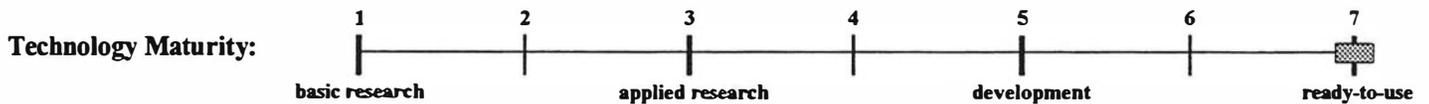
Laboratory: Lawrence Livermore National Laboratory

Contact: Nancy Del Grande (510) 422-1010, delgrande1@llnl.gov

Title: Site Characterization for Exploration and Production Systems

**Description:** Ice-thickness maps in cold-weather regions and near-surface aquifer maps in temperate regions facilitate the siting of drill rigs. Sea ice mapping helps optimize shipping routes for heavy equipment along established channelways. Precise temperature surveys, using dual-band infrared methods pioneered at LLNL, characterize both ice thickness and the near-surface hydrothermal regime to depths of 60 meters. Work performed under a research grant from the Finnish Government proved that aerial infrared mapping is a cost effective method of siting arctic exploration and production systems.

91-95 Funding (\$K): 120      Dates: 1977 - 1994



**Technology Transfer:** 20 publications on dual-band infrared imaging for buried and obscured object imaging and detection; chaired 5 conferences; two patents.

**Key Documentation:** J. E. Lewis, N. K. Del Grande, I. McKendry, P. F. Durbin, M. Lepparanta, "Thermal Mapping" in ERS-1 Baltic Sea Ice Calibration Validation Post-Experiment Report / Pipor/Finland, Finnish Institute of Marine Research Report 1992 (9), Ed. M. Lepparanta and M. Lensu, Helsinki (1992).  
 N. K. Del Grande, "Method for Identifying Anomalous Terrestrial Heat Flows", Patent No. 4,005,289.

**Key Personnel:** Phil Durbin (510) 422-7940, durbin2@llnl.gov

**Lab Capabilities Applied:** Ultra sensitive temperature mapping of: 1) ice thicknesses & Structures; 2) aquifers 6-60 meters deep; 3) soil-moisture variations; 4) energy resource development sites; 5) buried military objects



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Category: Exploration (14, 3, 4)

Laboratory: Lawrence Livermore National Laboratory      Contact: Norman R. Burkhard (510) 422-6483, burkhard1@llnl.gov

Title: Synthetic Seismic Data (SSD) Calculations - part of the GONII project

**Description:** Description: As the complexity of the structures being explored and developed increases, new models that contain a level of complexity consistent with today's exploration and development targets are required. The applications of the model data include testing seismic processing algorithms, better understanding wave propagation in complex subsurface structures, and choosing proper seismic survey parameters in order to obtain an adequate amount of information about the geology and reservoir properties in the most cost-effective manner. In addition, the seismic models can be used for training and for benchmarking different hardware and software platforms and/or configurations.  
 This project is a joint initiative between the DOE labs and the SEG/EAEG 3-D seismic modeling committee. The SEG/EAEG has devised two models of interest: a salt dome model and an overthrust model. LLNL is using a finite difference modeling algorithm to simulate a realistic 3-D seismic survey of these models. The computational resources required to produce the SSD are very large. In order to produce a meaningful simulation within today's computational resources, a phased calculational program has been developed jointly with the SEG/EAEG. Each phase of program is defined to produce SSD that is a meaningful 3-D simulation at each step and that is valuable to the industry after each phase is completed. The SSD are being delivered on-line to the industry as each phase is calculated.

91-95 Funding (\$K): 500      Dates: 1993 - Present



**Technology Transfer:** SEG/EAEG 3-D Modeling Committee, SEG Research Committee, SEG Annual Meeting Presentations, SEG publications, trade journal articles, SEG Home Pages, SEG Summer Workshop

**Key Documentation:** Aminzadeh, F., Burkhard, N., Kunz, T., Nicoletis, L., Rocca, F., "3-D Modeling Project: 3rd Report", The Leading Edge, p. 125-128, February, 1995.  
 Aminzadeh, F. and Burkhard, N., "Joint Initiative Produces 3-D Models", The American Oil & Gas Reporter, p. 63-69, February, 1995.

**Key Personnel:** Shawn Larsen, 510-423-9617, larsen8@llnl.gov

**Lab Capabilities Applied:** Seismic data acquisition survey design, seismic computer modeling, massively parallel processor (MPP) computer code design and optimization, finite difference capabilities



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Category: Production (27, 25)

Laboratory: Lawrence Livermore National Laboratory

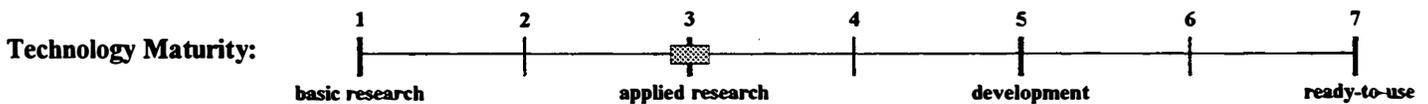
Contact: Lewis A. Glenn (510) 422-7239, glenn@s54.es.llnl.gov

Title: Perforation Dynamics in Geological Media

**Description:** Gas storage companies use depleted oil and gas fields for interim storage of natural gas. In the process, the fields are cycled through gas pressurization and depletion every year, with reperforation of the wells performed on a multiyear basis. The perforation process is poorly understood and improvements in operational performance would have a major impact on reducing the annual \$100M spent on storage deliverability. The industry has developed an extensive data base on the performance of particular wells, with the ability to characterize the productivity of a particular well bore as a function of perforation conditions. LLNL will design and implement an artificial neural network (ANN) to evaluate the extensive parameter space that has been explored, and use the results to guide a combined effort of simulation and experiment to improve operational performance. The active-participation of the industry team will ensure the timely transfer of the results to the production fields. In addition to aiding in the transfer process, deliverables will include : 1) a report describing the results of the ANN analysis of perforation data and derived regions of parameter space for optimum performance with existing perforators, 2) a report describing hydrodynamic simulations performed of selected perforations and the resulting damage, along with results from supporting core-sample perforation tests, and 3) a final report that includes complete results and an assessment of results from downhole tests, along with a discussion of key parameters and mechanisms pertinent to perforation.

91-95 Funding (\$K): 700

Dates: 1995 - Present



Technology Transfer: Reports, meetins with industrial partners.

Key Documentation: ACTI Proposal

Key Personnel: Lewis A. Glenn (510) 422-7239, glenn@s54.es.llnl.gov; Dennis Baum (510) 423-2236, dbaum@llnl.gov

Lab Capabilities Applied: Application of ANNs and GAs to geophysics and mechanics, multidimensional hydro simulations, development and application of complex inelastic rock models, design and testing of shaped charges.



**Index:** 168

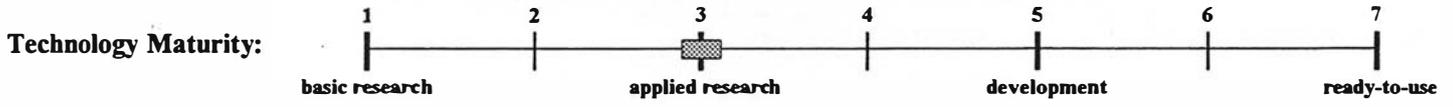
**Category:** Oil Processing & Refining (6)

**Laboratory:** Lawrence Livermore National Laboratory      **Contact:** Otis R. Walton (510) 422-3947, waltonor@llnl.gov

**Title:** Granular Flow

**Description:** A wide variety of industries utilize and/or process large quantities of granular solids; however, industrial plants that process solids have historically been much less reliable than those that use only gases or liquids. Shell Oil, Alcoa and Pall Corporation have acted as "industry observers" on the DOE/FE Granular Flow Advanced Research Objective (GFARO) providing advice on potential application areas. The discrete particle numerical models developed at LLNL have been verified against experimental flows performed at University of Florida. The model input is all based on measurable individual particle properties (tests conducted at Cornell University) with no free, adjustable parameters. No-cost licenses to share "software in development" have been established with Alcoa and Pall Corp. The models are also being transferred to the new NSF Engineering Research Center for Particle Science and Technology at the University of Florida where further development (in collaboration with LLNL) will continue. Engineering design tools that can simulate flows of at least bench-top scale can be developed directly from the existing models. For applications with large particles (i.e., millimeter-scale particles like agricultural grains) engineering design simulations are possible with massively parallel computers.

**91-95 Funding (SK):** 4900      **Dates:** 1984 - Present



**Technology Transfer:** Publications in open literatures, no cost license agreement to share software and development.

**Key Documentation:** Walton, O.R., and R.L Braun, "Simulation of Rotating-Drum and Repose Tests for Frictional Spheres and Rigid Sphere Clusters," in proceedings of DOE/NSF Workshop on Flow of Particulates and Fluids, Sept. 1993, Ithaca, NY.  
 Chapter 25, Numerical Simulation of Inelastic, Frictional Particle-Particle Interactions," O.R. Walton, Particulate Two-Phase Flow, M. C. Roco, ed., Butterworth-Heinemann, Boston, p884-911 (1993).

**Key Personnel:** Anthony J.C. Ladd (510 422-4596, tony-ladd@llnl.gov)

**Lab Capabilities Applied:** Molecular-Dynamics and Statistical Mechanics Expertise, Advanced Numerical Methods, Computer Graphics, Engineering Mechanics Models, Finite Element Calculations (DYNA and NIKE), Scientific Workstation and Mainframe Supercomputer implementation of models.



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Category: Development (22, 5)

Laboratory: Lawrence Livermore National Laboratory      Contact: Daniel J. Schneberk (510) 423-3531, schneberk1@llnl.gov

Title: Evaluation of Geologic Specimens with CT

**Description:** The cost effective, rapid, and quantitative evaluation of soil and rock samples (of up to 1 cubic foot) is an important capability for oil and gas formation evaluation and for assessment of building site characteristics. Computed tomography techniques and codes have been adapted to provide quantitative information on soil and rock samples without the need for tedious and destructive cutting and polishing methods. Specific physical properties can be measured such as porosity, density, grain size, and mineralogy. We have a very unique tomographic capability in that we can scan samples on both the micro- (small samples 1-2 mm o.d. with micrometer spatial resolution) and macro- (samples of 30 cm o.d. with submillimeter spatial resolutions). This can be used to evaluate scaling relations for physical properties. This work is synergistic with work being performed by the University of Texas, the University of California at Davis, Scientific Measurements Systems, and with an ongoing program to scan cores from The Geysers geothermal field.

91-95 Funding (\$K): 7000      Dates: 1986 - Present



Technology Transfer: Publications, BAA, CRADAs, Work For Others, Small Business Technical Assistnace Projects

Key Documentation: 1. B. P. Bonner, et al, "X-Ray Tomography of Preserved Samples From The Geysers Scientific Borehill" UCRL-JC-119573  
 2. B. P. Bonner, et al, "Determining Water Content And Distribution In Reservoir Graywacke From The Northeast" Geysers With Computed Tomography

Key Personnel: Nancy DelGrande (510) 422-1010, delgrandel@llnl.gov; Graham Thomas (510) 422-7325, thomas26@llnl.gov; Albert Brown (510) 422-7089, al-brown@llnl.gov; Hal Brand (510) 422-6312, brand1@llnl.gov; Harry Martz (510) 423-4269, martz2@llnl.gov

Lab Capabilities Applied: Computerized Tomography Systems and NDE Facilities B327, B239, T3226



**Index:** 170

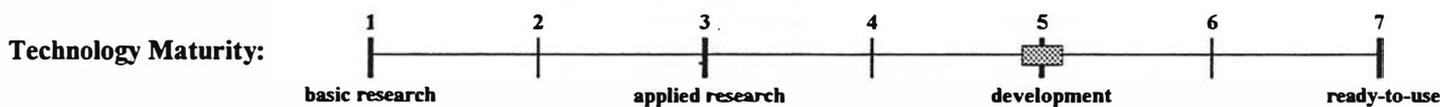
**Category:** Oil Processing & Refining (4), Production (24)

**Laboratory:** Lawrence Livermore National Laboratory      **Contact:** Robert Cena (510) 422-7336, cena1@llnl.gov

**Title:** Oil Shale Technology

**Description:** LLNL formed a cooperative effort with major U.S. oil companies/entities to conduct a research and development project involving the recovery of oil from shale resources in the western United States. The project used a four ton per day retort test unit and other facilities to advance the state of the art as far as practical with that equipment and to identify the next steps and facilities required to further advance the technology. The oil companies involved in the project were Amoco Corp., Chevron-Conoco Joint Venture and Unocal Corp. For the past decade, LLNL has pioneered an oil shale recovery (retorting) process that would form the basis of a cost-effective model that U.S. industry can commercialize. Industrial CRADA partners have equally extensive experience in oil shale development and own or control resources amenable to shale development. Production of unique, high valued products from oil shale combine with technology advances to allow demonstration of advanced retorting technology at significant scale. A first field test plant at the 100-300 barrel-per-day scale would pave the way for this development. The LLNL original oil shale project started in the early 1970's and devoted hundreds of man years to modified-in-situ combustion retorting. Residual capability from that effort would apply to fire-flooding EOR.

**91-95 Funding (\$K):** 5000      **Dates:** 1992 - 1995



**Technology Transfer:** CRADA, open publications and lab reports

**Key Documentation:** P.H. Wallman, "Coproduction of Oil and Electric Power from Colorado Oil Shale", Energy, Vol 17, No. 4, pp 313-319, 1992.  
 R. J. Cena, "A Hot-Recycled-Solid Oil Shale Retorting Process for the Production of Shale Oil and Specialty Chemicals", Preprint: American Chemical Society, Division of Fuel Chemistry, Vol 39, No. 4, pp 1248-1252, 208th ACS National Meeting, Washington D.C, August 20-25, 1994.

**Key Personnel:** Chuck Thorsness (510) 422-8124, thorsness1@llnl.gov

**Lab Capabilities Applied:** 4-tonne-per-day Hot-Recycled-Solid oil shale retorting pilot plant, oil shale crushing/sizing facil., bench scale fluidized bed & cont'd screw feeder shale pyrolysis units, hydropyrolysis unit & extensive hardware/software/modeling cap., two decade proj.



**Index:** 171

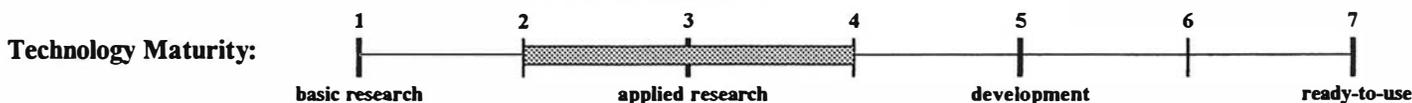
**Category:** Environmental & Regulatory (7)

**Laboratory:** Lawrence Livermore National Laboratory      **Contact:** Robert S. Glass (510) 423-7140, glass3@llnl.gov

**Title:** Gas Phase Sensors

**Description:** The California Air Resources Board (CARB) and the EPA have developed regulations which require auto makers to incorporate comprehensive on-board diagnostics systems onto new vehicles, starting in 1994. The intent of the regulations is to ensure that the vehicle operator is informed when emission control systems are no longer performing adequately. Once operators are informed of a malfunction, they will then take the vehicle in for repairs, so the exhaust emissions are again within the standards. The objective of this program is to develop a prototype sensor, or a sensor array, which could be used for measuring tailpipe or engine-out emissions from an internal combustion engine designed for a low-emission vehicle (LEV). Specifically, this sensor would monitor the performance of the catalytic converter system, demonstrating the potential to quantify the level of deterioration, to ensure compliance with environmental regulations. The sensor may also be used in a feedback control system for fuel control. Our efforts center on the development of solid-state electrochemical sensors for this purpose. Sensors are needed for monitoring gaseous species such as O<sub>2</sub>, NO<sub>x</sub>, CO, H<sub>2</sub>, SO<sub>2</sub>, hydrocarbons, and other species. At LLNL, we are specifically concentrating on the development of oxygen and hydrocarbon sensors. In this effort, LLNL works collaboratively with LANL in basic materials research. General Motors and the automobile consortium, USCAR, provide overall guidance and function as test centers for prototypes. The unique thin film deposition capabilities, ion beam modification, microfabrication, and materials science strengths of LLNL are being utilized in this work. Solid-state sensors of this type may also find use in monitoring industrial stack emissions to ensure environmental compliance, lessening the need for costly maximum achievable control technology.

**91-95 Funding (\$K):** 310      **Dates:** 1993-present



**Technology Transfer:** publications in open literature,; publication in Lab capabilities catalog, presentations in national conferences

**Key Documentation:** G.B. Balazs and R.S. Glass, "AC Impedance Studies of Rare Earth Oxide Doped Ceria, "accepted for publication in Solid State Ionics (November, 1994)  
G.B. Balazs, R.S. Glass, and L.W. Hrubesh, "Characteristics of Ceria-Based Amperometric Oxygen Sensors Utilizing Porous Silica Diffusional Coatings," Extended Abstracts of the 184th Meeting of The Electrochemical Society, Vol. 93-2, 947 (1993)

**Key Personnel:** Quoc Pham (510) 423-3394, no e-mail

**Lab Capabilities Applied:** microfabrication; thin film deposition; ion implantation; sensors; electrochemical measurements



Index: 172

Category: Development

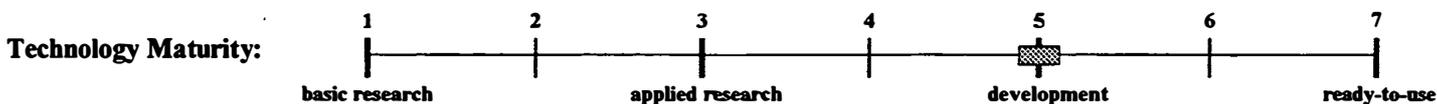
Laboratory: Lawrence Livermore National Laboratory

Contact: Jeff Wagoner (510) 422-1374, wagoner1@llnl.gov

Title: Oil and Gas Well Log Imaging

**Description:** Through a FE-funded project to create a data-base for the Santa Maria Basin (including well logs) and the DP-funded GO-NII project, we have found substantial similarities between needs of the weapons program and the oil and gas industry for the conversion of historic paper and microfiche records to more computer-accessible forms. These existing projects lead to a new ACTI project, whose objective is to 1) develop and optimize software for well log raster imaging, 2) optimize the storage and retrieval of the well-log data, and 3) provide a pilot which produces raster well log images of major fields/plays/basins in the U.S., as a means of proving that this information is both vital and commercially produceable. Geophysical well logs are a component of the well records that California and Texas keep about their respective states' wells. Since 1978, paper well logs have been converted to microfiche by a data provider for more convenient commercial access and storage, with a copy sent to the state. Current mechanisms for converting from the microfiche to electronic forms of a raster picture file and then the numerical format required by analysis programs are each too expensive for any data provider to do on a widespread basis. Additionally, the raster forms require large amounts of storage such that only a few hundred wells would fit on a CD and electronic file transfers over a standard modem line would be prohibitively time consuming and expensive. A pilot program is needed to both reduce the cost and storage requirements of providing these electronic well log forms and to provide the commercial data providers with the market drive to justify investment in expanding the base of electronic data provided so that producers have ready access to the information needed to increase their ability to find oil and gas at lower costs. Our objective is to have organizations in each participating state define the field/play/basin of highest interest to the producers in that state, and to involve a state university in the scanning and rasterization of the data in that state. We will replicate two of MJ's systems to be loaned to the universities for the scanning and rasterization of the data of interest.

91-95 Funding (\$K): 2000      Dates: 1994-present



Technology Transfer: Software will be licensed by MJ Systems; there will be publications describing the project and results.

Key Documentation: ACTI Proposal

Key Personnel: Carol Hunter (510) 422-1657, chunter@llnl.gov; Oscar Nazario (510) 423-0918, nazario@llnl.gov; Bruce Lownsbery (510) 423-4974, bel@llnl.gov

Lab Capabilities Applied: Signal processing, digitization, database development, electronic hardware development, software development, computations



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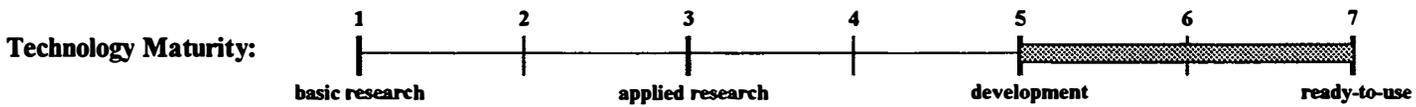
Category: Environmental & Regulatory (9)

Laboratory: Lawrence Livermore National Laboratory      Contact: C.R. Carrigan (510) 422-3941, carrigan@s94.es.llnl.gov

Title: 3-D Simulation of Multiphase Contaminant Transport and In Situ Remediation of Low Permeability Soils Using an Alternating Current Based Ohmic Heating Technique

Description: A numerical simulation capability has been developed that couples a 3-D nonisothermal, multiphase flow and transport computer program (Nitao, JJ, Reference Manual for the NUFT Flow and Transport Code, Version 1.0, LLNL Report, May, 1993) to an in situ ohmic heating model (Carrigan, CR and Nitao, JJ, A Fully Coupled Model for 3-D Partially Saturated Flow and Transport in Soil Ohmically Heated by Application of Multiphase A.C. Electrical Potentials. To be submitted to Journ. of Environmental Science and Technology, 1995) that simulates the heating rate produced by passing an alternating current through the soil by energized electrodes emplaced at different locations in a hydrologic system of arbitrary complexity. The heating model is dependent on temperature, saturation, cation exchange capacity and ionic conductivity through the use of the Waxman-Smits model of electrical conductivity. The OHM/NUFT simulator is intended to provide a predictive and diagnostic capability for the Dynamic Underground Stripping Project at LLNL. This project uses ohmic heating of tight clay formations to partition contaminants (gasoline, TCE) into a vapor phase that bleeds into surrounding higher permeability formations where the contaminant can be extracted by vacuum extraction and steam injection techniques. This method has been used at LLNL to extract several thousand gallons of gasoline from spill sites. The modeling capability has been used to diagnose the occurrence of non-uniformities in the heating distribution. It can also be used to facilitate the design of a remediation facility and to maximize the efficiency of its operating program, for example, maximizing the ratio of remediation to energy usage through the simulation guided manipulation of the schedule of ohmic heating and steam injection.

91-95 Funding (\$K): 385      Dates: 1991 - Present

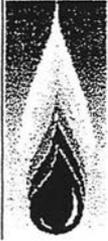


Technology Transfer: Papers in the open literature and internal LLNL reports, presentations at meetings and workshops.

Key Documentation: Carrigan, CR and Nitao JJ, Development of a Predictive and Diagnostic Modeling Capability for Joule Heating in "Dynamic Underground Stripping Project LLNL Gasoline Spill Demonstration Report" (R. Newmark, ed.), Vol. 3, UCRL-ID-116964, p 5-195, 1994. Carrigan, CR and Nitao, JJ, Appendix 5: "Modeling of ARV Sparging and Electrical Heating Using NUFT and an Ohmic Heating Module" in Treatment Facility F: Accelerated Removal and Validation Project, UCRL-ID-116621, p.. A5-1, 1994.

Key Personnel: John J. Nitao (510) 423-0297, nitao@s13.es.llnl.gov

Lab Capabilities Applied: Large scale modeling of electrical heating, fluid flow and transport using in-house 3-D simulators on high speed, minicomputers.



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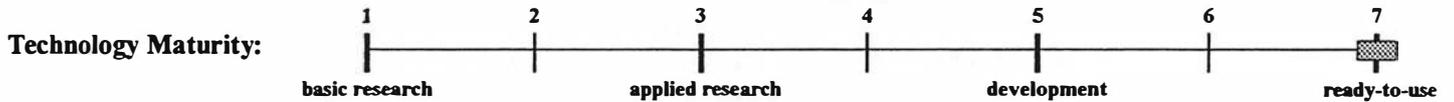
Category: Development (18)

Laboratory: Lawrence Livermore National Laboratory      Contact: William Daily (510) 422-8623, daily1@llnl.gov

Title: Laboratory Analysis of Rock Core Using Electrical Resistance Tomography

Description: Electrical Resistance Tomography, an electromagnetic technique using the principles of computerized tomography, provides an ability to produce high resolution images of electrical resistivity distribution within rock cores under test in the laboratory. The technique has been especially valuable for imaging water movement through fractured cores which are under pressure and temperature. It permits the study and mapping of fluid infiltration in the core and is especially useful when the sample is in a pressure vessel and at high temperatures. The technique enables quality scientific measurements under difficult experimental conditions.

91-95 Funding (\$K): 50      Dates: 1991



Technology Transfer: None

Key Documentation: Daily, W. D., W. Lin and T. Buscheck, Hydrological Properties of Topopah Spring Tuff: Laboratory Measurements, J. Geophys. Res., 92, 7854-7864, 1987.  
 Lin, W. and W. Daily, Laboratory-Determined Transport Properties of Core from the Salton Sea Scientific Drilling Project, J. Geophys. Res., 93, 13047-13056, 1988.

Key Personnel: Abe Ramirez (510) 422-6909, ramirez3@llnl.gov

Lab Capabilities Applied: Geophysical and remote sensing expertise and tools, rock properties laboratory



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Category: Exploration (4, 6, 10, 12), Development (3, 9, 11)

Laboratory: Lawrence Livermore National Laboratory      Contact: P.A. Berge, 510-423-4829, Pat\_Berge@quickmail.llnl.gov

Title: Velocity Analysis, Parameter Estimation, and Constraints on Lithology for Transversely Isotropic Sediments

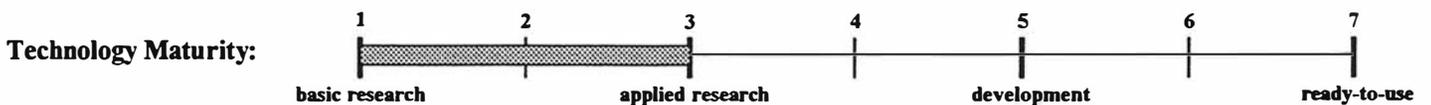
**Description:** This research addresses a key issue of concern to the petroleum exploration industry. New methods are being developed for processing and interpreting seismic reflection data acquired in regions where the rocks and sediments do not have isotropic sound-wave velocities. The influence of anisotropy leads to significant distortions in seismic reflection data processing and errors in interpretation that can result in drilling in the wrong place or to the wrong depth, and errors in data analysis that may turn a play into a non-play or vice versa.

Industry involvement includes: collaborators who will provide expertise in seismic anisotropy (Amoco, Chevron) and processing reflection data in complex areas (Western Geophysical); funding for visiting scientists from industry to work with the Colorado School of Mines group on seismic data processing (Mobil) and with LLNL researchers on modeling stress-induced anisotropy in granular media (Schlumberger-Doll); and in-kind support including making appropriate seismic reflection data-sets available for this research (Chevron). Industry participants also support the research at the Colorado School of Mines Center for Wave Phenomena through consortium fees.

Deliverables to be pursued in parallel over the next three years include algorithms and codes for processing seismic reflection data and determining elastic wave velocities in transversely isotropic media; theoretical expressions needed for incorporating shear wave data into inversion for the complete set of parameters describing the anisotropy; analysis and resulting database showing the correlation between anisotropic parameters and rock properties so that the seismic data can be interpreted for constraints on rock and sediment composition.

Known applications and impacts include improved processing and interpretation of seismic reflection data in the oil exploration industry; increased understanding of the connections between seismic properties and other physical properties of rocks containing hydrocarbons; imaging the earth more accurately to find oil more reliably.

91-95 Funding (\$K): 600      Dates: 1995 - Present



Technology Transfer: Publications in open literature, staff exchange

Key Documentation: The proposal written to describe and request funding for this new project can be found in: Burnham, A. K., 1994 DOE Advanced Computational Technology Initiative Proposals, Lawrence Livermore National Laboratory report UCRL-PROP-118997.

Key Personnel: James Berryman, (510) 423-2905, berryman@s123.es.llnl.gov

Lab Capabilities Applied: Theoretical seismology; Exploration geophysics; Rock physics



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Category: Development (33); Environmental & Regulatory (9)

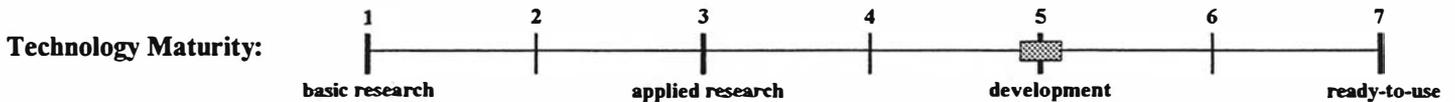
Laboratory: Lawrence Livermore National Laboratory      Contact: Virginia M. Johnson, (510) 423-2005, vmjohnson@llnl.gov

Title: Optimization Methods for Reservoir Management

**Description:** Over the last five years, LLNL has evolved a "soft computing" approach (integrating fuzzy logic, neural networks, and genetic programming methods) to the optimization of engineering design tasks. The ANN-GA methodology for optimizing groundwater remediation strategies links artificial neural networks (ANNs) to the genetic algorithm (GA) to search for designs which best balance regulatory, economic, and engineering goals. By training networks to stand in for CPU-intensive reservoir simulators, millions of designs are evaluated in practical time limits using conventional workstations. The ANNs are further employed in Monte Carlo experiments to test the contributions of individual design components.

These methods have been developed and tested on field data, contaminant transport models, and treatment facility design problems from a western Superfund site. Work is currently underway to apply them to gas-storage and secondary/tertiary oil recovery problems. In the gas-storage problem, historical production data supplied by independent gas producers (see the project description for Perforation Dynamics in Geologic Media) will be analyzed by means of ANNs, which will then be linked to the GA to search for formation and operator-controllable factors that optimize yield. In the oil recovery problem, a consortium of oil companies represented by the Petroleum Science and Technology Institute of Edinburgh, U.K., will be contributing data, full-field reservoir simulations, and development planning problems from a mature North Sea reservoir.

91-95 Funding (\$K): 1500      Dates: 1991 - present



Technology Transfer: publications in open literature, conferences

**Key Documentation:** Rogers, L. L. and F. U. Dowla. 1994. Optimization of groundwater remediation using artificial neural networks and parallel solute transport modeling. *Water Resources Research*, 30(2), 457-481. Johnson, V. M. and L. L. Rogers. 1995. Location analysis in ground water remediation using artificial neural networks. UCRL-JC-117289, Lawrence Livermore National Laboratory, Livermore, CA. See also *Ground Water* (in press).

Key Personnel: Leah L. Rogers, (510) 422-3538, rogersl1@llnl.gov

Lab Capabilities Applied: Neural Computing, Heuristic Search Techniques, Distributed Processing, Reservoir Simulation, Decision Analysis



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**Category:** Deepwater Offshore (16), Environmental & Regulatory (14)

**Laboratory:** Lawrence Livermore National Laboratory      **Contact:** Dr. Robert Murray (510) 422-0308, murray6@llnl.gov

**Title:** Seismic Hazard Assessment for Santa Barbara Channel Offshore Platforms

**Description:** The US Minerals Management Service is re-evaluating the seismic hazard for offshore platforms in the Santa Barbara Channel of California. The impetus for this work came from a need to develop modern seismic design and reevaluation criteria for offshore platforms in regions of high seismicity. These criteria will be based on currently available seismological and geological data and state-of-the-art hazard methodologies being developed in California. The project draws on capabilities from a much larger LLNL Computational Earthquake Initiative (Hutchings, L.J., (1994), Kinematic Earthquake Models and Synthesized Ground Motion Using Empirical Green's Functions, Bul. Seis. Soc. Am., Vol. 84; D.B. McCallen, F.E. Heuze and P.W. Kasameyer, (1993), A Methodology for Calculating the Response of Structures to Earthquakes on Specific Faults, Proceedings of the 6th International Conference on Soil Dynamics and Earthquake Engineering, Bathe, England.)

**91-95 Funding (\$K):** 250      **Dates:** 1994 - Present



**Technology Transfer:** Publications in the open literature, and presentations at selected conferences.

**Key Documentation:** A.C. Boissonnade, R.C. Murray and W. Foxall, "Seismic Hazard Characterization and Mapping for Offshore Platforms in the Santa Barbara Channel," Proceedings of the 2nd International Workshop on Wind and Earthquake Engineering for Offshore and Coastal Facilities, UC Berkeley, January, 1995.

**Key Personnel:** Auguste Boissonnade (510) 423-0872, abois@llnl.gov; Jean Savy (510) 423-0106, jbsavy@llnl.gov; Larry Hutchings (510) 423-0354, hutchings2@llnl.gov

**Lab Capabilities Applied:** This project utilizes the probabilistic hazard techniques and seismology expertise developed at LLNL



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Category: Production (21), Environmental & Regulatory (12)

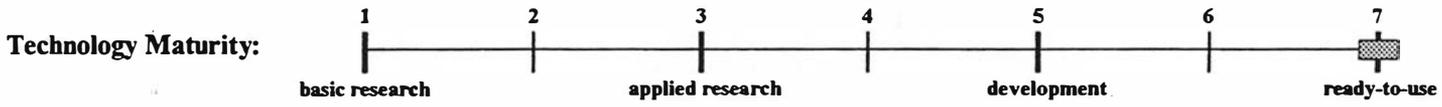
Laboratory: Lawrence Livermore National Laboratory      Contact: M. Allen Northrup (510) 422-1638, northrup1@llnl.gov

Title: Battery-powered Portable Micro-machined DNA Detector

**Description:** The object of this project is to develop a portable (real-time) system to detect the presence of specific deoxyribonucleic acids (DNA) by ultra-selective amplification with the polymerase chain reaction (PCR). The PCR technique, whose inventor recently received the Nobel Prize, has many applications, including the detection of HIV, other pathogens, forensic analysis and the detection of bacterial contaminants in the environment. Previous PCR machines have been massive and extremely power hungry. Using micro-fabrication techniques, LLNL researchers have recently built and operated the world's first battery-powered hand-held PCR machine. The instrument, which is readily fieldable, can be used to monitor the DNA signature of enzymes which can signal either the propagation or death of the particular microbes being used in the enhancement process. The instrument can be used in downhole measurements.

Industrial involvement has been focused on pharmaceutical firms and neither microbial enhanced oil recovery nor bioremediation have yet been pursued.

91-95 Funding (\$K): 1600      Dates: 1993 - Present

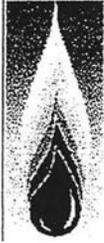


Technology Transfer: CRADA process, licensing process

Key Documentation: Patent Application pending; publication in professional journals for the healthcare industry

Key Personnel: M. Allen Northrup (510) 422-1638, northrup1@llnl.gov

Lab Capabilities Applied: MicroTechnology facility, microfabrication and microstructure expertise, biomedical engineering, Biology/Biotechnology Project



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Category: oil Processing & Refining (12)

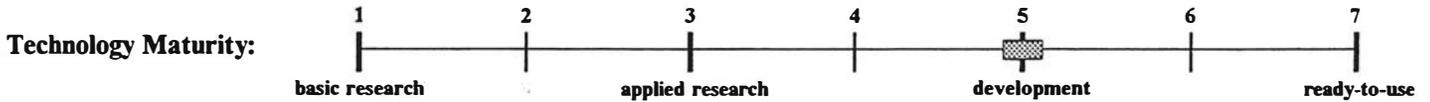
Laboratory: Lawrence Livermore National Laboratory      Contact: Arden Dougan (510) 422-5549, adougan@llnl.gov

Title: Compact Analytical Neutron Interrogation System

**Description:** LLNL has developed a technique to identify chemical elements using a portable, electrically-driven ion-tube accelerator, which can produce pulses of 14-MeV neutrons. The neutrons react with chemical elements, producing gamma radiation. The characteristics of the gamma radiation identify the chemical elements and their relative quantities. The technique is highly penetrating, illuminating 1 meter depths in common objects. Our system is field-portable so it can perform in-situ measurements and analysis or can be employed in a process line. Our system is approximately 1/10th the volume of conventional oil-logging systems and will fit in two suitcases. The system is easy to operate remotely from a PC-computer. The size and portability make the system extremely flexible.

Neutron activation analysis techniques are applicable for determining the amount of oxygen, sulfur, or metal loading in fuel, or process line monitoring, and can be used where the lines are under high temperature or high pressure. It can be used to determine the amount of sea water that is mixed with the crude oil as it is off-loaded from ships.

91-95 Funding (\$K): 100      Dates: 1993- present



Technology Transfer: CRADA (negotiations in progress), open publications, and lab reports

Key Documentation: R. A. Alvarez, A. D. Dougan, M. R. Rowland, and T. F. Wang, "Neutron Interrogation to Identify Chemical Elements with an Ion-Tube Neutron Source (INS)", to be published in J. Radioanalyt. Nucl. Chem.

Key Personnel: Arden Dougan (510) 422-5549, adougan@llnl.gov

Lab Capabilities Applied: Experience in active neutron interrogation and gamma spectrometry measurements and analysis, radiation transport modeling, radiation sensor development



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Category: Oil Processing &amp; Refining (23)

Laboratory: Lawrence Livermore National Laboratory

Contact: Bruce Watkins (510) 423-5188,  
watkins1@llnl.gov

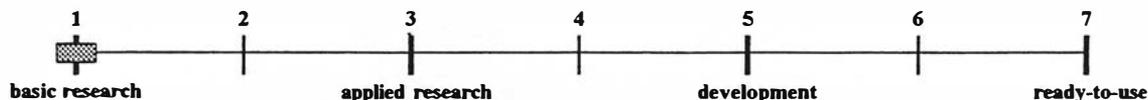
Title: Biomimetic Catalysts for the Conversion of Methane to Methanol

**Description:** The object of this project is to develop catalysts that will perform the selective oxidation of methane directly to higher hydrocarbons (liquids) or alcohols (methanol). These catalysts should be robust enough to survive in commercial catalyst reactors. The original approach was to develop a rational design for inorganic metal oxide catalysts. Experimental and computer modeling showed that this approach will not produce a catalyst with sufficient selectivity for industrial applications. We then changed our approach to first gain an insight to the mechanism of action of enzymes that already perform a selective oxidation of methane to methanol, and to use this information to design catalysts that mimic the function of the enzyme, but be more robust for commercial reactors. Amoco's role is to monitor LLNL's progress, provide insight from years of in-house research, and to evaluate catalysts in pilot plants. This project is expected to a) add to the understanding of the structure/function relationships of enzymes; b) generate catalysts that perform the selective oxidation of methane to methanol; c) scale-up to industrial-sized catalyst reactors. This technology has application to the conversion of natural gas at remote sites to a liquid product (methanol, liquid transportation fuel), to the treatment of hazardous waste, remediation of contaminated sites, destruction of explosives, and the manufacture of fine chemicals. It could have a \$1 billion impact in the transportation sector alone.

91-95 Funding (\$K): 3000

Dates: 1990 - Present

Technology Maturity:



Technology Transfer: Publications in open literature, meetings with CRADA partners, presentations at public meetings.

Key Documentation: GRI Final Research Report: "Conversion of Methane to Higher Hydrocarbons", B.E. Watkins, et al., UCRL-CR-119242.

Cooperative Research and Development between Amoco Corporation and the Regents of the University of California, "Biomimetic Catalysts for the Conversion of Methane to Methanol", LLNL Case No. TC-548-93.

Key Personnel: Joe Satcher (510) 422-7794, satcher@cmsi.llnl.gov

Lab Capabilities Applied: Organic and inorganic synthesis, cell culture and enzyme biochemistry, EXAFS spectroscopy, rational catalyst design



**Index:** 181

**Category:** Exploration (1), Development (2)

**Laboratory:** Lawrence Livermore National Laboratory      **Contact:** G. Goudreau (510) 422-8671  
goudreau@llnl.gov

**Title:** Massively Parallel Computing

**Description:**

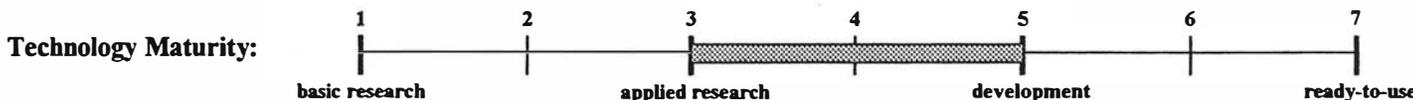
a) Massively parallel computers enable next-generation applications in solid and structural mechanics with problem sizes in the millions of elements. Parallel algorithms for both explicit and implicit finite element models require new algorithms for (1) partitioning meshes for arbitrary geometries, (2) dynamically-load balanced algorithms for modeling material interface interactions, and (3) scalable parallel I/O software and storage technology for binary databases with up to a terabyte of data.

b) Research in scalable parallel I/O for structured and unstructured grid applications is being conducted in collaboration with Gary Montry from Southwest Software. Other industry-related projects at the LLNL include the Gas and Oil National Infrastructure Initiative and the High Performance Storage Systems Initiative. This latter project is developing software tools for searching, browsing, and accessing of datasets with approximately 2 terabytes of data.

c) Deliverables for the ParaDyn research project at LLNL include (1) integrated software for mesh partitioning using state-of-the-art partitioning methods, (2) new parallel algorithms for contact at material interfaces including a novel algorithm for dynamically load-balancing the contact surfaces, and (3) demonstration applications (one hundred thousand to one million elements) in penetration, crashworthiness, and metal forming.

d) The ParaDyn project and follow-on projects for implicit methods provide the parallel algorithm expertise which is being implemented in all our structural, thermal, and fluid finite element models. Parallel applications in computational mechanics are expected to impact engineering design efforts in all industries by reducing the turnaround time for design studies.

**91-95 Funding (\$K):** 1000      **Dates:** 1993 - Present



**Technology Transfer:** DYNA3D pioneered vector supercomputing in solid dynamic over 15 yrs via collaborators program, liscensed in last 5; MPP collaborators just starting w/several sites & few platforms; Algorithms published, and expect to stimulate commercial code w/new tech.

**Key Documentation:**

- Whirley, R.G. and B.E. Engelmann (1993), DYNA3D: A Nonlinear, Explicit, Three Dimensional Finite Element Code for Solid and Structural Mechanics - User Manual, Lawrence Livermore National Laboratory, Livermore, California, UCRL-MA-107254 Rev. 1.
- Hoover, C.G., DeGroot, A.J., Maltby, J.D., and Procassini, R.J., ParaDyn - DYNA3D for Massively Parallel Computers, in Engineering Research Development and Technology Thrust Area Report FY94, Lawrence Livermore National Laboratroy, Livermore, California, in publication.

**Key Personnel:** C. Hoover (510) 422-1556, hoover1@llnl.gov

**Lab Capabilities Applied:** Comp. engrs & phys. to develop parallel algorithms; 256 processor T3D parallel computer, Cray Research, Inc./256 processor Meiko CS-2 parallel computers at Livermore; Facility for Advanced Scalable Tech. - 48 processor Meiko CS-2 w/scalable I/O Facility



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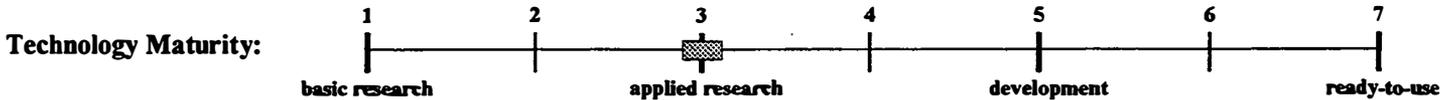
Category: Oil Processing & Refining (25, 21, 4)

Laboratory: Lawrence Livermore National Laboratory      Contact: John G. Reynolds (510) 422-6028, reynolds3@llnl.gov OR john\_reynolds@lccmail.ocf.llnl.gov

Title: Heavy Crude Oil Processing

**Description:**  This research addresses key industry issues in the production, transportation and refining of heavy crude oils. Metals removal in heavy crude oils before refining allows more utilization of heavy crude by existing refinery technology such as FCC and hydrotreating. Hydrogen addition upgrading of heavy oils by water processing, carbon rejection upgrading of heavy oils by moving packed bed pyrolysis, and computational optimization these processes address utilizing more of the non-distillable portion of the heavy crude oil for transportation fuels than conventional bottom-of-the-barrel processing such as coking and asphalt production. Well head (field) and refinery are potential applications. Industry is intimately involved many ways. For all projects industry is providing input during demonstration and development and will provide assistance when scale-up occurs. Some metals removal reagents have shown promise in the laboratory, water processing experiments are just beginning, low severity pyrolysis processing shows upgrading of Kern River crude, computational modelling has not begun yet. Success of these projects will greatly assist in the utilization of heavy crude oil processing as produced today. Removal of metals prior to upgrading has huge impact on every refinery world wide. Water and pyrolysis upgrading has particular importance to field upgrading for producers of heavy oils in California (particularly secondary production by steam flooding).

91-95 Funding (\$K): 1550      Dates: 1992 - Present



Technology Transfer: Open publications, patents, licensing of patented technology, personal communication.

Key Documentation: CRADA TC-400.92

Key Personnel: Glenn Fox, (510) 422-0455, fox7@llnl.gov; Alan Burnham, (510) 422-7304, burnham1@llnl.gov

Lab Capabilities Applied: Heavy oil processing and characterization laboratory; 4 tonne/day oil shale retort, high pressure aqueous pyrolysis laboratory, analytical chemistry division facilities, Pyromat II micropyrolyzer



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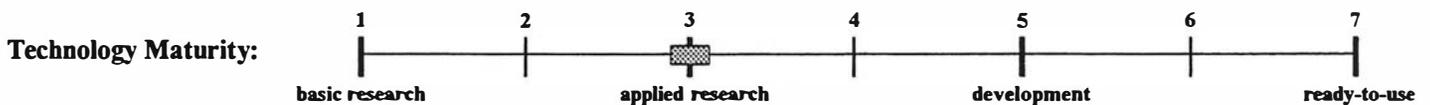
Category: Environmental & Regulatory (2, 10, 11)

Laboratory: Lawrence Livermore National Laboratory      Contact: Joseph C. Farmer, (510) 423-6574, no e-mail

Title: Capacitive Deionization

**Description:** Carbon aerogel-based capacitive deionization (CDI) is a novel technology which offers significant economic and environmental benefits over traditional deionization processes, including ion exchange and evaporation. CDI is a broad-based technology that will be applied to a wide range of industrial and environmental applications including ion removal from waste water, treatment of boiler water in nuclear/fossil fuel plants, production of high purity water for semiconductor manufacturing, electrically driven water softeners for residential use, removal of salt water for agricultural irrigation and desalinization of sea water. The CDI process is relatively simple. Water containing salt, heavy metals, or even radioactive isotopes is pumped through a series of electrochemical cells. An electric potential is then applied across the electrodes, which attract the negatively and positively charged ions. Carbon aerogels are used to make the electrodes because of their high specific surface area. A number of detailed parametric studies have been conducted to date, utilizing different types of solutions, concentrations and stack sizes and voltages. A proof-of-principle prototype containing 384 electrodes is currently in operation at LLNL; a dual-stack system has also been made in which one stack is dedicated to purifying while the other is regenerating. The next step is to scale-up to enable processing of larger concentration gradients (from 1000 to 10,000 ppm) and higher flowrates. Carbon aerogel-based CDI eliminates waste generation inherent in processes such as ion exchange by substituting nontoxic and nonpolluting electricity for the acids, bases, and salts.

91-95 Funding (\$K): 1800      Dates: 1994 - Present

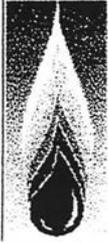


Technology Transfer: Technology is being licensed to large corporations involved in water treatment.

Key Documentation: A US patent has just been received.

Key Personnel: Greg V. Mack (510) 423-1905, mack2@llnl.gov; David V. Fix (510) 423-1740, no email

Lab Capabilities Applied: Key capabilities utilized include aerogels, electrochemical process engineering, and computer controls.



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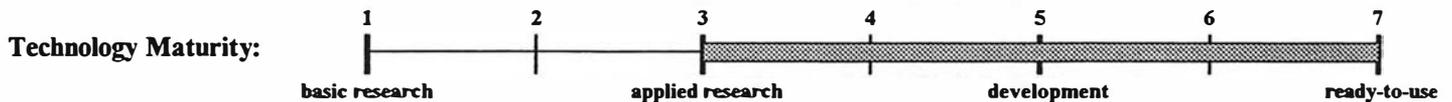
Category: Development (10), Environmental & Regulatory (5)

Laboratory: Lawrence Livermore National Laboratory      Contact: William Daily (510) 422-8623, daily1@llnl.gov

Title: Electrical Resistance Tomography for Subsurface Imaging and Leak Detection

**Description:** Electrical Resistance Tomography (ERT) is a cross borehole electromagnetic method for mapping subsurface resistivity with variations in the resistivity indicative of the presence of inhomogenities in the material. Cross-well Electrical Resistance Tomography (ERT) has been used to map a steam flood used for environmental remediation. The technology could be used for detailed subsurface mapping of EOR steam floods as well as surfactant floods, or almost any fluids moving in the subsurface. Any time borehole electric logs might be useful for looking at formation fluid, ERT could be used to image the same electrical properties between wells. ERT has been used at many sites to describe characteristics such as the location of sand lenses and continuity of clay layers. ERT has also been used to monitor steam flood, air sparging, vadose infiltration, ohmic heating, RF heating and LNAPL release. Oil reservoir scales are much larger that those encountered at environmental sites but ERT has already been used to image between wells of 200 feet separation and well separation of 1000 feet should not be difficult. The approach can significantly improve the ability to perform site characterization and process monitoring at lower costs than presently possible. Several environmental companies are negotiating licenses with LLNL for the technology to be used in site characterization and process monitoring. ERT is also well suited to detecting and locating leaks in lined storage ponds, landfills, and in steel tanks (surface or buried). The technology has been demonstrated to work on small, field scale models of holding ponds and landfills. Furthermore, the method has been proven in the field during a detection test for leakage from a full scale surface tank in Hanford, WA that was enabled by support from Westinghouse. BP America funded some of the early work in this project and expressed significant interest as have Westinghouse and other environmental concerns. This interest results mainly from the methods ability to provide a capability to detect, locate and image the extent of fluids released from a pond, landfill, or tank.

91-95 Funding (\$K): 1120      Dates: 1988 - Present



Technology Transfer: CRADA; license

**Key Documentation:** Daily, W., A. Ramirez, D. LaBrecque and J. Nitao, Electrical Resistivity Tomography of Vadose Water Movement, Water Resources Research, 28,1429-1442, 1992.  
 • Ramirez, A., W. Daily, D. LaBrecque, E. Owen and D. Chesnut, Monitoring an Underground Steam Injection Process Using Electrical Resistance Tomography, Water Resources Research, vol. 29, no. 1, pp 73-88, 1993.

**Key Personnel:** Abe Ramirez (510) 422-6909, ramirez3@llnl.gov

**Lab Capabilities Applied:** Geophysical and remote sensing expertise and tools



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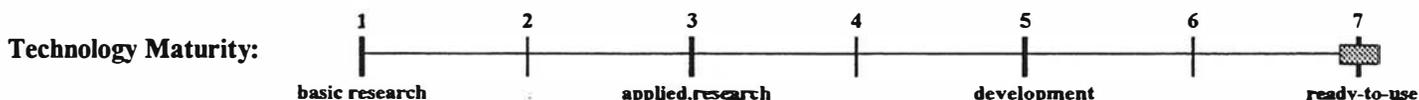
**Category:** Oil Processing & Refining (26)

**Laboratory:** Lawrence Livermore National Laboratory      **Contact:** Alan Lamont (510) 423-2575, lamont1@llnl.gov

**Title:** Economic Analysis and Modeling

**Description:** Several energy market studies have been conducted to assess the impact of new technologies or proposed changes in energy policies. Typically, a quantitative model is developed using optimization techniques and economic principles. Data for the models are derived from commercial or government databases and supplemented with expert opinion. Results of studies identify preferred courses of action and the robustness of decisions. Examples include: 1) development of a database of U.S. energy and economic statistics to support modeling efforts, 2) analyses of the U.S. emissions trading markets, natural gas deregulation proposals, and the Polish and Chinese energy economies using a generalized network equilibrium modeling package developed in-house, 3) production cost modeling to estimate the impact of a proposed carbon tax on the economics of coal, nuclear, and natural gas based electric power generation, 4) energy technology R&D project selection using decision analysis and resource allocation models, and 5) issues paper on the distributed utility concept, where generation, energy storage, and control is dispersed throughout the distribution rather than concentrated at the transmission level.

**91-95 Funding (\$K):** 600      **Dates:** 1991 - Present



**Technology Transfer:** Collaboraton software agreements for use of software, Laboratory reports

**Key Documentation:** Distributed Utility Valuation Project, EPRI Report TR-102807, July 1993  
User's Guide to the META\_Net Economic Modeling System, Alan Lamont, August 1993

**Key Personnel:** Thomas Edmunds (510) 422-5156, edmunds2@llnl.gov  
Thomas Altenbach (510) 422-1285, altenbach2@llnl.gov

**Lab Capabilities Applied:** energy economics, systems optimization, decision analysis



Index: 186

Category: Environmental & Regulatory (12)

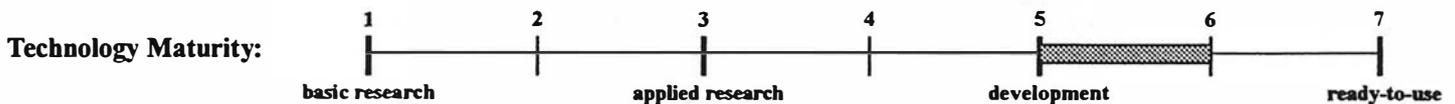
Laboratory: Lawrence Livermore National Laboratory      Contact: Roger Aines, 510-423-7184, e-mail aines@s63.es.llnl.gov

Title: Dynamic Underground Stripping

**Description:** Dynamic Underground Stripping (DUS) is a combination of in-situ steam injection, electrical resistance heating and fluid extraction for rapid removal and recovery of subsurface contaminants such as solvents and fuels. Underground imaging and other advanced measurement techniques monitor the system in-situ for process control. Field tests at a deep gasoline spill (120'-160') at LLNL recovered over 7,000 gals in under a year of operations. Initial estimates of gasoline within the treatment area were 6,300 gals plus or minus 30%, so a major success at removing the source term contaminating groundwater was accomplished. An estimated 750 gals remain in and around the treatment zone. The initial estimate of full remediation using pump and treat was from 50 to 200 years. Analysis of system cost and performance compares favorably with conventional pump and treat methods and vacuum extraction for removing non-aqueous phase liquids (NAPLs) such as gasoline from deep surface plumes. ROI is estimated at 4:1 with cleanup times reduced to under 1 year.

Dynamic Stripping has been proposed to quickly clean up the major concentrated source of the groundwater contamination. It is a major improvement because pump & treat assumes straight line removal when in fact it may never fully clean a site because of mass transfer limits at low concentrations. The removal of the concentrated free product eliminates the major source of the groundwater contamination and may allow the residual to be removed by natural bio-remediation.

91-95 Funding (\$K): 10500      Dates: 1992 - 1994



**Technology Transfer:** The technology is being proposed at numerous DOE, other Federal and industrial sites with license negotiations underway with at least five commercial firms.

**Key Documentation:** 1) "Dynamic Underground Stripping to Remediate a Deep Underground Spill", J. Yow, R. Aines, R. Newmark, K. Udell & J. Ziagos, GEOENVIRONMENT 2000 Conference, New Orleans, LA, Feb. 24-26, 1995  
 2) "Cleaning Up Underground Contaminants", R. Aines, R. Newmark, A. Copeland, J. Ziagos, ENERGY & TECHNOLOGY REVIEW, May 1994, pgs 11 - 21

**Key Personnel:** Robin Newmark (510) 423-3644, e-mail newmark@s95.es.llnl.gov  
 John Ziagos (510) 422-5479, e-mail john\_ziagos@quickmail.llnl.gov

**Lab Capabilities Applied:** Reservoir Engineering, Engineering Analysis Instrumentation, Field Testing, Simulation, Underground Imaging



Index: 187

Category: Development (15, 14, 20)

Laboratory: Lawrence Livermore National Laboratory      Contact: James M. Ferguson (510) 424-4768, ferguson@viper.llnl.gov

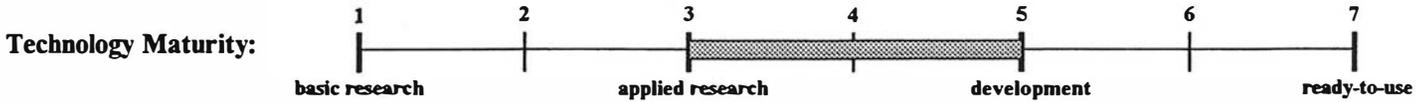
Title: Computer Simulation of Nuclear Well Logging Devices

**Description:** Nuclear well logging is a method of studying the materials surrounding boreholes. A tool consisting of a neutron or gamma-ray source and one or more detectors is lowered into the borehole. The response of the detectors to radiation returning from outside the borehole depends on the lithology, porosity, and fluid characteristics of the material. In principle, the characteristics of the materials outside the borehole can be inferred from the response of the detectors. The interpretation of the data is based on benchmark measurements and computer simulation of the measurements with neutron and gamma-ray transport codes.

Rapid advances in computer power have made it feasible to use deterministic methods for this application. Advanced algorithms have been developed to further reduce the computational expense. We are working to develop deterministic computer codes for modeling the response of neutron and gamma-ray logging tools, using advanced methods developed at LLNL. Initial funding came from a LDRD project, and the work will now continue through H4P and ACTI funding. These codes will solve oil logging benchmark problems, based on real problems provided by industry. Industrial partners will dedicate an equivalent effort in time and databases, design information, and interpretive software and expertise developed over time within the industry. Industry participation will insure development of computational tools which meet the needs of industry.

The final product will be a system of codes to calculate the response of nuclear logging tools to an environment specified by the user. The code will run stand-alone on the powerful workstations used throughout the industry. The prototype codes will be made available to industrial personnel for purposes of code development, testing, and bench marking, but not for commercial purposes. The final code system will be available to all qualified US. industry users, including the partners of this project, with proper licensing agreements

91-95 Funding (\$K): 800      Dates: 1993 - Present



**Technology Transfer:** The technology transfer will be in the form of a computer system, which will be made available through the RSIC (at Oak Ridge) to eligible U.S. industrial users, through a licensing procedure like that now used to disseminate the LANL code MCNP.

**Key Documentation:** ACTI Proposal #26: Computer Simulation of Nuclear Well Logging Devices.

**Key Personnel:** Milo Dorr (510) 423-2423, dorr@llnl.gov; Peter Brown (510) 423-2098, pnbrown@llnl.gov; John Rogers (510) 423-0990, no e-mail address; Chris Clouse (510) 422-4343, no e-mail address; Maurice Aufderheide (510) 423-6174, no e-mail address

**Lab Capabilities Applied:** LLNL Computer Center  
 LLNL B-Division work station network  
 Expertise in Computational Physics in the LLNL B Division  
 Expertise in Computational Math in the LLNL CMRD Group



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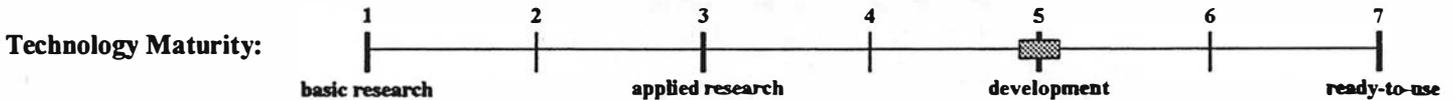
Category: Development, Production

Laboratory: Lawrence Livermore National Laboratory      Contact: Jeff Wagoner (510) 422-1374, wagoner1@llnl.gov

Title: Oil and Gas Data Infrastructure

Description: LLNL has two existing and one new project dealing with databases and data infrastructure for the oil and gas industry. A FE-funded project compiled an extensive data base on production history and associated formation information (e.g., well logs) for the Santa Maria Basin in California. Part of the DP-funded GO-NII project has used the extensive data storage and intelligent archive facilities at LLNL. The ACTI Oil and Gas Data Infrastructure Project grew out of these activities and will design, implement, and integrate inexpensive, standards-based, simple mechanisms for on-line access to all oil and gas data currently available at the California Division of Oil, Gas and Geothermal Resources and Texas Railroad Commission. Cost-effective access will be available through the existing Internet infrastructure using defacto Internet protocols and client/server tools. Eventually, widespread use of the system by oil and gas operators will facilitate electronic filing of documentation and permits required in both California and Texas. The range of beneficiaries from the system is broad. The primary target is the small, independent operator who is becoming the most important player in extending the life of our declining domestic resources. But in addition, city, county and state governments, county assessors, environmental consultants and analysts will, along with larger oil and gas producers, also benefit significantly from use of this system. We will deliver a demonstration system that will set the stage for an electronic infrastructure for access to oil and gas information with future extensibility potential to all states.

91-95 Funding (\$K): 2500      Dates: 1993-present.



Technology Transfer: Software developed will be icensed; there will also be publications and manuals; training sessions for users.

Key Documentation: ACTI Proposal

Key Personnel: Carol Hunter (510) 422-1657, chunter@llnl.gov; Sam Coleman (510) 422-4323, scoleman@llnl.gov; Oscar Nazario (510) 423-0918, nazario@llnl.gov; Bruce Lownsbery (510) 423-4974, bel@llnl.gov; Dwayne Chesnut (510) 423-5053, chesnut@llnl.gov

Lab Capabilities Applied: Computer data storage systems, database development, communication systems, hardware development, software development, earth sciences



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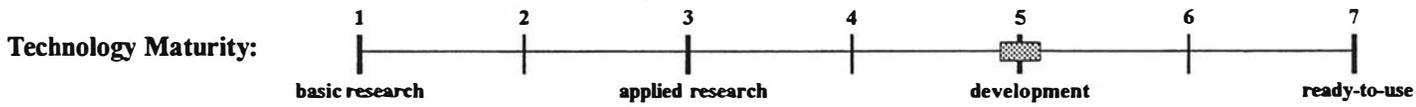
Category: Environmental & Regulatory (10, 12)

Laboratory: Lawrence Livermore National Laboratory      Contact: Conrad Yu (510) 422-7356, yu1@llnl.gov

Title: Portable Micro-machined Gas Chromatograph

**Description:** The object of this project is to develop a portable (real-time) gas detection system to insure the safety of personnel. Industrial plant processing of toxic gases and demilitarization type activities expose personnel to a high degree of risk in a potentially hazardous area. Gas chromatography has proven to be a reliable means of gas detection having very high detection sensitivity. Conventional laboratory GCs are bulky units (many cubic feet in size) which take a long time (typically 20 minute) to analyze a sample gas. LLNL is applying microelectromechanical technology (MEM) and has developed an innovative circular cross-section GC column on silicon wafers. These column's were tested and the results showed high resolution for a mixture of gases. LLNL currently is developing a zero-dead-volume high-temperature injection valve and a high speed to enable packaging of all the components to form a hand-held gas chromatograph. The device can be used to detect gases in the environment, to promote safety near toxic gasses, to monitor gases in tanks and to detect leaks in closed areas. A local industrial firm is seeking participation.

91-95 Funding (\$K): 480      Dates: 1993 - Present



**Technology Transfer:** Micro Technology Inc (MTI) in Fremont is interested in doing miniture GC, and tech transfer operations have been established between LLNL and MTI.

**Key Documentation:** Patent Application

**Key Personnel:** Conrad Yu (510) 422-7356, yu1@llnl.gov

**Lab Capabilities Applied:** MicroTechnology, microfabrication, chemistry



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Category: Oil Processing &amp; Refining (12)

Laboratory: Lawrence Livermore National Laboratory

Contact: Kenneth W. Dolan (510) 422-7971,  
dolan2@llnl.gov

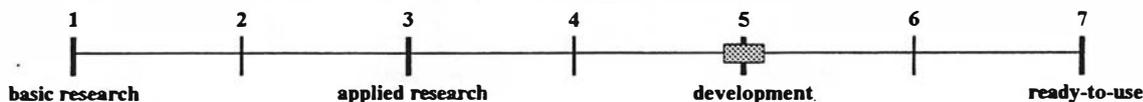
Title: Quantifying Corrosion Damage

**Description:** Advanced infrared, ultrasonic, digital radiography, acoustic, and signal and image processing instrumentation and methods have been developed for federal agency and manufacturing CRADA partners. Dual-band infrared imaging systems have been used to quantify corrosion in pipes for Dow Chemical Corporation, corrosion thinning and pitting in airframes for the FAA and corrosion related delaminations in concrete slabs and bridge decks for FHWA. Customized ultrasonic and acoustic systems, real time radiography, digital radiography and computerized tomography systems, and signal and image processing systems have been developed for CRADA manufacturing partners for on-line and final product inspection for component and weld certification, thickness gauging and dimensioning.

91-95 Funding (\$K): 7800

Dates: 1991 - Present

Technology Maturity:



**Technology Transfer:** Publications in open literature, staff exchanges, cooperative research and development agreements, broad agency announcements, open seminars and training sessions, software co-development agreements, transfers of software to public domain.

**Key Documentation:** N. K. Del Grande, P. F. Durbin and M. R. Gorvad, "Infrared Computed Tomography", and K. W. Dolan, J. J. Haskins, D. E. Perkins and R. D. Rikard, "X-Ray Imaging: Digital Radiography" in Engineering Research, Development and Technology Thrust Area Report FY93, UCRL 53868-93, May 1994.

**Key Personnel:** Nancy Del Grande, (510) 422-1010, delgrande1@llnl.gov; Harry Martz, (510) 423-4269, martz2@llnl.gov; Daniel Schneberk (510) 422-6792, schneberk1@llnl.gov; Graham Thomas (510) 422-7325, thomas2@llnl.gov

**Lab Capabilities Applied:** Dual-band infrared imaging for precise temperature mapping, ultrasonics, acoustic microscopy, laser acoustics, and acoustic monitoring; real-time radiography, digital radiography and computerized tomography at 5 kV to 9MeV; signal and image processing.



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Category: Development (33)

Laboratory: Los Alamos National Laboratory      Contact: Ron Daniel, 505-665-0597, rdaniel@lanl.gov

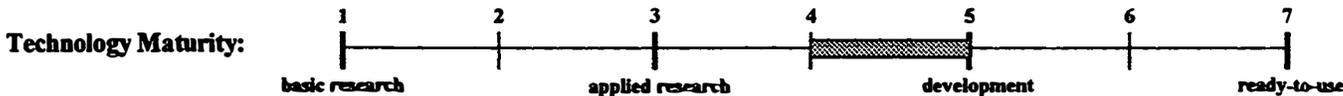
Title: Development of a Uniform Resource Characteristics Service

**Description:** The World Wide Web and its best-known browser, NCSA Mosaic, have taken the world by storm. However, the web's phenomenal growth has revealed a fundamental weakness at its foundation - the system is entirely based on the locations of resources, not their identity. URLs (Uniform Resource Locators) specify a protocol, a host, and a path. This is analogous to citing references by their position on the shelves of a particular library. Identifying a single host and path leads to a bevy of problems with fault-tolerance, network hotspots, and excessive traffic. The web also has fundamental security problems since it was never designed with encryption, authentication, data integrity, or scalable access control in mind.

We have been participating in an Internet Engineering Task Force effort to overcome these problems by allowing people to cite network-accessible resources with a URN (Uniform Resource Name). A name-to-location resolution service, similar in some respects to the Domain Name System, would provide the level of indirection necessary to provide multiple copies of resources and to deal with their migration. The data structure that holds the information for the name to location mapping is known as the URC (Uniform Resource Characteristics). In addition to name and location, we are providing the capability for storing arbitrary metadata about the resource in the URC. Frequently this will be bibliographic information, but more esoteric information such as sensor wavelengths, lattice spacings, price, poetic meter, digital signature, etc. will be necessary depending on the nature of the resource. We plan to accommodate this range of information by using named attribute sets, similar to SGML Document Type Definitions, that can be composed in inheritance hierarchies. The attribute sets are uniquely identified by using a URN, which also lets us retrieve them from across the world if necessary.

The work of discussing usage scenarios and setting requirements is mostly complete. We are now ready to prototype a few approaches to the URC service and compare them. Our goal is to have a prototype URC server, based on the S-HTTP work of CommerceNet, implemented by the end of the summer. We will compare this server with the whois++-based server being developed at Georgia Tech. The results of that comparison would be presented to the IETF at their December meeting.

91-95 Funding (\$K): 300      Dates: 1995 - present



Technology Transfer: Internet Engineering Task Force, Mosaic team at NCSA, Spyglass, S-HTTP technology, Commerce Net

Key Documentation: 1) Ron Daniel and Michael Mealling: URC Scenarios and Requirements; Internet Draft; <URL:ftp://cnri.reston.va.us/internet-drafts/draft-ietf-uri-urc-req-00.txt>

Key Personnel: Ron Daniel, 505-665-0597, rdaniel@lanl.gov  
 Dave Forslund, 505-665-1907, dwf@lanl.gov

Lab Capabilities Applied: Distributed computing, computer security, large databases



Index: 192

**Category:** Exploration (15, 2)

**Laboratory:** Los Alamos National Laboratory      **Contact:** Nancy L. Marusak, 505-667-5698, nmarusak@lanl.gov

**Title:** Facility for Information Management, Spatial Analysis, and Visualization

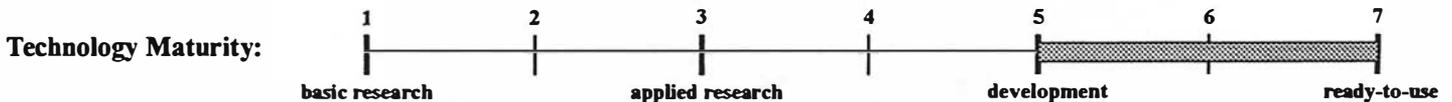
**Description:** The Environmental Restoration (ER) Project office established the Facility for Information Management, Analysis and Display (FIMAD) to provide the tools, systems and expertise needed to support the large amount of spatial and tabular data collected as part of the ER effort at LANL. The information is readily accessible to project participants through a variety of media.

The FIMAD has developed a combination of a Geographic Information System (GIS) using ESRI's Arc/info and Arcview and database management system (Oracle) to provide the tools for customers. Los Alamos has been working using this proven software for three years and has built a highly sophisticated, mature system. The FIMAD encompasses a variety of specialists each concentrating on a different aspect of the ER project's data needs, yet working together to solve complex problems in data analysis, visualization and data manipulation and storage. Specific applications include risk assessment, site characterization, 3D visualization and remediation.

Applications to the oil and gas industry includes a wide range of tasks. Typical analysis are spatial relationship of existing wells, proposed wells, land ownership, cultural features, surface soils, geology and surface sampling locations and topography. Examples of tabular data include well construction, stratigraphy, lithology, wireline logs, pay zone intervals, and seismic information.

With these tools and this type of data, FIMAD provides the capability to display surface locations combined with 3D visualization of the subsurface. In addition, metadata such as production histories, actual lease agreements and legal definitions for wells, land parcels etc. could be scanned into a document management system and accessed via the world wide web.

**91-95 Funding (\$K):** 10000      **Dates:** 1991 - present



**Technology Transfer:** Mosaic, American Society for Photogrammetry & Remote Sensing, American Congress on Surveying and Mapping, New Mexico Geographic Information Council, Jemez Area GIS Users Group, Geographic Information/Land Information System

**Key Documentation:** 1) Color Orthophotography: To Scan or Not, Jan Benson, NCSM/ASPRS Annual Convention and Exposition Technical Papers, Volume 3 Charlotte, North Carolina, Feb 27-Mar2, 1995.  
2. The Ring that Weds GIS and CAD Systems, Tom Garrison, National DOE/Contractors and Facilities CAD/CAE User's Group, Los Alamos, New Mexico, May, 1994.

**Key Personnel:** Thomas McVittie, 505-665-3674, mcvittie@lanl.gov  
Tom Garrison, 505-665-2404, tom@fimad5.lanl.gov  
Jan Benson, 505-667-7665, benson@fimad6.lanl.gov  
Liz Zeiler, 505-665-3610, liz@fimad2.lanl.gov

**Lab Capabilities Applied:** Geology, hydrology, systems engineering, cartography, spatial analysis, database administration, chemical analysis, software development.



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Category: Environmental & Regulatory (10, 7,14)

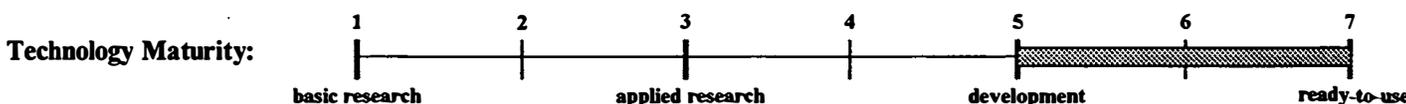
Laboratory: Los Alamos National Laboratory      Contact: W. B. Cottingame, 505-667-8339, wcottingame@lanl.gov

Title: Advanced Lidar Systems for Pollution Monitoring

**Description:** The Lidar / Environmental Applications Project Team at LANL is working to apply recent advances in optical remote sensing and electro-optics to the development and application of a new generation of laser-based systems for air-quality monitoring. This remote sensing technology known as light detection and ranging (LIDAR) provides the means to detect remotely, with high spatial resolution, the constituents making up the atmosphere. This project is for development of enabling technologies for both aerosol lidar, which is sensitive to the atmospheric aerosol and particulate burden, and for species-specific Raman, DIAL, and LIF lidar, which are types of lidar that provide spatially resolved concentrations of molecules and gases through exploitation of unique, species-specific optical characteristics of the individual atmospheric constituents. This technology is applicable to species-specific monitoring of wide areas, such as could be the case for fugitive emissions, and localized sources, such as stacks. Development of industrial-class, laser-based systems that remotely monitor many emissions sources for many chemical species, (the criterion pollutants and a large variety of air toxics) at one time can save installation of individual monitors, which cost over \$100,000 each initially with significant yearly maintenance cost. Such economic benefits ease the burden of compliance and speed realization of the benefits of higher air-quality standards to the public.

This project focuses LANL's twenty-five years of defense and civilian lidar remote sensing experience on conversion of the fruits of recent defense related laser developments toward advanced air-pollution monitoring capabilities. This project is directed toward the realization of significant advancements to reduce the size, complexity, and operational cost and to increase versatility, reliability, and applicability that have to date been effective barriers to commercial acceptance. Our work in developing lidar for air quality was recognized with an R&D 100 Award in 1993 and our "miniature" aerosol lidar was selected as "What is Best in Environmental Science" by Popular Science in 1992.

91-95 Funding (\$K): 5000      Dates: 1991 - present



Technology Transfer: Licensed product, User facility agreements, Funds-in agreements, Joint industrial partnerships, Publications, Field measurements, R&D 100 Award winner

Key Documentation: 1) D. I. Cooper and W. E. Eichinger, Jou. Geo. Res. - Atmospheres 99, 22,937 (1994).  
2) W. T. Buttler, et al., Los Alamos National Laboratory Report, LA-UR 94-2902.

Key Personnel: W. E. Eichinger, 505-665-8062, 72400.3635@CompuServe.com  
D. I. Cooper, 505-667-7537, dcooper@lanl.gov

Lab Capabilities Applied: Lidar remote sensing, Atmospheric science, Laser and optics, Computer science, Atmospheric chemistry, Field Experimentation, Instrumentation



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Category: Environmental & Regulatory (10, 5, 7)

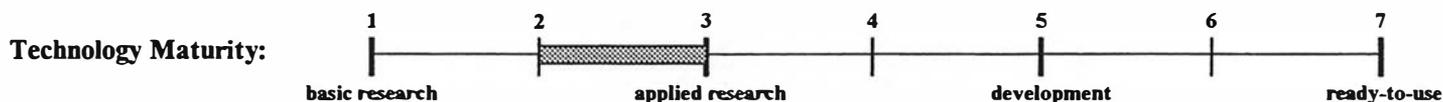
Laboratory: Los Alamos National Laboratory      Contact: Matthew Monagle, 505-665-7422, monagle@lims1.lanl.gov

Title: A Simple New Monitor For Air Emissions

**Description:** Pollution from volatile organic constituents (VOCs) is a problem associated with many petrochemical operations from production through refining to commercial distribution. The objective of this work is to fabricate two simple, rugged and field-deployable monitors for the detection of these VOCs. Currently, we envision one monitor to be developed for organo- sulfur compounds (such as thiophene or H<sub>2</sub>S) while the other would be for non-selective hydrocarbon monitoring. At the heart of this new monitor is a technology being developed at LANL for waste destruction. Using this waste destruction technology on a smaller scale allows us to monitor for constituents in air. We have already demonstrated the monitor for halogenated hydrocarbons in air and we are currently funded to build a continuous air monitor for the local waste management group. We are currently speaking to several commercial instrument vendors regarding the licensing of this technology for environmental applications.

Specific applications for the two monitors would include a sulfur monitor for the measurement of H<sub>2</sub>S in natural gas streams during the sweetening process to measure effectiveness in real-time. Another application of this monitor technology might be the measurement of leaks using the non-specific hydrocarbon monitor. Additional applications of this technology are expected under the Clean Air Act Amendments. The key advantage of this technology, which sets it apart from many existing technologies, is its ability to support these analytical operations without additional reagents. This should make implementation and operation of these monitors a much simpler task.

91-95 Funding (\$K): 3100      Dates: 1994-present



Technology Transfer: Patent application in progress, license specific applications of technology to commercial manufacturers, CRADAs with users and manufacturers of technology

Key Documentation: 1) Patent Application  
2) Due to the novel nature of the technology and the need to protect patent privileges, there is no published literature on this specific technology.

Key Personnel: Jeff Roberts, 505-667 4086, Roberts@lims1.lanl.gov

Lab Capabilities Applied: Instrument development, Environmental chemistry, Analytical chemistry, Waste destruction



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**Category:** Oil Processing & Refining (1, 7)

**Laboratory:** Los Alamos National Laboratory

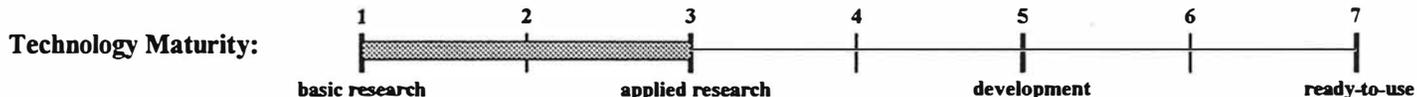
**Contact:** David C. Smith, 505-667-2424, d.smith@lanl.gov

**Title:** Synthesis and Evaluation of New Mixed Metal Nitride Catalysts for Petroleum Refining and Specialty Chemical Manufacturing

**Description:** Transition metal carbides and nitrides possess unique chemical characteristics. These materials are found to have very attractive catalytic properties. For example, molybdenum and tungsten carbides and nitrides resemble the noble Group VIII metals (Pt, Pd, Rh, ...) in catalytic activity and offer superior selectivity, stability and resistance to poisoning. These ceramics also often form continuous solid solutions over large composition ranges. The combination of these provisions has led to the speculation that optimum catalytic activity for specific reactions can be found among the mixed metal materials.

The goal of the Los Alamos effort is to develop high specific surface area bimetallic nitride catalysts,  $M_xM_yN_z$ , with desired catalytic activity and/or selectivity. We will demonstrate the applicability of a new low-temperature synthetic technique. The catalytic activity and/or selectivity of these systems will be determined. From these results the effects of metal stoichiometry on surface electronic structure and catalytic activity and/or selectivity will be quantified. Through our efforts, it will be possible to intelligently choose alloying schemes to optimize a catalytic compound.

**91-95 Funding (\$K):** 100      **Dates:** 1994 - present



**Technology Transfer:** CRADA, publication in open literature

**Key Documentation:** None

**Key Personnel:** David C. Smith, 505-667-2424, d.smith@lanl.gov  
 Joseph Barrera, 505-665-0907

**Lab Capabilities Applied:** Synthetic Chemistry, Materials Characterization



Index: 196

Category: Development (16, 3, 8, 10)

Laboratory: Los Alamos National Laboratory      Contact: D.S. Dreesen, 505-667-1913, dreesen@lanl.gov

Title: Mapping Conductive Fractures Using a Through-Tubing Geophone Receiver Array (Slimline Through-Tubing Geophone Receiver Array)

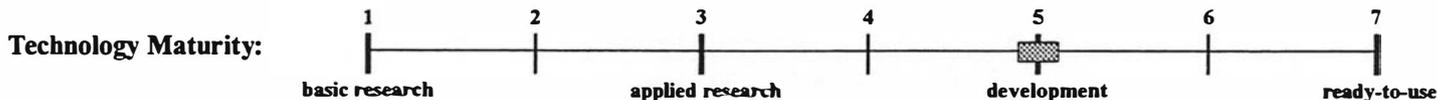
**Description:** Seismic mapping and VSP surveys in oil and gas reservoirs require costly well preparation and extended instrumentation deployments to locate natural features and conduct deep structural investigations of a reservoir. Preparation of wells for deployment of seismic receivers typically includes removal of tubing and installation of bridge plugs. Other costs include returning the well to production and delayed production. Through-tubing tools will significantly reduce well preparation and return to production costs.

A CRADA with Schlumberger Well Service (SWS) was approved in July 1994. Schlumberger has provided operational support for the Alaskan geophone deployment, consultation and support for the 1-11/16" tool design, and cable heads, housings, and running hardware for the array tool. Los Alamos has designed and tested the sonde anchoring system and all of the electronics. Successful through-tubing operations have been demonstrated using a single modified Los Alamos 3-1/4" diameter geophone tool deployed in Prudhoe Bay wells with large diameter tubing.

Prototype Tools: Los Alamos has designed a modular, 1-11/16" diameter tool using SWS 22-pin connections. Design features include a 3-orthogonal-axis geophone receiver, an electric motor powered anchor, weight bar, a 3-axis inclinometer, a Casing Collar Locator, downhole amplification, and a modem to receive operating commands from the surface. One conductor will be used for power while the remaining conductors in the 7-conductor wireline will be used for signals. The spacing between the sondes can be set from 20 ft to 200 ft.

Well Testing: ARCO, Exxon, Texaco, Enserch, and Meridian have expressed interest in fielding the tools in test wells, for VSP demonstrations, and in microseismic mapping demonstrations.

91-95 Funding (\$K): 780      Dates: 1992 - present



Technology Transfer: CRADA No. LA93C10075, Project Review Meetings, Internal/External Quarterly Reports, SPE Papers, SPE Presentations,

Key Documentation: 1) Brady, J.L. et al: "Microseismic Monitoring of Hydraulic Fractures in Prudhoe Bay," Tech Paper SPE 28553, Sept., 1994.  
2) Rutledge, J.T. et. al: "Subsurface Fracture Mapping Using Microearthquakes Detected During Primary Oil Production. Clinton County, Kentucky," Tech Paper SPE 28384, Sept., 1994.

Key Personnel: D.A. Anderson, 505-667-1441, anderson@seismo5.lanl.gov  
T.D. Fairbanks, 505-665-4159, fair@seismo5.lanl.gov  
J.T. Rutledge, 505 667-8938, rutledge@seismo5.lanl.gov

Lab Capabilities Applied: Microseismic Mapping, Well Deployed Seismic Receivers, Petroleum Reservoir Engineering, Well Completion and Downhole Instrumentation, Engineering Analysis, Well Logging and Downhole Measurement, Diagnostics, Instrumentation, Field Testing



Index: 197

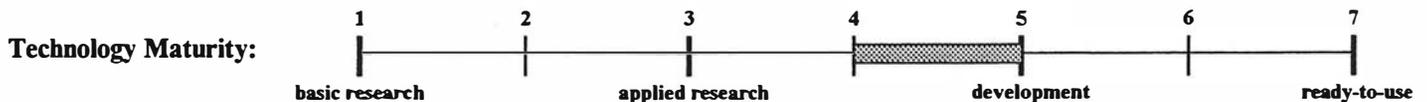
Category: Environmental & Regulatory (11)

Laboratory: Los Alamos National Laboratory      Contact: Joseph R. Duke, Jr., 505-667-1328, jduke@lanl.gov

Title: Microcellular Foams for the Separation of Heavy Metal-Ions from Waste Streams

**Description:** In the late 70's Los Alamos began to study the development of ultra-low density, microcellular foams for applications in a variety of physics experiments which required substances that simulated the presence of "high pressure gases". The results of these studies produced low density, homogeneous, open-celled, and highly porous polymeric foams and a significant technology base for production of these types of materials. Work on these polymeric foams continued throughout the 80's and into the 90's for applications including structural materials and most recently for use in actinide separations in our waste streams. Due to the open-celled nature of the foams and their high porosity, studies in the early 90's focused on using the materials for resins, similar to ion-exchange resin-beads. Various methods of functionalizing these materials with chelating ligands specific for actinides and water soluble polymers with chelating groups were investigated. Our studies to date indicate that these materials out perform resin beads, of similar compositions, when used to remove metal-ions from solutions. Presently, we are investigating flow through these materials under Laboratory Directed Research and Development funding and are investigating their use for separations of cesium, strontium, uranium, and plutonium from waste and processing streams. These materials can be used as hydrophobic materials for absorbing oil-spills when unfunctionalized and as resins for removing metal-ions from waste and processing streams. Depending upon the composition of the waste stream the foams need to be tailored to achieve specificity and separations efficiency.

91-95 Funding (\$K): 500      Dates: 1992-Present



Technology Transfer: Patents, Publications in open literature, Presentations at technical meetings

Key Documentation: 1) Williams, Joel M., et al. "Composite Foams" US Patent 5,037,859, Aug. 6, 1991, 2) Steckle, Warren P., Duke, Joseph R., Jorgensen, Betty S.; "Cobalt Dicarbolide Containing Polymer Resins for Cesium and Strontium Uptake"; Metal Containing Polymeric Materials; Pittman, C. U., et al., eds.; Plenum Publishing, New York, NY; 1995.

Key Personnel: Warren P. Steckle, 505-667-3619, steckle@lanl.gov  
Betty S. Jorgensen, 505-667-3619, betty@lanl.gov  
Robert E. Hermes, 505-667-6862, hermes@lanl.gov

Lab Capabilities Applied: Polymer chemistry, low density foam fabrication, foam characterization.



Index: 198

Category: Environmental & Regulatory (8, 14)

Laboratory: Los Alamos National Laboratory      Contact: Sumner Barr, 505-665-2868, barr@lanl.gov

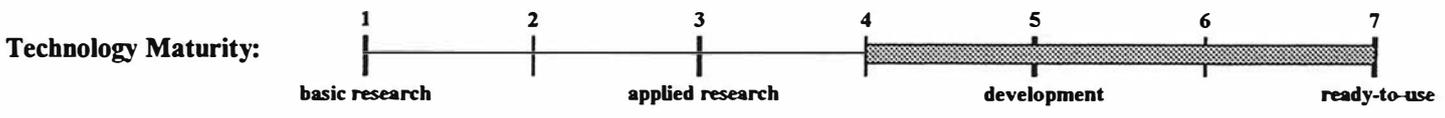
Title: Atmospheric Transport and Fate of Pollutants Over Complex Terrain

**Description:** The traditional perspective on atmospheric pollution is driven by regulatory compliance which invariably has a strong simplistic and conservative bias. As we follow the current trend to go beyond compliance, many companies are finding long term profitability by using air pollution assessment tools that emphasize accuracy and flexibility by incorporating the most complete physics and chemistry. Advanced computational methods have enabled us to build models that run on users' workstations and couple chemistry, aerosols, complex terrain, deposition and other processes into fully 3D time dependent forecasts of pollutant distribution and fate.

The requirements for accurate prediction of the fate of atmospheric emissions from industrial processes go far beyond regulatory compliance. They include facility siting, design, and operations as well as emergency preparedness and post-event dose reconstruction.

As a result of decades of research into the processes affecting pollutant dispersal and transformation in settings of complex terrain, vegetation, and land use, Los Alamos has developed high performance models that we tailor to meet the clients' special needs (e.g. emergency response, site specificity vs. generic, user friendly, scale of interest). We usually couple the model application with an experimental phase for validation, establishment of the optimum network of model inputs, and assurance that the important physical/chemical processes are highlighted. The product is much more than a computer code but is a highly responsive capability directed to the client's application. We support both software and data collection until the customer feels ready for independence.

91-95 Funding (\$K): 5250      Dates: 1979-present



Technology Transfer: Journal publications, book chapters, computer codes, collaborations with users

Key Documentation: 1) Barr, S., and M. M. Orgill, "Influence of External Meteorology on Nocturnal Valley Drainage Winds," Journal of Applied Meteorology, 28, 497-517 (1989)  
 2) Williams, M. D., T. Yamada, G. L. Stone, S. Barr, and W. E. Clements, "Chemical Downwind Hazard Modeling Study: Evaluation of Model Concepts and Site Assessment," Los Alamos National Laboratory Report LA-UR-87-897 (January 1987).

Key Personnel: Jim Bossert, 505-667-6268, bossert@lanl.gov  
 Chih-Yue Jim Kao, 505-667-9226, kao@vega.lanl.gov  
 James T. Lee, 505-667-8352, lee@vega.lanl.gov  
 Keeley Costigan, 505-665-4788, krc@vega.lanl.gov  
 Scott Elliott, 505-667-0949, selliot@kokopelli.lanl.gov

Lab Capabilities Applied: Atmospheric physics, atmospheric chemistry, aerosol science, computational fluid dynamics, high performance computing, cloud dynamics



**Index:** 199

**Category:** Development (16, 3, 8, 10)

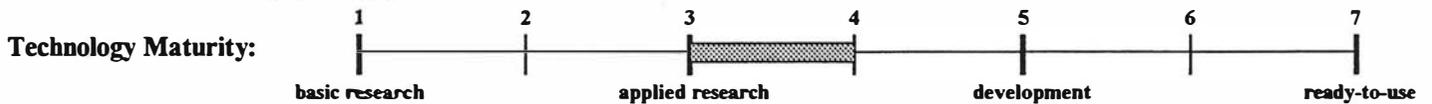
**Laboratory:** Los Alamos National Laboratory      **Contact:** Jim Albright, (505) 667-4318, albright@seismo5.lanl.gov

**Title:** Advanced Sensor Technology for Microholes and Other Seismic Applications

**Description:** A broad based technology integration and development program has been embarked upon with the goal of demonstrating the feasibility of substantially reducing the costs of subsurface deployment of geotechnical instrumentation. Discussions with the drilling industry, engineering calculations, and cost analyses have provided encouragement to explore the use and advantages of 1" diameter boreholes (referred to as microboreholes) drilled with coiled tubing to depths ranging from 100 to 10,000 ft. In comparison to production hole drilling, scale factors ranging up to 40 are possible for reductions in pipe weight, circulating fluid volume, and drill site foot print. Consequently, microholes have the potential to be drilled for much less than conventional-size holes. Similarly, substantial cost reductions can be expected for wireline draw works, hoisting and telemetry cables, and borehole instrumentation.

The focus of this project is on borehole seismic instrumentation. Tasks include: the identification or development of miniature geophones and accelerometers meeting microborehole size constraints; fabrication of borehole instrumentation packages; fabrication and testing of a wireline unit for deployment of the packages; installation of the packages in simulated microboreholes; and performance comparisons with existing technology at oil industry test sites. In addition to microborehole installation, these sensors will be suitable either for wireline deployment in 5/8" coiled tubing, or for 5/8" packed tubing deployment in the tubing-casing annulus of producing wells. Applications include crosswell, vertical seismic profiling, exploration seismic, and monitoring of induced reservoir seismicity. Geophones meeting these rigid size requirements have been fabricated by a commercial source and are undergoing prototype testing.

**91-95 Funding (\$K):** 225      **Dates:** 1994-present



**Technology Transfer:** Presentations at workshops, symposia and meetings, publication in professional society journals, field testing at commercial sites, collaboration with geophone manufacturers.

**Key Documentation:** None to date. Multiple expanded abstracts will be submitted for presentations at upcoming Society of Petroleum Engineers and DOE-sponsored symposia.

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Tom Fairbanks, (505) 665-4159, fair@seismo5.lanl.gov  
Dave Anderson, (505) 667-1441, anderson@seismo5.lanl.gov

**Lab Capabilities Applied:** Logging tool design, borehole seismic analysis and interpretation, field testing, drilling and completions, reservoir analysis, mechanical and electrical engineering, well test facilities.



Index: 200

Category: Development (16, 3, 8, 10)

Laboratory: Los Alamos National Laboratory

Contact: D.S. Dreesen, 505-667-1913, dreesen@lanl.gov

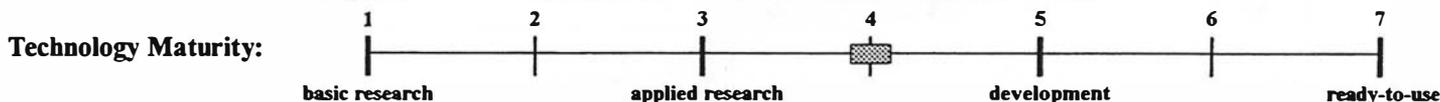
Title: Advanced Instrumentation for Fracture Mapping/Microseismic (Downhole Microprocessor for Mono-cable Telemetry Systems)

**Description:** Seismic mapping in oil and gas reservoirs requires costly well preparation and extended instrumentation deployments to locate natural features and conduct deep structural investigations of a reservoir. For longer deployments, wireline costs will be an increasing fraction of the total cost. Methods to reduce the wireline costs include (1) replace 7-conductor wirelines with mono-cables, and (2) develop park-and-release instrumentation that allows the wireline to be demobilized during long deployments. The data rate for commercial mono-cable telemetry systems is too slow to monitor multiple on-line geophones. The use of downhole processors promises a method to reduce the required telemetry rate by discriminating seismic events of interest from background noise and feeding data to the telemetry system at a constant rate.

While park-and-release systems will require technology breakthroughs in batteries, downhole cooling, and downhole data storage beyond the scope of the current project, downhole processors will be a critical component of a future park-and-release system.

Mono-cable is typically fielded at a significantly lower cost, is more widely available, is normally used for cased-hole logging, and is much better suited for operations in wells with a potential for high shut-in pressure. The possibility of leaks or spills in the operation of pressure control equipment is reduced significantly using a smaller diameter mono-cable instead of larger diameter, 7-conductor lines. Schlumberger will provide a commercial mono-cable telemetry system and limited technical support to conduct a bench top demonstration of a prototype system.

91-95 Funding (\$K): 265 Dates: 1995 - present



Technology Transfer: Quarterly Reports once project is initiated, Trade Journal Articles, Internet Home Pages

Key Documentation: 1) Brady, J.L. et al: "Microseismic Monitoring of Hydraulic Fractures in Prudhoe Bay," Tech Paper SPE 28553, Sept., 1994. 2) Rutledge, J.T. et. al: "Subsurface Fracture Mapping Using Microearthquakes Detected During Primary Oil Production, Clinton County, Kentucky," Tech Paper SPE 28384, Sept., 1994.

Key Personnel: T.D. Fairbanks, 505-665-4159, fair@seismo5.lanl.gov J.T. Rutledge, 505-667-8938, rutledge@seismo5.lanl.gov

Lab Capabilities Applied: Borehole tool development, borehole seismology, microseismic mapping, reservoir characterization and engineering, well completion and downhole instrumentation, well logging and downhole measurement.



Index: 201

Category: Deepwater Offshore (11)

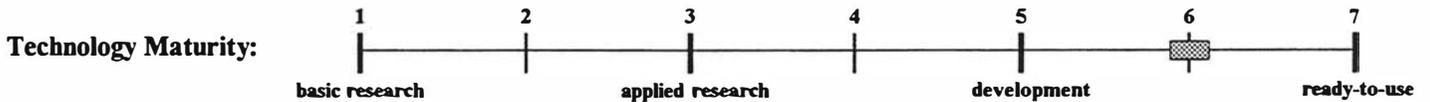
Laboratory: Los Alamos National Laboratory      Contact: Ronnie B. Parker, (505)667-8587, parker@lanl.gov

Title: Fatigue Failure of Top Drive Drilling Rigs to Jarring Operations

**Description:** Los Alamos will evaluate the structural loads that are transmitted to a top drive drilling rig during jarring operations. Past performance of top drives while jarring indicate potential safety problems during the event. The Los Alamos effort will characterize the loading associated with jarring by reviewing literature, providing instrumentation, and performing numerical modeling on pertinent components. We plan to familiarize ourselves with the operation of top drives and particularly their operation during a jarring operation.

An instrumentation package consisting of numerous accelerometers and strain gages has been designed and fabricated. This package was tested during dynamometer tests on a Varco rig at the factory. It is now ready for field testing on a top drive rig during production offshore operations. With help from Varco BJ International and Shell Drilling we plan to instrument a top drive during jarring operations. These tests will gather accelerometer and strain data during the event. We will use this data to characterize the loading events transmitted to the top drive during the jar. The test data will be used to numerically model components of the top drive to determine structural response to the load environment. The data and analysis will then be used to develop jar limiting criteria for existing top drive systems, and will provide loading conditions for future designs of top drive systems.

91-95 Funding (\$K): 175      Dates: 1993 - present



Technology Transfer: Drilling Engineering Association Seminars, Trade Journal Articles, SPE Papers, INTERNET Home pages

Key Documentation: Pending Completion of the field tests on a top drive rig.

Key Personnel: Ronnie B. Parker, 505-667-8587, parker@lanl.gov  
William E. Baker, 505-667-7776, webaker@carina.unm.edu

Lab Capabilities Applied: Engineering Analysis, Mechanical Engineering, Diagnostics, Instrumentation, Simulation, Field Testing, Finite Element Methods, Fatigue Analysis, Structural Response Analysis to Dynamic Loading



Index: 202

Category: Oil Processing & Refining (1, 11), Environmental & Regulatory (10)

Laboratory: Los Alamos National Laboratory      Contact: Ray Stringfield, 505-667-1477, stringfield\_r@lanl.gov

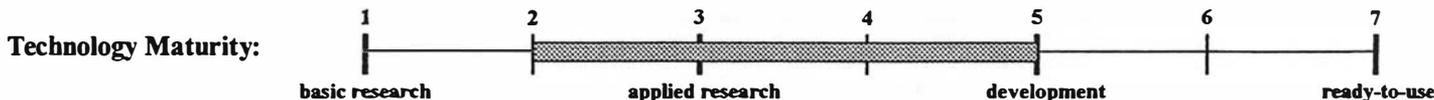
Title: Microwave Driven Chemistry

**Description:** The project goals are to design methods to scale-up microwave processes to the industrial scale and also to develop new chemistry processes using microwaves instead of conventional heating. Examples of new processes include organic chemical synthesis, waste decomposition, chemical separation, plasma chemistry, and plasma surface processing. The technical approach uses state of the art microwave technology developed for particle accelerators and the nuclear weapons program.

Microwaves have the advantages of localized heating, low thermal inertia, flexible control, and feasible production scaling to small size plants to minimize the environmental impact of accidents and transportation from the point of use from centralized plants. In addition, new chemistry processes have been discovered that have not been possible using thermal heat sources. Uses have been identified in several areas of chemistry, including refinery combustion emissions, petroleum demetallization, improved chemical reactor design, separations science, energy efficiency improvements, catalysis, combustion science, waste water treatment and waste slugs, solid waste disposal, and gaseous emissions.

Advanced computer modeling is used to design microwave applicators with great detail. Supercomputers, work stations, and sophisticated semi-analytical models are all used as needed to appropriately design each aspect of these applicators. Other computer models study the chemistry induced from first principles. In addition to unique computational and theoretical capabilities, Los Alamos has a large variety of microwave sources ranging in frequency from 200 MHz (1 MW average power) to 84 GHz (30 kW average power), rf control system technology able to control both microwave power and frequency, magnetic field engineering design and construction facilities capable of building systems of 1 meter and larger cross section. Industrial partners have collaborated in identifying chemistry problems of commercial interest, and have provided crucial insight into the requirements of final production system reliability and adaptability. We anticipate that adapting conventional processes to microwave based production systems (for solids, liquids, gases, and plasmas) can reduce the cost of product manufacture by up to ten percent, and also enable manufacture in smaller economic units, with more flexible product requirements than conventional processing.

91-95 Funding (\$K): 3000      Dates: 1990 - present



Technology Transfer: Publications, industry staff exchange, CRADAs,

Key Documentation: Not Available (CRADA Protected)

Key Personnel: Ray Stringfield, 505-667-1477, stringfield\_r@lanl.gov

Lab Capabilities Applied: Accelerator design, supercomputer modeling, microwave diagnostics, advanced optical and laser diagnostics, chemistry and chemical engineering/plant design



Index: 203

Category: Deepwater Offshore (16, 9)

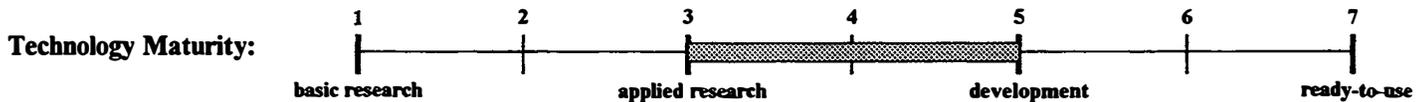
Laboratory: Los Alamos National Laboratory      Contact: Chuck Farrar, 505-667-4551, farrar@lanl.gov

Title: Damage Detection and Health Monitoring of Structures and Mechanical Systems

**Description:** The interest in the ability to monitor a structure and detect damage at the earliest possible stage is pervasive throughout the civil and mechanical engineering communities. Current damage detection methods are either visual or localized experimental methods such as acoustic or ultrasonic methods, magnet field methods, radiographs, eddy-current methods and thermal field methods. All these experimental methods require that the vicinity of the damage is know a priori and that the portion of the structure being inspected is readily accessible. The need for more global damage detection methods that can be applied to complex structures has lead to the development of methods that examine changes in the vibration characteristics of the structure. Damage or fault detection, as determined by changes in the dynamic properties or response of structures, is a subject which has received considerable recent attention in the literature. The basic idea is that modal parameters, notably frequencies, mode shapes, and modal damping, are a function of the physical properties of the structure (mass, damping, and stiffness). Therefore, changes in physical properties of the structure, such as its stiffness or flexibility, will cause changes in the modal properties.

Much of the early work in this field was performed by oil companies in the 1970s and early 1980s because of interest of in offshore oil platform safety assessment. Since these investigations, many advances have been made in this field. Currently, Los Alamos is applying neural network technology to examine vibration characteristics that are indicative of damage and the location of the damage. We are also studying the various damage identification algorithms described in the technical literature and applying them to experimental and analytical data obtained form an actual bridge structure that was systematically damaged. Los Alamos has also developed state-of-the-art sensors and signal processing hardware for specific application to the damage identification problem.

91-95 Funding (\$K): 1400      Dates: 1991 - present



**Technology Transfer:** Quatro Corporation has commercialized the electronic hardware and sensors developed for damage identification, technical reports and presentations.

**Key Documentation:** 1) C. R. Farrar, et al., "Dynamic Characterization and Damage Detection in the I-40 Bridge over the Rio Grande," Los Alamos National Laboratory report LA-12767-MS, (June 1994).  
2) D. J. Jauergui and C R. Farrar, " A Comparison of Various Damage Identification Algorithms Using Experimentally Measured and Analytically Generated Vibration Data," Los Alamos National Laboratory report (in preparation).

**Key Personnel:** Chuck Farrar, 505-667-4551, farrar@lanl.gov  
Al Migliori, 505-667-2515, miglioni@lanl.gov  
Norm Hunter, 505-667-2099, hunter@lanl.gov

**Lab Capabilities Applied:** Digital signal processing, advanced sensor design, design of signal processing hardware, finite element analysis, nonlinear system identification, advanced vibration analysis, neural network algorithms, experimental vibration measurements.



Index: 204

**Category:** Development (25,2,6), Exploration (15)

**Laboratory:** Los Alamos National Laboratory      **Contact:** Richard P. Kendall, 505-667-0961, rpk@vega.lanl.gov

**Title:** National Information Infrastructure Technologies Applied to Database Synthesis and Remote Problem-Solving for the Carpinteria Reservoir Re-Development Project

**Description:** To forestall the premature abandonment of fields (perhaps as many as 20) along the California coast, the development practices of the sixties must be updated with advanced reservoir management techniques. These techniques reduce re-development costs and implementation time. They depend on high quality, integrated computer models and databases.

The current project includes four tasks: (1) POSC-compliant database generation for geological, petrophysical and reservoir engineering data; (2) integration of petrotechnical applications; (3) development of geological models of the Carpinteria Field ("models" is plural because of the use of geostatistical methods to distribute geological attributes throughout the reservoir; and (4) development of engineering models to forecast production from alternative re-development scenarios. Although the specific focus of this project is a California offshore field, the methodology is applicable to other re-development projects where re-characterization of the reservoir is important. This project is industry-lead through working groups which provide guidance and promote technology transfer.

**91-95 Funding (\$K):** 100      **Dates:** 1994 - Present



**Technology Transfer:** SPE Papers (pending), INTERNET Home Pages, collaboration with Carpinteria field producers

**Key Documentation:** In preparation.

**Key Personnel:** Richard Kendall, 505-667-0961, rpk@vega.lanl.gov  
George Zivoloski, 505-667-1581, gaz@vega.lanl.gov  
Earl Whitney, 505-667-3595, earl@vega.lanl.gov

**Lab Capabilities Applied:** Petroleum Engineering, Reservoir Engineering, Geostatistics, Geological Modeling, Flow Simulation, Distributed Databases, Distributed Computing



Index: 205

Category: Gas Gathering (1), Gas Storage (7)

Laboratory: Los Alamos National Laboratory      Contact: Greg Swift, 505-665-0640, swift@lanl.gov

Title: Thermoacoustic Natural Gas Liquefier

**Description:** In a collaboration with Cryenco Inc. (Denver CO) and with NIST-Boulder, we are developing a combustion-powered natural gas liquefier with no moving parts and requiring no electrical power. It will have high efficiency, remarkable reliability, and low cost.

This thermoacoustic natural gas liquefier (TANGL) will be maintenance-free, inexpensive, portable, and environmentally benign. It will be used for economic recovery of natural gas from wells too remote to justify construction of a gas pipeline, for small scale local liquefaction of gas as a transportation fuel, for offshore gas recovery from sites inaccessible to pipelines, for recovery of gas entrained in petroleum, and for recovery of gas from biowaste.

The liquefier will comprise a thermoacoustically driven orifice pulse tube refrigerator. In short, the device uses acoustic phenomena to produce refrigeration from heat, with no moving parts. The system will comprise nothing more than heat exchangers and pipes, made of common materials, without exacting tolerances.

91-95 Funding (\$K): 850      Dates: 1993 - present



Technology Transfer: Publications in the open literature, talks at cryogenic engineering conferences, announcement in Commerce Business Daily, news releases, patent licensing, cooperative R&D

Key Documentation: 1) G. W. Swift, R. A. Martin, and R. Radebaugh, "Acoustic Cryocooler", US patent 4,953,366, September 4, 1990.  
 2) G. W. Swift, "Thermoacoustic engines", Journal of the Acoustical Society of America, Vol. 84, p. 1145 (1988).

Key Personnel: Greg Swift, 505-665 0640, swift@lanl.gov  
 David Gardner, 505 665-4318, gardner@rayleigh.lanl.gov

Lab Capabilities Applied: Thermal physics, acoustics, cryogenics, heat pipes, heat transfer engineering



Index: 206

**Category:** Environmental & Regulatory (12, 2, 11), Oil Processing & Refining (11)

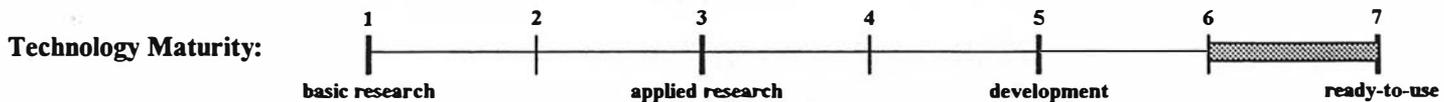
**Laboratory:** Los Alamos National Laboratory      **Contact:** W. J. Parkinson, 505-667-7021, parkinson@lanl.gov

**Title:** An Intelligently Controlled Three-Phase Centrifuge for Petroleum Waste Separation

**Description:** A portion of our project was to demonstrate the technical and economic feasibility of using centrifuge technology for separating petroleum tank bottoms and refinery wastes into salable oil, clean solids, and clean water. We demonstrated that it could be done with a unique 3-phase centrifuge for a break-even cost, using some very difficult-to-separate wastes. We are now improving the process, by developing an intelligent control system for more economical operation and fluid dynamic modeling for improved future centrifuges. Our modifications to the centrifuge system will make the process better and more economical.

This excellent and unique process was developed by a small company. It would make economic sense to make this centrifuge process an integral part of every refinery and oil field operation in the country. It would eliminate hazardous wastes and increase oil production in all cases. Unfortunately, it requires a great deal of skill and experience to run the process. Highly skilled operating labor is the largest contributor to the cost of the operation. Our advanced intelligent control and set-up system will make it possible for an ordinary operator to set up and operate the process. The fluid dynamic modeling will help us understand flow patterns, which will in turn help improve separations and reduce wear in future centrifuges. Maintenance due to wear is the second-most costly part of this technology.

**91-95 Funding (\$K):** 1830      **Dates:** 1993-present



**Technology Transfer:** Cooperative research and development agreement, field demonstrations at waste sites, publications in the open literature, presentations at national technical conferences

**Key Documentation:** 1) CRADA, An Intelligently Controlled 3-Phase Centrifuge for Waste Separation, LANL and Centech Inc.  
2) Parkinson, W.J., et.al.: "Centrifuge Technology for Minimizing Petroleum Waste", International Journal of Environmentally Conscious Design & Manufacturing, Vol. 2, No. 1, 1993.

**Key Personnel:** Ron Smith, 505-667-7002, ronsmith@lanl.gov  
Alan Graham, 505-665-5259, graham@lanl.gov  
Ray Steele, 505-667-5463, steele@lanl.gov

**Lab Capabilities Applied:** Chemical Engineering, Petroleum Engineering, Electrical Engineering, Advanced Process Control, Fluid Dynamic Computer Modeling, Artificial Intelligence



Index: 207

Category: Drilling & Completion (5, 1, 6), Production (5, 18, 25)

Laboratory: Los Alamos National Laboratory      Contact: Peter M. Roberts, 505-667-1199, proberts@lanl.gov

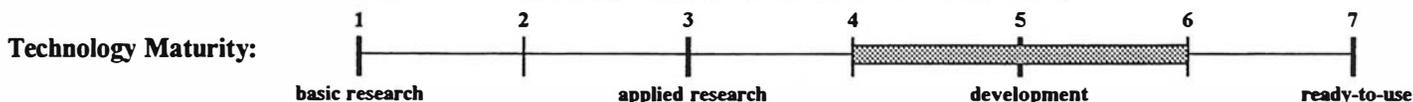
Title: Ultrasonic Reduction of Wellbore Deposits and Formation Damage

**Description:** Oil recovery procedures historically have been hindered by various types of wellbore and near-wellbore formation damage that either plug up perforations in the wellbore casing or reduce the effective permeability of the oil-bearing formation around the wellbore. Existing methods used by the oil production industry to remedy these problems are often costly, environmentally unsound and can produce additional damage if not carried out carefully.

The primary goal of this project is to investigate the effectiveness of using ultrasonic waves for removing particulates and chemical precipitates from wellbores and the surrounding formation, thereby restoring permeability and increasing the economics of producing older wells that might otherwise be abandoned. The main deliverable will be a fully-functional downhole-deployable ultrasonic cleaning tool. When the hardware and methods have been developed to the point where a formula for a successful cleaning treatment can be established, the technology will be transferred to industry.

Currently, this project involves a collaboration between Schlumberger-Doll Research, ForcEnergy, Perf-Clean International, The Measurement Group, University of Texas at Austin, and Los Alamos National Laboratory. Schlumberger-Doll is responsible for performing high-pressure cleaning tests in their laboratory, using a downhole-compatible ultrasonic source developed by The Measurement Group. ForcEnergy will provide support for field cleaning tests that are planned for the upcoming year. Perf-Clean International owns a fluid-driven shock wave device for use in similar applications. They will provide access to their technology and support for field comparison tests with the ultrasonic tool.

91-95 Funding (\$K): 550      Dates: 1991 - present



Technology Transfer: Prototype downhole ultrasonic cleaning tool, field performance characterization data, comparisons with existing technologies, journal publications, network home pages

Key Documentation: Venkitaraman, A., P. M. Roberts and M. M. Sharma: "Ultrasonic Removal of Near Wellbore Damage Caused by Fines and Mud Solids", Proc. Soc. Petrol. Eng. Intl. Symp. Formation Damage Control, SPE 27388: 441-449 (1994).

Key Personnel: Peter M. Roberts, 505-667-1199, proberts@lanl.gov  
Mukul M. Sharma, 512-471-3257, mukul\_sharma@utpe.pe.utexas.edu  
Timothy Jones, 203-431-5248, tjones@ridgefield.sdr.slb.com

Lab Capabilities Applied: Petroleum Engineering, Formation Damage Characterization, Physical Acoustics, Ultrasonic Testing, Instrumentation, Electrical and Mechanical Engineering, Wave Propagation Modeling, Source Characterization, Field Deployment and Testing



Index: 208

Category: Exploration (4, 3)

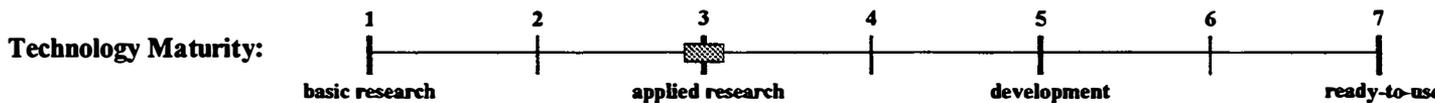
Laboratory: Los Alamos National Laboratory      Contact: Michael Fehler, 505-667-1925, fehler@lanl.gov

Title: Testing Advanced Computational Tools for 3D Seismic Analysis Using the SEG/EAEG Model Dataset

**Description:** The development of a 3-D structural and stratigraphical model of hydrocarbon reservoirs is crucial for the future ability of the exploration industry to economically discover and produce oil and gas. 3-D model building requires extensive use of accurate imaging and modeling of 3-D seismic data. These computational tasks are extremely expensive and new ideas and methods are necessary for making them cost-effective. An important step for the advancement of the state of the art in 3-D seismic technology is the collaborative 3-D Seismic Modeling project undertaken by the Society of Exploration Geophysicists (SEG), the European Association of Exploration Geophysicists (EAEG), and the U.S. Department of Energy (DOE). This collaboration has designed realistic subsurface models for two challenging and relevant exploration plays: a sub-salt reservoir and an overthrust structure. Two extensive 3-D seismic surveys will be computed over these geological models, employing thousands of supercomputer CPU hours and generating hundreds of GigaBytes of data. In this project we aim to enhance the value to the oil industry of the 3-D Modeling Project by developing several new 3-D seismic methods and by testing them using the results of the 3-D Modeling Project.

This project is a collaborative effort between Los Alamos, Oak Ridge National Laboratory and Lawrence Livermore National Laboratory, five universities, the Society of Exploration Geophysicists, and several US petroleum companies. The computational resources of the Los Alamos Advanced Computing Laboratory will be used to support this project. This effort is also complemented by other ongoing 3-D seismic processing efforts at Los Alamos.

91-95 Funding (\$K): 775      Dates: 1995-present



**Technology Transfer:** Internet documentation, meetings with industry and university partners, presentations/workshops at technical meetings, publications in open literature, availability of codes to partners, porting of codes to participants during development.

**Key Documentation:** New project just being initiated, Advanced Computational Technology Initiative Proposal.

**Key Personnel:** Michael Fehler, 505-667-1925, fehler@lanl.gov  
Leigh House, 505-667-1912, house@seismo5.lanl.gov

**Lab Capabilities Applied:** Seismology, mathematics, parallel computing, numerical analysis and algorithms development, laboratory acoustics facilities, prestack migration of seismic data, advanced computing laboratory.



Index: 209

Category: Oil Processing & Refining (25,6)

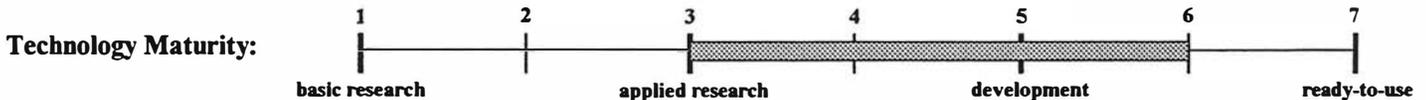
Laboratory: Los Alamos National Laboratory

Contact: B. A. Kashiwa, 505-667-8812, bak@lanl.gov

Title: Computer Simulation of Reactive Multiphase Flow

**Description:** Our CRADA projects with both Amoco and Exxon are aimed at adapting existing Los Alamos multiphase flow computer codes, (referred to as CFDLIB for Computational Fluid Dynamics Code Library), to provide detailed 2 and 3-dimensional simulations of reactive multi-phase flows in refinery units with complex geometries on modern workstations, supercomputers and massively parallel supercomputers. The refinery units to be simulated are Amoco's Ebullated Bed Resid Hydrocracking Unit and Exxon's Fluid Catalytic Cracking Units. These projects combine Los Alamos' unique capabilities in computational flow simulation, multiphase and turbulence theory and massively parallel supercomputing with the industrial partners' experimental, computational and process know-how. The industrial partners' contributions include performing experiments, assisting with theory and code development and testing simulation predictions against proprietary and non-proprietary benchmarking data. Once fully developed, CFDLIB will provide optimization capabilities well beyond current state-of-the-art. CFDLIB will be of a very general nature and will be applicable to a variety of additional refinery processes such as H2SO4 alkylation reactors, delayed and fluid cokers, trickle-bed reactors, fluidized bed combustion reactors, etc.

91-95 Funding (\$K): 2100      Dates: 1992-present



**Technology Transfer:** CRADAs with Amoco and Exxon, open literature publication, e-mail, teleconferences, presentations, workshops

**Key Documentation:** 1) B.A. Kashiwa and R. M. Rauenzahn, "A Multimaterial Formalism," Proceedings, ASME Symposium on Numerical Methods for Multiphase Flows, Lake Tahoe, NV, 19-23 June 1994. 2) B. A. Kashiwa, N. T. Padial, R. M. Rauenzahn and W. B. VanderHeyden, "A Cell-Centered ICE Method of Multiphase Flow Simulations," Proceedings ASME Symposium on Numerical Methods for Multiphase Flows, Lake Tahoe, NV, 19-23 June 1994.

**Key Personnel:** D. B. Kothe, 505-667-9089, dbk@lanl.gov  
N. T. Padial, 505-665-0931, nelylanl@lanl.gov  
W. B. VanderHeyden, 505-667-0371, wbv@lanl.gov

**Lab Capabilities Applied:** Chemical Engineering, Mechanical Engineering, Computational Fluid Dynamics, Engineering Analysis, Multiphase Flow, Turbulence, Parallel Computing



Index: 210

Category: Environmental & Regulatory (9, 6, 12, 14)

Laboratory: Los Alamos National Laboratory      Contact: Nina Rosenberg, 505-665-0183, rosenberg@lanl.gov

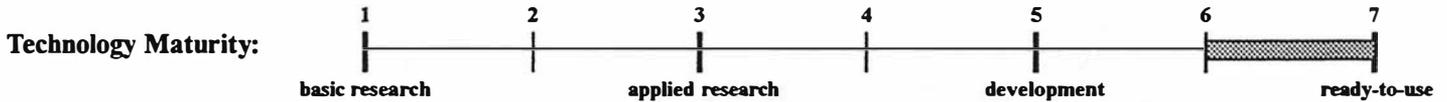
Title: Modeling Transport and Remediation of Soil and Groundwater Contaminants

**Description:** The petroleum industry faces many complex and expensive soil and groundwater remediation problems. These problems demand decisions concerning risk assessment, remediation design, and cleanup technologies. Establishing an engineering basis from which to make these decisions requires an understanding of contaminant flow and transport in the subsurface, the ability to model the system, and the ability to incorporate the technical solutions into the model.

The availability of tools to address these problems is limited because of the difficulty in incorporating the necessary complex physical processes and hydrostratigraphy. Los Alamos National Laboratory's Earth and Environmental Science Division has developed computer codes that can address many of the systems of interest. These codes are designed to simulate complexities, including fully 3-D non-isothermal, multiphase flow in heterogeneous and fractured media. The codes include modules to analyze chemical reactivity, biokinetics, horizontal, vertical and angled well systems, air sparging and barometric effects. In addition, we have coupled the flow and transport codes with advanced grid generation tools which include the ability to generate realistic meshes directly from hydrostratigraphic data.

Los Alamos can provide experience and expertise in applying these codes to a variety of environmental problems. We have been called upon to help with performance assessments for novel remediation techniques, determining effectiveness of remediation scenarios, designing monitoring activities, and predicting potential contaminant migration. Our codes have been successfully used by consultants, industry, and universities.

91-95 Funding (\$K): 5000      Dates: 1991 - present



Technology Transfer: Computer codes, Conference presentations, Journal articles, World Wide Web/Internet pages

Key Documentation: 1) Zyvoloski, G., Z. Dash and S. Kelkar (1992), FEHMN 1.0: Finite element heat and mass transfer code, Los Alamos National Laboratory Report LA-12062-MS.  
2) Travis, B.J. and N.D. Rosenberg (1994), Numerical simulations in support of the in situ bioremediation demonstration at Savannah River, Los Alamos National Laboratory Report, LA-12789-MS.

Key Personnel: Bryan Travis, 505-667-1254, bjtravis@lanl.gov  
George Zyvoloski, 505-667-1581, gaz@vega.lanl.gov  
Ken Eggert, 505-667-3544, kge@lanl.gov

Lab Capabilities Applied: Computational fluid dynamics, Subsurface multiphase flow and contaminant transport modeling, Visualization, High performance computing



Index: 211

Category: Oil Processing &amp; Refining (1, 19, 25)

Laboratory: Los Alamos National Laboratory

Contact: Antonio Redondo, 505-667-9738,  
redondo@lanl.gov

Title: Modeling and Simulation of Hydrocarbon Catalysis in Zeolites.

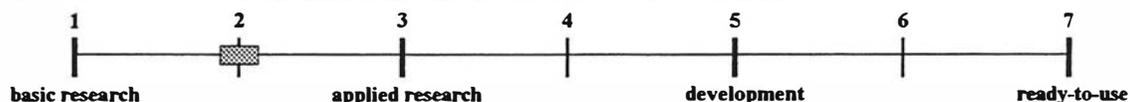
**Description:** We are currently carrying out theoretical research on catalysis (cracking and partial oxidation of hydrocarbons) in zeolite-type catalysts. Current activities are focused on calculating thermochemistries, structures and reaction barriers for hydrocarbon reactants and products in zeolites such as zeolite Y and ZSM-5. Capabilities include quantum mechanical techniques. For accurate studies on smaller systems we use ab initio and density functional theory, for systems containing hundreds of atoms we employ semiempirical techniques, and for even larger systems (up to thousands of atoms) we use classical methods, such as Monte Carlo and molecular dynamics. This work has been carried out in collaboration with industrial laboratories, such as W.R. Grace and Amoco Oil.

An additional project involves modeling zeolite synthesis pathways and identifying the important factors that determine specific zeolite structures formed from organic structure-directing templates in solution. The goal of the work with W.R. Grace is to develop kinetic models of fluid catalytic cracking (FCC) of gasoils that include all aspects of the FCC process. We are particularly interested on the effect of different catalyst configurations on the product distributions and selectivities as a function of gasoil composition. Parts of this work, in collaboration with ARCO Chemical, address the problem of activation of low molecular weight hydrocarbons by catalytic partial oxidation.

91-95 Funding (\$K): 2300

Dates: 1991-present

Technology Maturity:



Technology Transfer: open literature, staff visits, confidential reports.

**Key Documentation:** 1) A. Redondo and P.J. Hay, "Quantum Chemical Studies of Acid Sites in Zeolite ZSM-5," J. Phys. Chem. 97 (1993) 11754.  
2) B. Calef and A. Redondo, "Initial Stages of Electrophilic Substitution Studied with Quantum Molecular Dynamics," Chem. Phys. Lett. 223 (1994)

Key Personnel: P. Jeffrey Hay, 505-667-3663, pjh@t12.lanl.gov

**Lab Capabilities Applied:** Computational Theoretical Chemistry, Molecular Quantum Mechanics, Molecular Dynamics, Monte Carlo Methods, Molecular Simulations, Statistical Mechanics, Catalysis Theory.



Index: 212

Category: Development (10), Production (25)

Laboratory: Los Alamos National Laboratory      Contact: Jim Albright, (505) 667-4318, albright@seismo5.lanl.gov

Title: Binary Liquid Explosive and Initiator System for Wellbore Applications

**Description:** Originally intended for use in a logging tool as a source of seismic energy but now available for many wellbore explosive applications, an inherently safe explosive and initiation system has been developed. A liquid explosive has been developed and characterized that consists of two chemicals, neither of which are classified as explosives and consequently require no special provision for transportation to the site at which it is used. When mixed on the surface or in a logging tool, an insensitive explosive is formed that can only be detonated by sophisticated technical means. Detonation of the mixture produces no toxic or corrosive decomposition products. Gaseous decomposition products are completely soluble in wellbore fluids. Detonation is accomplished by electrical discharge to a slapper initiator specially designed to operate under hydrostatic pressures and temperatures commonly encountered in production wells. Final design of the explosive-initiator systems required testing and optimization of various design parameters including bridge dimensions, discharge voltage, gap width, barrier material properties, flyer velocity, initiation pressure, temperature stability, and failure diameter. Reliable detonation has been accomplished in the laboratory at 125 C and 2000 psi. The binary explosive chemicals and electrical slapper initiators are commercially available and low in cost.

91-95 Funding (\$K): 1000      Dates: 1991-1993



**Technology Transfer:** Patent disclosure pending, presentations at the Borehole Seismic Forum, slapper initiator technology transferred to a service company, Internet Home pages

**Key Documentation:** Los Alamos National Laboratory Report being prepared for publication

**Key Personnel:** Jim Albright, (505) 667-4318, albright@seismo5.lanl.gov

**Lab Capabilities Applied:** Explosives chemistry and physics, explosives test facilities, electrical and mechanical engineering, logging tool development, explosive safety analysis, materials science, downhole explosive tools, electrical initiation of explosives.



Index: 213

Category: Exploration (2), Development (33)

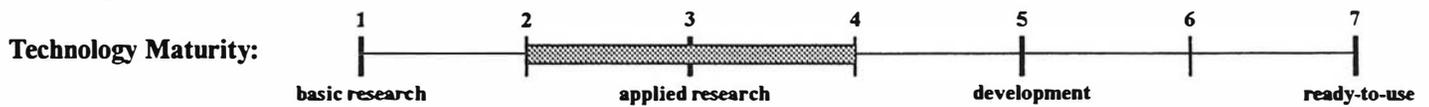
Laboratory: Los Alamos National Laboratory

Contact: Robert Malone, 505-667-5925, rcm@lanl.gov

Title: Modeling Ocean Currents and Eddies for Offshore Operations

**Description:** The oil industry is concerned about understanding and dealing with ocean processes that interfere with exploration and production operations on platforms in the ocean. This concern has increased as drilling operations have moved to deeper waters. Their initial interest was in the Gulf of Mexico, where platform operations are affected by anti-cyclonic ocean eddies that form several times a year. The Eddy Joint Industry Project (EJIP) was formed (present membership is 11 oil companies) to sponsor the collection of data on eddies in the Gulf. New joint projects have been formed to study ocean circulation in other parts of the globe, including the North Sea and Indonesia. The oil industry is also interested in ocean modeling. Models can be used to provide guidance for the optimal location of current meters in regions where exploration is just beginning. They can also be used to develop a Climatology of eddies and circulation patterns, and possibly to develop a predictive capability that could take advantage of recent progress in satellite altimetry measurement of the sea surface height. However, the industry lacks in-house modeling capability and has begun collaborating with Los Alamos. Los Alamos has provided selected output for many areas of the world from our high-resolution global simulations. Several oil companies have used these model results to guide exploration efforts, most recently near Nigeria.

91-95 Funding (\$K): 150      Dates: 1994 - present



**Technology Transfer:** Publications in open literature, exchange of model output and analysis, participation in Eddy Joint Industry Project

**Key Documentation:** 1) Smith, R.D., J.K. Dukowicz and R.C. Malone, "Parallel Ocean General Circulation Modeling," *Physica D*, 60, 38-61 (1992).  
2) Dukowicz, J.K. and R.D. Smith, "Implicit Free-surface Method for the Bryan-Cox-Semtner Ocean Model," *J. Geophys. Res.*, 99, 7991-8014 (1994).

**Key Personnel:** James Sanderson, 505-665-6605, jgs@lanl.gov  
Sumner Dean, 505-667-0708, shd@lanl.gov  
Aaron Lai, 505-665-6635, cal@vega.lanl.gov

**Lab Capabilities Applied:** Ocean modeling, visualization tools, high performance computing, computational fluid dynamics.



Index: 214

Category: Development (25, 1, 27)

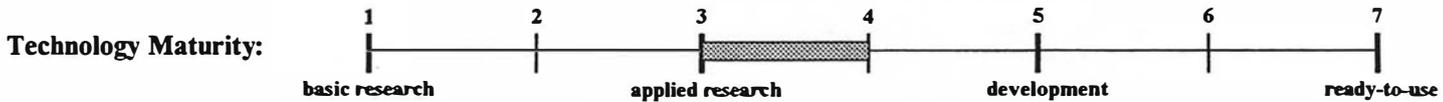
Laboratory: Los Alamos National Laboratory      Contact: H.J. Wasserman, 505-667-2136, hjw@lanl.gov

Title: Innovative Gridding and Solution Techniques for High-Performance Reservoir Simulation

**Description:** Current reservoir models do not adequately use fine-scale data that 3D seismic imaging has provided. Although using such data could decrease risk in field development, extremely fine-scale numerical grids in three dimensions are required. Such fine-scale reservoir models have put a tremendous burden on computational resources. Two key areas of concern are gridding and solution techniques. Gridding issues directly affect the quality of the representation of the geologic and hydrologic structure of a given reservoir. Both adaptive structured grids and unstructured grids allow complex geologic structures to be modeled with a minimum of nodes. These techniques, however, can lead to more complexity in numerical methods, solution matrices, software design, and computational performance challenges. These challenges must be addressed on a variety of computing platforms in a cost-effective manner.

The objective of this project is to further the development of the next generation of gridding and solution techniques. Through a cycle of algorithm development and extensive benchmarking, we plan to characterize and implement methods that are optimal for the desired computing environments. We will compare structured grids, adaptively-refined structured grids, and unstructured grids on computing platforms ranging from workstations to massively parallel machines. The associated linear system solver techniques, including multigrid, domain decomposition, and unstructured linear equation solvers, will be explored in a similar manner.

91-95 Funding (\$K): 2100      Dates: 1995 - present



Technology Transfer: SPE Papers, News Releases, open literature journal articles, licensed software

**Key Documentation:** 1) K. D. Brislawn, D. L. Brown, G. S. Chesshire, and J. S. Saltzman. Adaptively-refined Overlapping Grids for the Numerical Solution of Systems of Hyperbolic Conservation Laws, Los Alamos National Laboratory Unclassified Release.  
 2) J. E. Dendy, Multigrid Methods for Three-Dimensional Petroleum Reservoir Simulation on SIMD Machines, SPE 25243, 1993.

**Key Personnel:** Jeff Saltzman, 505-667-4285, jss@lanl.gov  
 George Zyvoloski, 505-667-1581, gaz@lanl.gov  
 Olaf Lubeck, 505-667-6017, oml@lanl.gov  
 Joel Dendy, 505-667-5929, jed@lanl.gov  
 Wayne Joubert, 505-667-7374, wdj@lanl.gov

**Lab Capabilities Applied:** Fluid Dynamics, High-Performance Computing, Simulation, Finite Element Methods, Mathematical Software, Parallel Processing, Numerical Methods



Index: 215

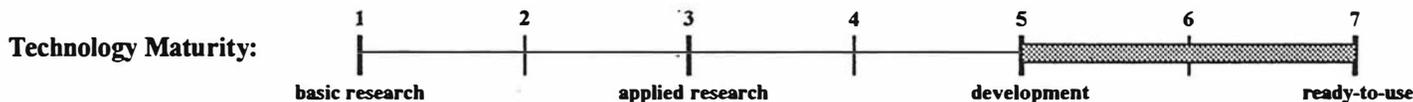
Category: Environmental & Regulatory (15, 4, 14)

Laboratory: Los Alamos National Laboratory      Contact: Mike Murrell, 505-667-4845, mmurrell@lanl.gov

Title: Naturally Occurring Radioactive Materials (NORM) Analysis For Oil And Gas Operations

**Description:** Over the past five years, industry and government have become increasingly concerned about the issue of naturally occurring radioactive materials or NORM in waste and equipment from oil and gas operations. The isotopes <sup>226</sup>Ra and <sup>228</sup>Ra are the two principal radioactive nuclides of interest due to the long half-life (1600 y and 5.75 y, respectively) of each daughter. The most precise and sensitive technique for the determination of these radionuclides is thermal ionization mass spectrometry. This technique was first developed at LANL. This mass spectrometric capability, along with our capabilities for radionuclide assay by radioactive decay and our experience with data interpretation for environmental samples, makes us a unique resource for NORM issues. We can provide technical expertise in analytical methods such as sampling protocol, preparation and certification of reference materials, commercial laboratory certification, and custom chemical separation schemes. We can also provide risk assessment for source term characterization - especially at low levels, transport modeling, and in uncertainty and sensitivity analysis. We have a great deal of experience in dealing with regulatory compliance issues such as providing proof of compliance at very low levels.

91-95 Funding (\$K): 120      Dates: 1994 - Present



Technology Transfer: Publications in open literature, exhibits at national and regional meetings

Key Documentation: 1) A. M. Volpe, J. A. Olivares, and M.T. Murrell, "Determination of Radium Isotope Ratios and Abundances in Geologic Samples by Thermal Ionization Mass Spectrometry," Analytical Chemistry 63, 913-916, (1991).

Key Personnel: Mike Murrell, 505-667-4845, mmurrell@lanl.gov  
Malcom Fowler, 505-667-5439 mmf@lanl.gov

Lab Capabilities Applied: Radiochemistry, mass spectrometry, actinide element geochemistry, environmental risk assessment



**Index:** 216

**Category:** Exploration (3, 4)

**Laboratory:** Los Alamos National Laboratory

**Contact:** Michael Fehler, 505-667-1925, fehler@lanl.gov

**Title:** Gulf of Mexico Sub-Salt Seismic Imaging Project

**Description:** As is well known, much of the oil and gas production in the Gulf of Mexico and Gulf Coast is associated with salt and mostly with vertical dome features. However, roughly 40% of the continental shelf is covered by more horizontal salt features. These horizontal features, known as canopies, swell, tongues, welds, and pillows have very irregular three-dimensional configurations and present a large velocity contrast from the surrounding sediments. Until recently, obtaining clear images of sediments beneath these salt features has been very difficult if not impossible. Conventional seismic processing techniques are not adequate to properly image the sedimentary layers beneath the salt. More comprehensive and extensive formulations are required. These advanced methods go by the name of 3-D prestack depth migration. They use massive amounts of data, require an accurate estimate of the subsurface structure and velocity field, and demand a considerable amount of computer resources. During this project we will develop and investigate the range of applicability of two or more methods of doing pre-stack depth migration of seismic data. The target is to develop methods that work well to image beneath salt structures in the U.S. Gulf Coast region. Our effort to date includes work on travel-time calculations using ray-tracing and numerical solutions of the Eikonal equation, data compression algorithms, methods for data anti-aliasing and integration, numerical modeling of the wave equation, and new visualization techniques for the seismic data. This is a joint project with Amoco Production Company, Marathon Oil Company, Phillips Petroleum Company, The Louisiana Land and Exploration Company, and Western Atlas International, Inc. The industry participants are providing seismic data tapes, results from their own in-house efforts, and technical guidance during all phases of this project.

**91-95 Funding (\$K):** 1625      **Dates:** 1994-present



**Technology Transfer:** Internet documentation, bimonthly meetings with industry partners, on-site industry consultant, staff exchange presentations at technical meetings, publications in the open literature, availability of codes to partners.

**Key Documentation:** 1) CRADA: Gulf of Mexico Subsalt Imaging Project.  
2) Advanced Computational Technology Initiative Proposal.

**Key Personnel:** Michael Fehler, 505-667-1925, fehler@lanl.gov  
Steve Hildebrand, 505-665-8904, sth@piglet.lanl.gov  
Tong Fei, 667-0488, tfei@seismo5.lanl.gov  
Eugene Gavrilov, 505-665-7448, gavrilov@acl.lanl.gov

**Lab Capabilities Applied:** Seismology, mathematics, parallel computing, numerical analysis and algorithm development, advanced computing laboratory, data compression techniques, advanced visualization technologies.



Index: 217

Category: Development (33, 25)

Laboratory: Los Alamos National Laboratory      Contact: J. M. Kindel, 505-667-3718, jkindel@lanl.gov

Title: Prepare Information for the Los Alamos/Petroleum Recovery Research Center Electronic Information System as a Means for Communications and Data Transfer to Independent Gas and Oil Producers

**Description:** The goal of the Los Alamos/Petroleum Recovery Research Center (PRRC) electronic information system (GO-TECH) is to provide a mechanism for the rapid exchange of ideas, data, and technology by providing the petroleum community with access to computer based services. The approach is to use computer technology, which is commonly available at Los Alamos, to provide information browsing, file transfer, electronic mail and news services to a geographically dispersed audience.

Using a personal computer and modem, the petroleum community can gain access via the Cisco terminal server provided and maintained by Los Alamos. Once the user has been verified by the terminal server as having a valid account with the PRRC, the user can access information at Los Alamos, PRRC and throughout the Internet. Users are provided access software which can be installed on their personal computer using an installation procedure prototyped by Los Alamos.

The information maintained on the World Wide Web document GO-TECH was jointly selected by Los Alamos, PRRC, and independent oil and gas producers in New Mexico. Refinements to the document are facilitated by an on-line suggestion form which is accessible from the home page document. There are currently in excess of 220 registered GO-TECH users. Usage statistics, greater than 600 accesses per day, indicate that this document has become a resource to the worldwide petroleum industry.

91-95 Funding (\$K): 500      Dates: 1994 - present



Technology Transfer: Internet Home Page, Independent Petroleum Association of New Mexico, New Mexico Oil and Gas Association, Seminars, SPE presentations, Interstate Oil and Gas Compact Commission, and the Petroleum Technology Transfer Council.

Key Documentation: Internet Home Page (<http://baervan.nmt.edu/>)

Key Personnel: David Forslund, 505-665-1907, dwf@lanl.gov  
 John Morrison, 505-667-1042, jfm@lanl.gov  
 Robert Webster, 505-665-4183, robw@lanl.gov

Lab Capabilities Applied: Distributed computing, visualization, large data bases, intelligent search, and data mining



**Index:** 218

**Category:** Drilling & Completion (5, 1, 3), Development (9, 8), Production (25, 13)

**Laboratory:** Los Alamos National Laboratory      **Contact:** Robert P. Swift, 505-665-7871, bswift@lanl.gov

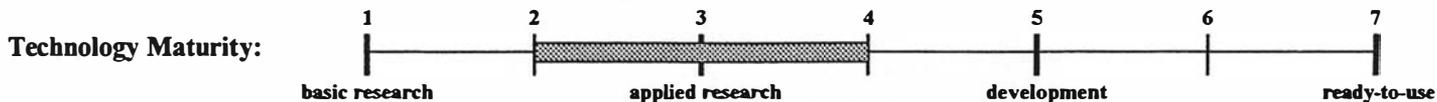
**Title:** Coupled Rock/Fluid Mechanics Numerical Simulations Applied to Well Completions

**Description:** The annual cost of inefficient well completion treatments exceeds \$100 million. Most of this inefficiency is attributable to perforation effects, such as created fines and sand production. Some operators report that ninety percent of perforations fail to establish communication with the formation. The gas and oil industry believes that a comprehensive study is needed that combines all the relevant physics for developing a better predictive capability to assess perforation damage and its effect on productivity. Operators can then evaluate alternative means to minimize and cleanup damage or use other stimulation methods.

The goal of Los Alamos's Coupled Rock Fluid Mechanic project is to increase understanding of the physics involved in well completions by combining numerical modeling, laboratory experiments, and field data. A broad spectrum of the industry will provide their expertise, share their data, and perform analyses in support of this project. Modeling will involve the use of current codes and techniques developed at Los Alamos, pursuit of new approaches, and hybridizing others. The project includes two tasks: 1) Perforation Damage Assessment and Cleanup examines perforation-induced damage and its effect on permeability reduction. 2) Soft Rock Deformation and Fracturing examines slurry transport in the near wellbore region to address cleanup, gravel packing, frac packing and proppant movement issues.

In addition, this work invaluablely impacts industry and National Laboratory goals. There is the potential for increased productivity and reduced completion costs for industry and the enhancement of fundamental core capabilities by advancing new concepts that benefits other Laboratory programs.

**91-95 Funding (\$K):** 1650      **Dates:** 1995 - present



**Technology Transfer:** Databases for perforation and sand production experiments, Publications in open literature, Workshop and Seminars, Code use training manuals and courses, collaborations with numerous industry participants.

**Key Documentation:** New project just being initiated, Advanced Computational Technology Initiative Proposal

**Key Personnel:** James Abbott, 505-667-9952, jra@lanl.gov  
 Alan Graham, 505-665-5259, graham@lanl.gov  
 Dave Mandell, 505-667-7145, dam@lanl.gov  
 Robert Stellingwerf, 505-667-8905, rfs@lanl.gov

**Lab Capabilities Applied:** Rock Mechanics, Fluid Mechanics, Well Completion Engineering, Shock Wave Physics, Shock Wave Experiments, Fracture Mechanics, Porous Flow, Slurry Movement, Perforation Mechanics, Micro-Mechanics, Discrete Element Methods



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Category: Development (16, 3, 8, 10)

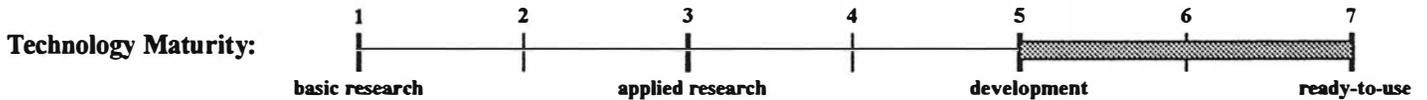
Laboratory: Los Alamos National Laboratory      Contact: Jim Albright, (505) 667-4318, albright@seismo5.lanl.gov

Title: Microseismic Fracture Mapping and Determination of Fluid Flow Paths in a Producing Reservoir

**Description:** Los Alamos personnel were first to observe microseismicity due to hydraulic fracturing in a pioneering experiment using borehole geophones at the Fenton Hill hot dry rock geothermal reservoir in 1975. Since that time, our research has broadened to include microseismicity associated with a wide variety of processes associated with primary and enhanced production from hydrocarbon and geothermal reservoirs in a variety of geologic settings. Included are seismicity related to hydraulic stimulation, acid treatment, waterfloods, reservoir subsidence, gas storage, and primary production. Seismicity has been observed in basement crystalline rock, metamorphic rocks, dolomite, sandstone, and chalk. Several phenomenon are common to these studies. All of the seismicity is associated with minute displacements along fracture or joint surfaces. The source areas and energies (magnitudes -6 to -1) that are involved are small so that it has only been possible to study the microseismicity using borehole instrumentation deployed close to the event location (usually within 3000 m).

Within the past 3 years, project personnel in collaboration with oil and gas producers have mapped seismicity due to primary production from shallow carbonate reservoirs in Clinton County Kentucky; deployed single station instrumentation in Logansport, Indiana to monitor seismicity associated with gas withdrawal from a gas storage facility; mapped hydraulic fracture seismicity in the Travis Peak Formation and the Austin Chalk; and completed analysis and mapping of seismicity observed in both the Prudhoe Bay, Alaska, and Ekofisk, North Sea reservoirs. This work was conducted in collaboration with over 10 oil and gas producers.

91-95 Funding (\$K): 1500      Dates: 1975-present



**Technology Transfer:** Presentations at meetings; publications in professional society journals and trade magazines, field experiments with over 10 oil and gas producers ranging from the largest majors to small independents, collaborations with well service companies

**Key Documentation:** 1) Rutledge, J. T., T. D Fairbanks, J. N. Albright, R. R. Boade, J. Dangerfield, and G. H. Landa, Reservoir Microseismicity at the Ekofisk Oil Field, EUROCK 1994, Rock Mechanics in Petroleum Engineering, A Joint SPE/ISRM Meeting, 29 August - 1 September, Delft University of Technology, The Netherlands, 1994.  
2) Brady, J., T. Fairbanks, and R. Withers, 1994, The First Test of Using Microseismicity to Monitor Hydraulic Fractures in Prudhoe Bay, Soc. of Pet. Eng., SPE 28553.

**Key Personnel:** Jim Rutledge, (505) 667-8938, rutledge@seismo5.lanl.gov  
Don Dreesen, (505) 667-4318, dreesen@lanl.gov  
Scott Phillips, (505) 667-8106, wsp@lanl.gov

**Lab Capabilities Applied:** Logging tool design, seismic data acquisition, well completions, borehole seismic analysis and interpretation, field testing, mechanical engineering, electrical engineering, well test facility.



Index: 220

Category: Oil Processing &amp; Refining (26, 3)

Laboratory: Los Alamos National Laboratory

Contact: K. L. Buescher, 505-667-1356,  
klb@lanl.gov

Title: Neural Networks for Chemical Process Control

**Description:** Many processes in the chemical industry, including chemical plants and petroleum refineries, have characteristics which make them difficult or impossible to control using conventional techniques based on linear or first-principles models. Often, these processes are too complicated or novel to make first-principles modeling economically feasible. They may be nonlinear enough that linear models will not result in adequate control, especially in unstable operating regimes or during startup and shutdown operations. More importantly, most processes drift with time and are subject to unpredictable disturbances, so that a model which adapts to changes in the process is necessary.

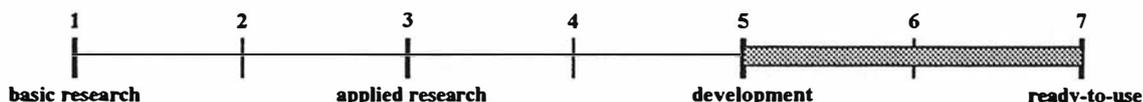
This project (which centers around a CRADA with DuPont) has successfully addressed these issues by using adaptive neural networks in a model predictive control scheme. The networks are first trained off-line, using historical process data, to mimic the process behavior. An appropriate control strategy is then found by using the network to predict the response of the process to various control strategies. Further, the network is trained on-line to allow it to adapt to changes in the process. In developing the neural network structure and the training algorithms, the emphasis was on reducing the amount of off-line characterization data required. Once the neural network model is trained, it can be used for purposes other than control, such as fault detection and operator training.

After convincing demonstrations on DuPont's benchmark simulations, we are installing the controller at a DuPont pilot plant. In conjunction with DuPont, we are taking steps to commercialize the software to make it widely available. This project has impacted and benefited from a number of ongoing technology-transfer projects at LANL that incorporate adaptive learning systems. The future direction of the project is to tie the controllers into a plant-wide, multi-level (materials, process, enterprise) optimization scheme.

91-95 Funding (\$K): 1300

Dates: 1993 - present

Technology Maturity:



**Technology Transfer:** LANL unlimited release technical reports, Seminars, Conferences (ACC and WCNN), CRADA, Patent Application, WWW pages, and papers available by ftp

**Key Documentation:** 1) C. C. Baum et al., "Adaptive Chemical Process Control: DuPont/Los Alamos Phase I Report," Tech. Rep. LA-UR-94-1039, Los Alamos National Laboratory, 1994.  
2) K. L. Buescher and C. C. Baum, "A Two-Timescale Approach to Nonlinear Model Predictive Control," to appear, 1995 American Control Conf. (Also, LANL report LA-UR-94-3256 available by anon. ftp from laws.lanl.gov in pub/control/chemical)

**Key Personnel:** Stanley K. Brown, 505-667-6178, skbrown@lanl.gov  
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Roger D. Jones, 505-667-8979, rdj@lanl.gov

**Lab Capabilities Applied:** Adaptive Computation and Control, Process Design and Optimization, Systems Integration





Index: 222

Category:

Laboratory:

Contact:

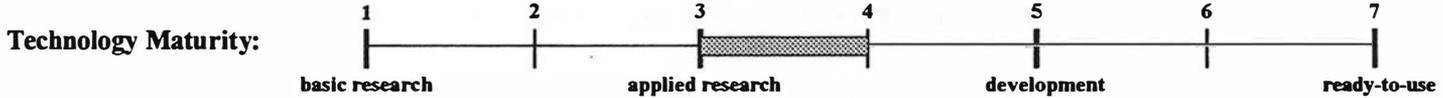
Title:

**Description:** Los Alamos entered into a user facility agreement with an industrial firm which applied Los Alamos computational design and test firing capabilities toward the development of an advanced perforator. The computations involved use of the MESA-2D two-dimensional wave-propagation code by the firm's staff engineers, with mentoring by Los Alamos staff. A design was developed which was predicted to provide the desired performance in terms of penetration in the rock formation and hole size opened in the casing.

Samples of the new perforator were built and test-fired at Los Alamos. The testing involved placement of a perforator into a realistic mockup of the downhole configuration. This included a carrier tube outside of which were water, casing, grout and sandstone. A 6-MeV dynamic flash radiograph was taken of the jet and its penetration into the sandstone in each of two experiments. The results of these experiments compared well with the computer predictions.

As a part of this activity, the MESA-2D code was transferred to the industrial firm for their use.

91-95 Funding (\$K):  Dates:



Technology Transfer:

Key Documentation:

Key Personnel:

Lab Capabilities Applied:



Index: 223

Category: Development (25, 5, 8, 30)

Laboratory: Los Alamos National Laboratory

Contact: Wendy Soll, 505-665-6930,  
wes@vega.lanl.gov

Title: Pore-Scale Flow and Examination of Effects of Scaling on Improved Oil Recovery Processes

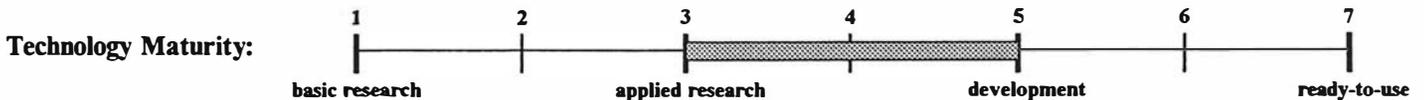
**Description:** The economically-based decisions to develop a reservoir are based on estimates of resources in the field and on simulations of the extraction process using reservoir models. For these field scale simulations to be accurate it is necessary to understand how smaller scale components of the system, core or pore level, influence system response, and to correctly represent this behavior in the large scale model. This work addresses improved simulation and prediction of fluid-rock interactions (e.g., relative permeabilities) that are utilized as input to reservoir scale models.

We have developed a computational approach that allows the user to replace empirical techniques and expensive laboratory measurements with a fast, highly accurate and robust numerical tool. This tool also makes it possible to examine the potential effects of other variables that are not easily measured in the laboratory, such as surface wettability. Using this computational tool to establish constitutive characteristics of the system also brings with it a potential savings of tens to hundreds of thousands of dollars for a reservoir characterization study.

This project has benefited significantly from a close collaboration between Los Alamos National Laboratory and Mobil Exploration and Producing Technical Center (MEPTEC). It has applied the strengths of Los Alamos (in computing, theoretical physics and porous flow) and the expertise and guidance of MEPTEC (in petroleum applications) to attack an important industry problem. It provides technology to industry, through transfer of computational models and databases, that can vastly improve estimates of recovery during EOR processes.

91-95 Funding (\$K): 1400

Dates: 1991 - present



Technology Transfer: Computer codes, Conference presentations, Journal articles, World Wide Web/Internet pages, Databases

Key Documentation: 1) Grunau, D.W. Lattice Methods for Modeling Hydrodynamics. PhD Dissertation, Colorado State University, Dept. of Math., 1993.  
 2) R&D 100 Award, 1994. Lattice Boltzmann Permeameter. R&D Magazine, Des Plaines, IL.

Key Personnel: Shiyi Chen, 914-945-2260, syc@t13.lanl.gov  
 Ken Eggert, 505-667-3544, kge@lanl.gov  
 Daniel Martinez, danielm@acl.lanl.gov  
 Gary Doolen, 505-667-8994, gdd@lanl.gov

Lab Capabilities Applied: Pore-scale Modeling, Theoretical and Computational Physics, Massively Parallel Computing, Multiphase Flow, Visualization Technology



Index: 224

Category: Development (25, 33)

Laboratory: Los Alamos National Laboratory      Contact: Ken Lee, 505-667-4370, ken\_lee@lanl.gov

Title: Reservoir Studies and Information Delivery Tools for Independent Oil Producers

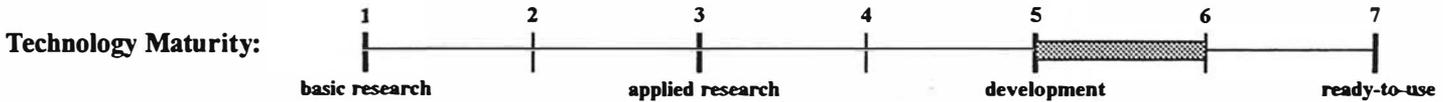
**Description:** The aim of this project is to make advanced simulation techniques available to Independent oil producers by reducing the level of technology required to access such techniques. By developing a distributed, basin-wide collection of such studies, early selection of improved oil recovery scenarios (e.g., water flooding, gas flooding) can be performed. This reduces the number of simulations required and thus the cost of developing reservoir management plans. A number of Independents have already indicated that they would be willing to share such data and that they believe that their productivity could be favorably impacted by a shared database.

One sub-goal is the demonstration of a distributed computational resource that can establish a match in the resources and training available to Independents with the tools available from service companies. This goal will be achieved by distributing the control of a reservoir simulation between the Independent and a consulting/engineering firm. The aim of this sub-goal is the reduction of the cost of delivery of simulation capability to the Independents.

Another sub-goal is the development of an on-line database of reservoir management case histories and a demonstration of the value of such a database. The development of this database includes performance of actual reservoir management studies that can be evaluated by the Independents for added value.

Los Alamos can provide experience and expertise in the development of information delivery tools and distributed databases as well as the performance of reservoir simulations.

91-95 Funding (\$K): 1600      Dates: 1994 - present



Technology Transfer: Computer Codes, World Wide Web/Internet Pages, Collaborations with Independent Producers

Key Documentation: 1) Advanced Computational Technology Initiative Proposal

Key Personnel: Bob Webster, 505-665 4183, robw@lanl.gov  
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Lab Capabilities Applied: Fluid Flow, Mass and Energy Transport, Development of High Performance Computing Environments, Reservoir Simulation



Index: 225

Category: Development (27, 25, 33)

Laboratory: Los Alamos National Laboratory

Contact: David H. Sharp, (505) 667-5266, dhs@t13.lanl.gov

Title: Scale-Up in Heterogeneous Reservoirs

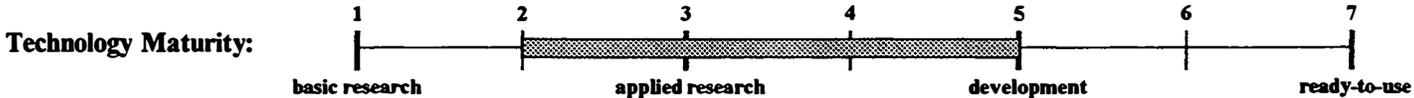
**Description:** Risk management and risk reduction are increasingly important in the development of new oil fields and in designing processes for the recovery of additional oil from existing resources. An ability to quantify accurately the various risks associated with different field development options will allow producers to evaluate complex projects reliably.

The specific risks we address result from uncertainties in geological models. Better risk management requires more accurate predictions of the recovery process and improved estimates of uncertainties. Because the fine scale geological variability often plays a dominant role in displacement processes, improved risk management will require the ability to simulate reservoir flows in highly detailed geological models. As the computational cost of such simulations is prohibitive, there is a compelling need for accurate scale-up methods that generate coarsened geological models resulting in flows in essential agreement with those obtained from detailed models.

Independent producers are increasingly important in the domestic oil industry. Reducing the cost of simulation will break technological and economic barriers to the more widespread use of simulations by independents. Improving the predictability of options such as infill drilling will encourage continuing production from declining oil fields.

In collaboration with our industrial and university partners (BP Houston, Chevron, and Stony Brook) we are developing novel scale up methods. Our goal is to deliver scale-up codes which: (i) are four orders of magnitude faster than conventional techniques, (ii) preserve the accuracy of fine scale simulations to within a few percent, and yet (iii) are easily applicable by practicing reservoir engineers.

91-95 Funding (\$K): 175      Dates: 1994 - present



**Technology Transfer:** Petroleum Technology Transfer Council (PTTC), direct interactions with service companies, presentations at technical meetings, publications in the open literature, porting of codes between collaborating partners

**Key Documentation:** Scale-up in Heterogeneous Reservoirs, M. A. Christie, L. J. Durlofsky, J. Glimm, K. S. Lackner, D. H. Sharp and T. C. Wallstrom, Los Alamos Report.

**Key Personnel:** David H. Sharp, (505) 667-5266, dhs@t13.lanl.gov  
 Klaus S. Lackner, (505) 667-5694, ksl@lanl.gov  
 Timothy C. Wallstrom, (505) 667-5675, tcw@t13.lanl.gov

**Lab Capabilities Applied:** Computational fluid dynamics, algorithm development, high performance computing, visualization technologies



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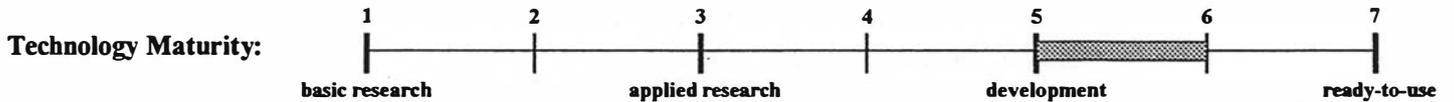
Category: Exploration (4, 3), Development (3)

Laboratory: Los Alamos National Laboratory      Contact: J.E. Pearson, 505-667-7585, pearson@demos.lanl.gov

Title: Society of Exploration Geophysicists Synthetic Seismic Database

**Description:** This program is a part of a multilab project involving Los Alamos, Lawrence Livermore, Sandia Albuquerque, and Oak Ridge. The project was overseen by the Society of Exploration Geophysicists (SEG). Industrial collaborators include The French Petroleum Institute, UNOCAL, Amoco and Politecnico di Milano Italy. Here we shall provide an overview of the project and describe the Los Alamos contribution. The goal is to generate a large scale synthetic seismic survey that can be used by oil exploration companies to validate the algorithms used for solving the inverse problem. (i.e. Given a seismic survey, what is the structure that produced it) The goal requires the repeated solution of the linear scalar wave equation with a highly nonuniform sound speed. The numerical method chosen was a second order in time and tenth order in space finite difference scheme. The numerical task was to run the simulation on a three dimensional mesh containing roughly 30 million points. This task was chosen so that it was large enough to tax the capabilities of the largest supercomputers. The boundary conditions that had been specified required a message passing implementation. This proved to be a nontrivial task on the Connection Machine which was the chosen Los Alamos Platform. We decided to write the entire code in CDPEAC, the C wrapper for the CM assembly language. This was a successful strategy. The Los Alamos code now runs at a sustained speed of 1 gigaflop on 32 nodes. The code is capable of up to 32 simultaneous runs on 1,024 nodes of the CM-5. Actual production runs comprising 16 simultaneous shots have been run on 512 nodes of the CM with sustained performances of 16 gflops. We expect further performance improvements after some optimization.

91-95 Funding (\$K): 1500      Dates: 1994 - present



Technology Transfer: Computer Codes, Conference Presentations, Journal Articles, collaborations between the project participants

Key Documentation: 1) Aminzadeh, F., Burkhard, N., Kunz, T. Nicolets, L., and Rocca, F. The Leading Edge, V14, No.2 (1995) 125-128.

Key Personnel: Bob Webster, 505-665-4183, robw@lanl.gov  
 Ken Lee, 505-665-7518, ken\_lee@lanl.gov  
 Eugene Gavrilo, 505-665-7448  
 Dave Forslund, 505-665-1907, dwf@lanl.gov

Lab Capabilities Applied: High Performance Computing, Numerical Techniques for Solving Partial Differential Equations, Solution Techniques for Advanced Supercomputers, seismology



Index: 227

Category: Development (14, 16, 20)

Laboratory: Los Alamos National Laboratory

Contact: Patrick Soran, 505-667-8103, soran@lanl.gov

Title: Computer Simulation in Support of Nuclear Well-Logging

**Description:** Nuclear well-logging is an inexpensive but very effective method for investigating subsurface lithology characteristics. A sonde consisting of source and detector(s) is lowered into a borehole. In the case of measurement while drilling (MWD), the sonde is an intimate part of the drilling string. The response of the detector(s) to the radiation returning from the borehole and formation allows some inference of the subsurface characteristics such as porosity, permeability, chemical constituents, and fluid saturation. The technique has two basic problems. First, the count rates from the detector(s) require a long chain of inference, empiricism, and experience to yield information on the lithology characteristics. Second, the interpretation of data is based on benchmark measurements and environmental corrections in a very limited set of known environments. Many of the environmental corrections are derived from computer simulation. Progress in nuclear logging will come with a resolution of these two major problems, smarter processing of tool readings, and development of computer tools that will provide the tool designer, field engineer, and interpretation engineer fast and simple methodologies for analyzing data.

The simulation of radiation transport as applied to nuclear well-logging is subject to several difficulties. (1) The transport problems are difficult because they are three-dimensional and sometimes time dependent, and they are optically thick, e.g., only one in a billion particles may get to a detector. Furthermore, the geometry is difficult since the critical dimensions of the tool are small relative to the particle interaction length. (2) Most radiation transport simulation codes are research tools and are very difficult to use. (3) The nuclear data are not always available, and those that are available are lacking in quality. (4) Finally, there is a need to develop algorithms to relate measurements and simulations to the parameters of the reservoir and wellbore. These are the issues being addressed by Los Alamos in this project.

91-95 Funding (\$K): 1200      Dates: 1994-present



Technology Transfer: Open literature publications, technical staff exchange, licensed product, collaborations with industry participants, CRADA

Key Documentation: 1) CRADA with Schlumberger - Doll Research  
2) Nuclear Science and Engineering Article (publication pending)

Key Personnel: Patrick Soran, 505-667-8103, soran@lanl.gov  
R. Arthur Forster, 505-667-7577

Lab Capabilities Applied: Radiation transport, MonteCarlo Codes, Nuclear database, High Performance Computing, Nuclear Weapons Experience



Index: 228

Category: Drilling & Completion (5), Production (25)

Laboratory: Los Alamos National Laboratory      Contact: J. E. Kennedy, 505-667-1468, jkennedy@lanl.gov

Title: Advanced Perforator Technology

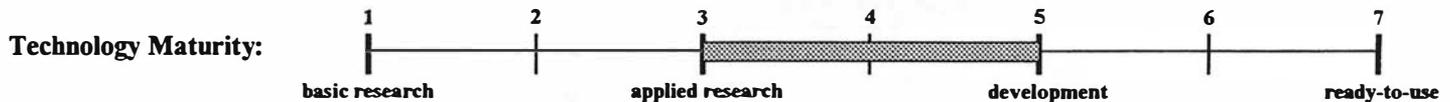
**Description:** This joint project with Schlumberger Perforating and Testing Center includes efforts on three aspects of perforator technology -- perforator design, high-temperature-stable explosive materials for use in perforators, and initiation of perforator detonation.

Design alternatives based upon Schlumberger proprietary ideas are being explored by computations performed with a Los Alamos two-dimensional wave-propagation code, MESA-2D. For an axisymmetric perforator and target geometry, this code simulates the detonation of the perforator, jet formation, and jet penetration through the gun tube, water, casing, cement and rock formation. Computer findings have been found to track well with results of Schlumberger above-ground experiments.

Work is under way on synthesis of high-temperature explosive materials suggested by Schlumberger. This includes novel methods of chemical synthesis aimed at improving the yield of the desired product (which simultaneously reduces hazardous waste generation) at reduced cost.

Slapper detonator technology is being developed according to proprietary Schlumberger approaches. Slappers are high-voltage detonators which utilize less hazardous secondary explosives. Their use therefore improves the safety of perforator system loading, transportation and insertion, and does not require cessation of electrical operations at the wellhead during insertion of the perforator gun. On this project, Schlumberger and Los Alamos have jointly developed suitable suppliers for the copper-Kapton laminate used to make slappers. Schlumberger test results with prototype slappers made by Los Alamos have been favorable.

91-95 Funding (\$K): 1800      Dates: 1993 - present



Technology Transfer: Limited to Schlumberger because information is proprietary.

Key Documentation: CRADA with Schlumberger Perforating and Testing Center

Key Personnel: J. J. Jacoby, 505-667-4312, jjj@lanl.gov  
 K.-Y. Lee, 505-667-7131, lee@dx16.lanl.gov  
 R. J. Yactor, 505-667-6655  
 E. C. Martinez, 505-667-7130, martinez\_ernesto\_c@lanl.gov

Lab Capabilities Applied: Explosive fabrication, computer simulation of explosive jets, slapper electrical detonator technology.



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**Category:** Development (4, 8, 21, 25, 30), Gas Gathering (2), Gas Storage (2)

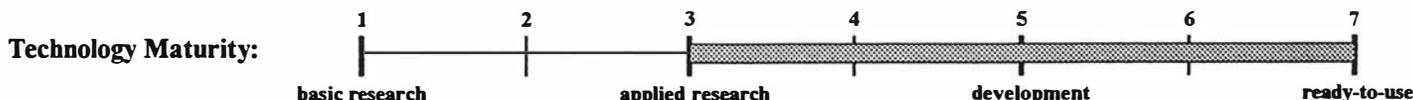
**Laboratory:** Los Alamos National Laboratory **Contact:** David R. Janecky, 505-665-0253, janecky@lanl.gov

**Title:** Multicomponent Labeled Tracer Technology: Characterization of Coupled Transport and Chemical Interactions in Petroleum Reservoirs

**Description:** Tracer approaches to characterization of oil reservoirs are being enhanced for both transport and chemical interactions. This chemical transport data for reservoirs is critical to validation and development of significantly enhanced simulators. New classes of conservative and reactive non-radioactive tracers for both laboratory and field experiments have been defined and are being tested using stable isotopic labeling schemes. An initial field test and demonstration is occurring in an actively producing reservoir. Physical processes to be investigated include flow, dispersion, sorption, partitioning, displacement, and chemical reaction. Tracer results will be used to constrain and validate oil field simulators and hydrologic codes, both operational and state-of-the-art versions. A robust set of tracers, field experience in their application, and interpretation methodology will be developed for large scale multi-well, multi-tracer flow and connectivity tests through continued efforts involving extensive collaboration with industry.

Existing collaborative activities include (1) a large scale field test (26 tracers) with Mobil Exploration and Producing, U.S. and Petrolite, (2) preparation for a second field test in a Mobil field also involving transfer of analytical technology to a commercial laboratory, (3) custody tagging demonstrations with ISOTAG, and (4) characterization analyses for ISOTAG and Exxon Production Research leading to joint laboratory core flood and field operations. The results of such experiments are providing a major critical step toward significantly enhanced characterization of reservoir flow paths; in effect overdetermining the state of the system and minimizing unconstrained terms in the models --- geochemical tomography.

**91-95 Funding (\$K):** 650 **Dates:** 1992 - present



**Technology Transfer:** SPE Papers, News Releases, Industry presentations, Industry collaborative agreements

**Key Documentation:** 1) Janecky, D. R., and Spall, W. D. (1990) New Tracer Technology for Geochemical Tomography. In Proceedings, SPE/UH Emerging Technologies Conference 281-283. 2) Spall, W. D., Janecky, D. R., Dixon, P. R., and Bayhurst, G. K. (1992) Integrated natural and injected multicomponent tracer experiments: Mammoth Hot Springs, Yellowstone National Park. In Proceedings, 7th International Symposium on Water-Rock Interaction.

**Key Personnel:** W. Dale Spall, 505-665-0475, wdspall@lanl.gov  
Walter F. Sandoval, 505-667-9756, wf-sandoval@lanl.gov

**Lab Capabilities Applied:** Analytical Chemistry particularly organic and isotopic, chemical design and isotopic labeling, speciation and geochemistry, high performance modeling, experimental implementation



Index: 230

Category: Drilling & Completion (10, 1, 2, 9, 12, 13)

Laboratory: Los Alamos National Laboratory      Contact: D.S. Dreesen, 505-667-1913, dreesen@lanl.gov

Title: Multi-Phase Fluid Simulator for Underbalanced Drilling (Hydrodynamic Modeling of Multi-Phase Drilling Fluid Flow to Simulate Underbalanced Drilling)

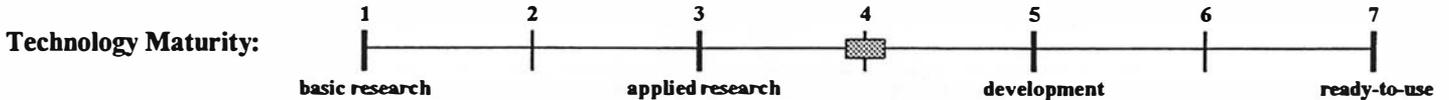
Description: Underbalanced drilling, which uses compressible drilling fluids such as air, nitrogen, natural gas, foams, or mists, is gaining widespread acceptance in the petroleum industry because it increases drilling rates and reduces formation damage. This project will develop a computational simulator for modeling the flow of compressible drilling fluids and cuttings in a wellbore. This simulator will be used by drilling companies and well designers in planning underbalanced drilling programs and as a diagnostic tool during actual drilling operations.

Physical phenomena to be included in the computational model will include: compressibility, heat transfer, friction and heads, relative motion and drag, re-grinding of cuttings, inflow and outflow of fluids, and various flow geometries. This model will be verified by comparison of computed results with laboratory data and actual drilling data furnished by the industrial participants. Los Alamos will provide code developers/modelers, systems engineering, drilling process characterization, and project coordination.

Collaboration. The Center for Drilling Hydraulics at Pennsylvania State University will provide experience in air drilling, drilling hydraulics, and pneumatic transport.

Industry Participation. Maurer Engineering Inc., Texaco Inc., Chevron, Pool Energy Services, and Mobil. Industry participants will support the project with in-kind contributions including: (1) Industry Advisory Committee/Technical Transfer; (2) Ongoing research and field operations for code and model verification; (3) Proprietary and public domain codes or output data for comparison with Los Alamos results; (4) Support of a research associate, post doctoral candidate, or graduate student.

91-95 Funding (\$K): 600      Dates: 1995 - present



Technology Transfer: Industry Advisory Committee, Drilling Engineering Association presentations, Quarterly Report, technical papers in appropriate journals

Key Documentation: New project just being initiated, Advanced Computational Technology Initiative Proposal.

Key Personnel: W.H. Reed, 505-665-6534, whr@lanl.gov

Lab Capabilities Applied: Multi-phase fluid flow simulation, dynamic fluid simulation, wellbore heat transfer simulation, unconventional drilling technology, well completion and downhole instrumentation, borehole tool design, well logging and downhole measurements



Index: 231

Category: Development (25,28), Exploration (13)

Laboratory: Los Alamos National Laboratory      Contact: David Forslund, 505-665-1907, dwf@lanl.gov

Title: Sunrise: A National Information Infrastructure Prototype

Description: Sunrise has the goal of providing a national scalable high-performance networked software environment which eases dynamic assembly of distributed industrial and scientific applications. The main focus of the project is to tie together enabling technologies (ATM networking, object-oriented distributed computing, graphical and multimedia user interfaces, security and privacy, and data-mining technologies) into several specific applications. A diverse set of application areas including materials modeling, environmental management, telemedicine, geographical information systems, and K-12 education are being used to ensure that the solutions developed are generic as possible. The TeleMed application, for example, enables a physician to navigate and analyze a complex, multimedia patient record including query-by-example of a radiographic image database. Such technology is applicable to a wide variety of complex information systems including integrating data acquired from reservoir management systems.

91-95 Funding (\$K): 3500      Dates: 1993 - present



Technology Transfer: Licensed product, publications in open literature

Key Documentation: <http://www.acl.lanl.gov/sunrise>

Key Personnel: David Forslund, 665-1907, dwf@lanl.gov  
 Dick Phillips, 665-1343, rlp@lanl.gov  
 Bob Tomlinson, 665-6599, bob@lanl.gov  
 Ron Daniel, 665-0597, rdaniel@lanl.gov  
 Pat Kelley, 665-4665, kelly@lanl.gov

Lab Capabilities Applied: High performance computing, networking, software engineering, visualization, telecollaboration, modeling and simulation.



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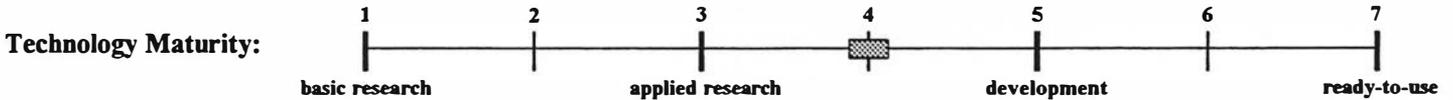
Category: Development (25,2)

Laboratory: Los Alamos National Laboratory      Contact: John Reynders, 505-665-7449, reynders@lanl.gov

Title: Parallel Object Oriented Methods and Applications

**Description:** Our goal is to develop a portable parallel simulation run-time system which supports several base types for scientific simulation. These foundation classes or object-libraries will consist of Arrays, Matrices, Particles, and Unstructured Meshes. A design requirement of this run-time system is that any code written with objects/components from these foundation classes will be portable between serial and parallel architectures with NO change to the source code. This framework focuses on object-oriented (OO) methodologies. OO paradigms have proven themselves in a variety of sectors (most notably, the PC software market) as being the methodology of choice for large-scale, team code development. We find this paradigm reduces code complexity and allows for expressions in the software which are closely related to the mathematical expressions which an engineer or physicist is attempting to solve in the first place. This framework is constructed in layers where at the highest level, a simple interface is presented to the user with a rich set of functionality and components. At layers lower in the class library there exist objects which the user never sees which mediates domain decomposition, data layout, and interprocessor communication. Moving to other architectures simply involves linking in the binary of the class library for the target architecture. This layered approach to software design and development also allows the users to penetrate the layers at any level. This allows rapid prototyping at the highest level where the object expressions are closely related to the actual equations being solved. At the same time, a user can access and manipulate objects hidden at a lower level to tune and optimize a particular application. This methodology is being used in a wide variety of applications and has great potential for the petroleum industry because of the rapid evolution of computing architectures.

91-95 Funding (\$K): 1250      Dates: 1994 - present



Technology Transfer: Technology publications in open literature

Key Documentation: <http://www.acl.lanl.gov/PoomaFramework>

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 Paul Hinker, 665-6396, hinker@lanl.gov  
 MaryDell Tholburn, 667-0619, marydell@lanl.gov

Lab Capabilities Applied: High performance computing, modeling, and simulation.



Index: 233

Category: Environmental & Regulatory (9,6)

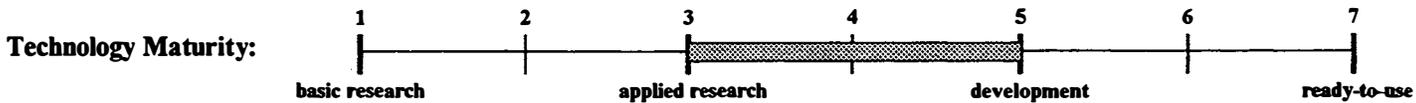
Laboratory: Los Alamos National Laboratory      Contact: Bradley Clark, 505-667-6287, bac@lanl.gov

Title: Lithology Characterization for Remediation of Underground Pollution

**Description:** Characterizing underground lithology is important in analyzing and comparing environmental remediation strategies for underground pollution. Lithology data, obtained from analysis of log records, is used in underground hydrological models to predict the impact of different remediation strategies. Continued borehole logging, testing, and analysis during the remediation process allow the actual performance of a remediation technique to be fed back into computer models, so the procedure can be modified to suit actual conditions. Existing nuclear borehole logging techniques have been used extensively for oil-bearing structures. However, environmental studies must function in the wider variety of geological and hydrological conditions found in both sedimentary and non-sedimentary formations near the earth's surface. Environmental analyses demand a more accurate characterization of lithology for use in hydrological models.

We propose to perform the transport code development and nuclear analysis to determine lithology data and map subsurface contaminant distribution. Others at Los Alamos, as well as elsewhere, would provide the tools to analyze underground flow, chemical exchange, and pollution removal. We plan to develop the transport codes for the next-generation massively parallel supercomputer with a user interface that will make these codes readily accessible to the petroleum industry and to the environmental community. The speed and the memory of the next generation of parallel architectures will enable the simulation of full-scale fields.

91-95 Funding (\$K): 875      Dates: 1994 - present



**Technology Transfer:** Collaborative project with Schlumberger-Doll Research, availability of transport models and efficient solution algorithms for massively parallel architectures.

**Key Documentation:** Proposal to the Department of Energy for a Cooperative Research Project in the High Performance Parallel Processor Program

**Key Personnel:** Bradley Clark, 505-667-6287, bac@lanl.gov  
Pat Soran, 505-667-8103, soran@lanl.gov

**Lab Capabilities Applied:** High performance computing, massively parallel computing, nuclear well logging, nuclear data base, modeling and simulation.



Index: 234

Category: Development (25), Exploration (13)

Laboratory: Los Alamos National Laboratory      Contact: Olaf Lubeck, 505-667-6017, oml@lanl.gov

Title: The Development of a General Reservoir Simulation for Massively Parallel Computers

**Description:** The need for a new reservoir simulator designed for massively parallel processor (MPP) computers has been researched and is considered to be a high priority agenda item by Amoco. An MPP reservoir simulator will make it possible to better quantify uncertainties in the performance of oil and gas reservoirs using geostatistical methods. It is estimated that several million cells per run will be needed for the type of methods employed. Demands for more accurate simulations over larger volumes necessitates the use of MPP's to perform the simulations within realistic time frames. Though production software for reservoir simulation is fairly well-developed, codes that fully exploit the power of MPP's to generate the model and solve the associated linear equations are practically nonexistent in the scientific and engineering communities.

This project will center around moving Amoco's current production reservoir simulator to the CRAY T3D system. The simulation will allow both black-oil and fully compositional fluid properties. The existing code will be adapted and rewritten to perform efficiently on massively parallel machines. In addition, efficient parallel iterative linear equation solvers will be incorporated into the software to perform the heavily computation-intensive linear system solutions required by the simulation. It is expected that one of the major spin-off products of the project will be in the area of massively parallel linear equation solvers.

91-95 Funding (\$K): 875      Dates: 1994 - present



**Technology Transfer:** Collaborative project with Amoco; it is anticipated that this technology will be licensed to a third-party company, who will make the simulation generally available to the petroleum industry.

**Key Documentation:** Proposal to the Department of Energy for a Cooperative Research Project in the High Performance Parallel Processor Program.

**Key Personnel:** Wayne Joubert, 505-665-7374, wdj@lanl.gov

**Lab Capabilities Applied:** High performance computing, modeling, and simulation.



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Category: Development (25, 28, 33)

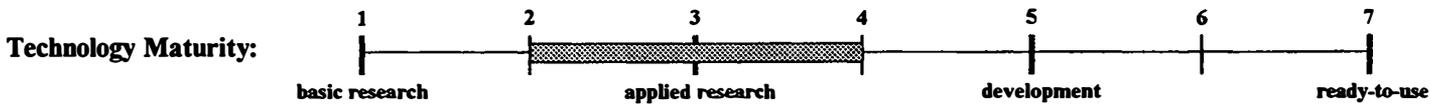
Laboratory: Los Alamos National Laboratory      Contact: J. M. Kindel, 505-667-3718, jkindel@lanl.gov

Title: Advanced Reservoir Management (ARM) for Independent Oil and Gas Producers

**Description:** This project involves a partnership between Los Alamos and key independents in six regions: Appalachia, Rocky Mountain, Mid Continent, Permian Basin, Pacific and Gulf Coast. The key interface is the Strategic Technologies Council whose member companies in eighteen (18) states will accomplish technology transfer through their state and regional independent producer organizations and the service industry.

This project involves gathering and generating advanced reservoir management techniques by working closely with independent producers on joint reservoir management projects. Drawing on advanced reservoir management techniques which exist for majors, Los Alamos National Laboratory is generating first order analogies to reservoirs and to recovery methods which emerge from similarities in reservoir geology, fluid behavior, other characteristics and appropriate recovery mechanisms. In particular, adaptive learning systems using techniques such as neural networks and expert advisory systems are being applied to diverse technology areas such as formation evaluation through log analysis, corrosion prevention, stabilization of well bores during drilling and well remediation. Applications of these adaptive learning approaches are also being made to determine oil and gas reserves, to assess recovery mechanisms, and to obtain more information from seismic data for exploration and infill drilling prospects. Information developed will be available through an internet archive.

91-95 Funding (\$K): 6500      Dates: 1995-present



**Technology Transfer:** Conference and workshop proceedings such as through PTTC and STC (Strategic Technologies Council); World Wide Web/Internet pages; licensing; journal articles

**Key Documentation:** 1) New project just being initiated, Advanced Computational Technology Initiative Proposal

**Key Personnel:** Joe Kindel, 505-667-3718, jkindel@lanl.gov  
 Kenneth Lee, 505-665-7518, ken\_lee@lanl.gov  
 Robert Webster, 505-665-4183, robw@lanl.gov  
 Kevin Buescher, 505-667-1356, klb@lanl.gov

**Lab Capabilities Applied:** System integration, adaptive computing, sensor modeling and interpretation, large data bases, modeling of nuclear well-logging, 3-D wave propagation models, distributed computing, visualization, data mining



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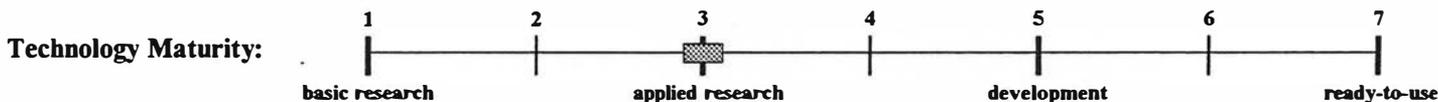
Category: Development

Laboratory: National Institute for Petroleum and Energy Research      Contact: Daniel Maloney, (918) 337-4364

Title: Characterization of Fractured Rock to Produce Remaining Oil in Place.

Description: Natural fractures pose significant challenges to petroleum recovery. For example, the estimated ultimate recovery from Spraberry/Dean sands of West Texas is only 5% of the estimated 9.4 billion barrels of the Original-Oil-In-Place (OOIP). Current knowledge is inadequate for describing capillary interaction between natural fractures and the matrix and the influence of changing stress fields on permeability. A model describing fluid imbibition from a fracture into a matrix was completed in FY 94. Laboratory tests will be conducted to provide data to refine and/or validate the model. The model will be used to assess Improved Oil Recovery (IOR) methods in fractured reservoirs.

91-95 Funding (\$K): 300      Dates: 1994-1995



Technology Transfer: Society of Petroleum Engineers meetings, technical presentations at Society of Core Analysts meetings, work-for-others projects, laboratory tours, communications with research staffs at other facilities.

Key Documentation: New project.

Key Personnel: Min Tham, (918) 337-4387 Daniel Maloney, (918) 337-4364 Ming-Ming Chang, (918) 337-4346

Lab Capabilities Applied: Flow through porous media laboratory including about \$300,000 in equipment (2-D linear X-ray scanner for saturation measurements, pumps, transducers, computers, specialized coreholders, explosion-proof ovens, solvent extraction systems, etc.).



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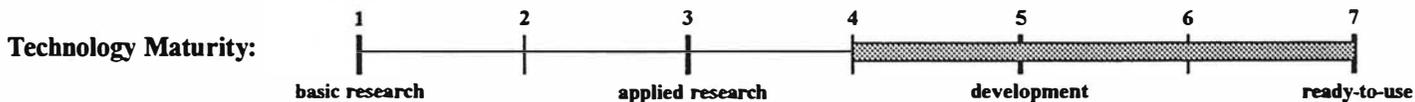
Category: Development (2), Production (3, 2, 11)

Laboratory: National Institute for Petroleum and Energy Research      Contact: Michael P. Madden, (918)337-4261

Title: Field Demonstrations in High Priority Reservoir Classes

**Description:** The objective of this program is to maximize the economically and environmentally sound recovery of oil from known domestic reservoirs and preserve access to the resource by demonstrating improved oil recovery processes and reservoir characterization methods and transferring the technology to the oil industry. The program is targeted toward classes of reservoirs having the highest potential for increased oil recovery and the highest probability of abandonment. Field projects are underway in eleven (11) Class 1, fluvial dominated deltaic, reservoirs and nine (9) Class 2, shallow shelf carbonate, reservoirs. Nine projects for Class 3, slope basin and basin clastic, reservoirs are under negotiation. The competitive solicitation for Class 4, strandplain and barrier island, reservoirs has just begun. These projects are demonstrating technologies in the following areas: digital databases, outcrop analysis, core analysis, biostratigraphy, core flooding, x-ray diffraction, scanning electron microscopy, nuclear magnetic resonance, fracture characterization, water and oil chemistry, biomarkers, PVT analysis, reservoir modeling and simulation, geostatistics, reservoir management, 3-D seismic, infill drilling, horizontal, deviated, and slant wells, short-radius laterals, recompletion, formation microscanning and imaging, borehole televiewer, pulse acoustic logging, well stimulation, pulse, interference, and tracer tests, pressure transient analysis, injectivity tests, drill stem tests, paraffin control, waterflooding, pressure maintenance, fault zone production, carbon dioxide, microbial, and polymer flooding, thermal processes, and alkaline assisted waterflooding. NIPER is planning, conducting solicitations, and monitoring the field projects. In addition, NIPER will participate with industry in demonstrating reservoir management technology using Cooperative Research and Development Agreements (CRADAs). These projects address industry-wide problems of declining production.

91-95 Funding (\$K): 17736      Dates: 1994 - Present



Technology Transfer: Workshops, Short Courses, Publications, Data Bases, Presentations, INTERNET Home Pages, Newsletters

Key Documentation: 1) Geological and Production Characteristics of Strandplain/Barrier Island Reservoirs in the United States, by E.L Cole, et al., DOE Report NIPER/BDM-0027, July 1994. 2) Research Needs for Strandplain/Barrier Island Reservoirs in the United States, by E.L Cole, et al., DOE Report NIPER/BDM-0054, September 1994.

Key Personnel: Michael Madden, 918-337-4261 Lance Cole, 918-337-4565 Mike Fowler, 918-337-4578 Susan Jackson, 918-337-4465 Gene Safley, 918-337-4318 Phillip Salamy, 918-337-4579 Mark Young, 918-337-4543

Lab Capabilities Applied: Petroleum Engineering, Reservoir Engineering, Reservoir Management, Geology, Numerical Simulation, Geological Modeling



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Category: Development

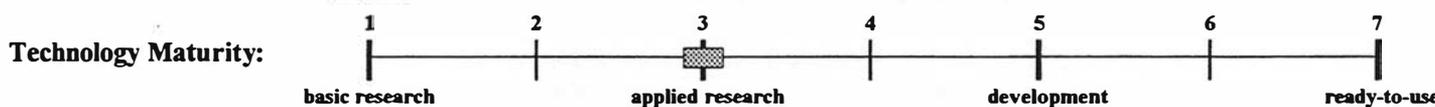
Laboratory: National Institute for Petroleum and Energy Research      Contact: Douglas Lawson, (918) 337-4589

Title: Integrated Geoscience/Engineering Methods of Optimal Reservoir Upscaling

**Description:** Independent operators are in need of more cost-effective methods for predicting production in depositionally heterogeneous reservoirs. NIPER is researching and developing a method for determining the optimum combination of grid refinement and block property averaging within a geological context. The work consists of:

- 1) Evaluating depositional heterogeneity for the barrier island/strandplain facies in the Almond Formation based on outcrop investigation along the Rock Springs Uplift, Wyoming.
- 2) Integrating observations into an architectural framework for Patrick Draw Field. Verifying from sampling and wireline logs.
- 3) Measuring properties within and among facies found in the outcrop.
- 4) Reviewing and improving current upscaling methods of deriving representative properties for larger units. Selecting grid size for an economical and representative model to calculate reservoir behavior. Testing techniques for reservoir at the Patrick Draw Field
- 5) Generalizing the results to other barrier island/strandplain reservoirs.
- 6) Transferring technology developed.

91-95 Funding (\$K): 3827      Dates: 1991- Present



**Technology Transfer:** Paper and presentations at Society of Petroleum Engineering Annual meetings, Rocky Mountain Geological Society meeting, New Technology for Independent Producers Workshop, Texas Independent Producers and Royalty Owners Technology Transfer Workshop,

**Key Documentation:**

- 1) Szpakiewicz, M.J., R.A. Schatzinger, M.M. Honarpour, M.K. Tham, and R.W. Tillman, 1989, Geological and Engineering Evaluation of Barrier Island and Valley-Fill Lithotypes in Muddy Formation, Bell Creek Field, Montana: In Coalson, E.B., ed., Petrogenesis and Petrophysics of Selected Sandstone Reservoirs of the Rocky Mountain Region, The Rocky Mountain Association of Geologists, Denver, Colorado, p. 159-182
- 2) Jackson, S.R., L. Tomutsa, M.J. Szpakiewicz, M.M. Chang, M.M. Honarpour, and R.A. Schatzinger, 1991, Application of an Integrated Methodology for Construction of a Quantified Transmissivity Model-Bell Creek Field, A Barrier Island Reservoir: In Lake, L., H.B. Carroll, Jr., and T.C. Wesson, eds., Reservoir Characterization II, Academic Press, Inc., N.Y., p. 524-556.

**Key Personnel:** Douglas Lawson, (918) 337-4589 Richard Schatzinger, (918) 337-4470 Ming Ming Chang, (918) 337-4346 Liviu Tomutsa, (918) 337-4472

**Lab Capabilities Applied:** Petroleum Engineering, Reservoir Engineering, Petroleum Geology, Reservoir Geology, Reservoir Simulation including Scale-up and Optimization, Log Analysis, Seismic Interpretational Structural Analysis, Petrographic Analysis including Scanning Elec



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**Category:** Environmental & Regulatory

**Laboratory:** National Institute for Petroleum and Energy Research      **Contact:** Raymond P. Anderson, Manager, Fuels & Engine Testing, (918) 337-4464

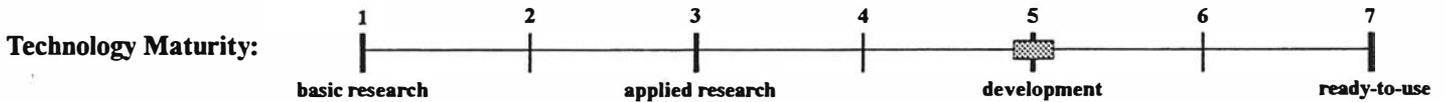
**Title:** Natural Gas Technology Enhancements

**Description:** The natural gas technology enhancements program involves the exploration and development of new concepts and components suitable for installation into both commercial and military vehicles. It is recognized that the utilization of natural gas powered vehicles and equipment will help improve air quality and ease this country's dependence on foreign fuel sources.

Through contract research with industry, the government is providing for development of advanced concepts and problem solutions for the following topic areas: natural gas storage systems; sensors and controls; and fueling equipment. The common focus is to reduce cost, improve performance, enhance safety, and improve the marketability of alternative fuel system. Work in these areas may include any aspect of the technical solution that will enable the use of natural gas in transportation vehicles either in the near term with a documented potential to increase the use of the fuel, or in the far term with the technological advancements that show the promise for the potential of the increased use of natural gas.

Proposals were solicited for work in the following areas: sensors and controls, CNG and LNG onboard storage, and CNG and LNG fuel supply. Contract awards are currently under negotiation.

**91-95 Funding (\$K):** 3000      **Dates:** 1994 - Present



**Technology Transfer:** Publications in open literature, technical presentations

**Key Documentation:** n/a

**Key Personnel:** Raymond P. Anderson, (918) 337-4464, Fax (918) 337-4342  
 M. Daniel Gurney, (918) 337-4379, (918) 337-4342

**Lab Capabilities Applied:** Emissions Testing, Physical Testing





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Category: Environmental & Regulatory

Laboratory: National Institute for Petroleum and Energy Research      Contact: Raymond P. Anderson, Manager, Fuels & Engine Testing, (918) 337-4464

Title: Establishing California Air Resources Board Reactivity Rating for Ethanol

**Description:** The use of alternative fuels has the potential for reducing emissions of photochemically reactive pollutants from automobiles. Although the mass emissions rates are not necessarily lower than those with gasoline, the photochemical reactivity of the Non-Methane Organic Gases (NMOG) can be significantly reduced with alternative fuels. California emissions regulations recognize the benefits of lower reactivity. For vehicles certified to operate on a fuel other than conventional gasoline, the NMOG mass emission value is multiplied by a Reactivity Adjustment Factor (RAF) applicable to the fuel and the vehicle emission control technology category. The reactivity adjusted NMOG emission rate is then compared to the emission standard to determine compliance.

Emissions tests of E85 fuel (85 percent fuel grade ethanol, 15 percent gasoline) were conducted using four identical model variable fuel vehicles calibrated for ethanol. Emissions and performances were comparable for the four vehicles. Detailed speciation of the exhaust was performed in order to determine the photochemical reactivity potential relative to gasoline. The ratio of the reactivities, the reactivity adjustment factor (RAF), was 0.68. With the application of the RAF to the NMOG emissions, the exhaust emissions were less than the California Transitional Low-Emission Vehicle standards. The repeatability of the results was well within the requirements for inclusion in the data base for establishing a generic reactivity adjustment factor for ethanol. The study was extended to other vehicles and other factors such as the effects of ethanol fuels on drivability and the effect of using blends of E85 and reformulated gasoline.

91-95 Funding (\$K): 185      Dates: 1992 - Present



Technology Transfer: Publications in open literature, technical presentations

**Key Documentation:** 1) Marshall, W. F.. Influences of Fuel, Driving Cycle, and Ambient Temperature on the Performance of Vehicles Designed for Ethanol Fuel. NIPER/BDM-0014. Prepared for the Department of Energy, January 1995  
 2) Marshall, W. F.. Reactivity Adjustment Factor for Vehicles Operating on E85. Presented at the Government Contractor's Coordination Meeting, Washington DC, October 1993.

**Key Personnel:** Raymond P. Anderson, (918) 337-4464, fax (918) 337-4342 William F. Marshall, (918) 337-4253, fax (918) 337-4342

**Lab Capabilities Applied:** Emissions Testing, Analytical Chemistry Laboratories



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Category: **Drilling & Completion**

Laboratory: **National Institute for Petroleum and Energy Research**      Contact: **Herb Carroll, (918) 337-4558**

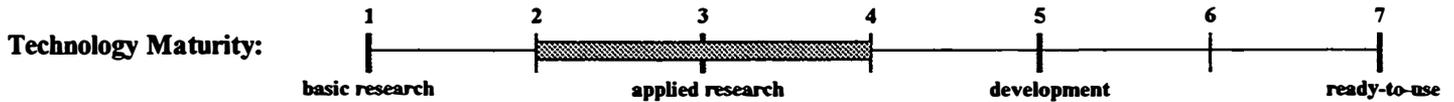
Title: **Drilling, Completion and Re-Completions (Underbalanced Drilling, Wellbore Stability, Coiled Tubing and Slimhole Drilling)**

**Description:** Drilling and completing new wells can account for 30% - 70% of the initial capital cost. The current economic climate requires that operating and capital costs be reduced if development is to continue in mature areas. Without new technology and/or improved equipment/fluids, the domestic active rig count will continue to be dismal, and existing wells will continue to be shut in at an accelerated rate. Independent producers operating with marginal cash flow and return on investment are particularly vulnerable.

The drilling program will develop improved, more cost-effective techniques, equipment and/or fluids for drilling and completion of new wells or recompletion of existing wells in an environmentally sound and operationally safe manner. The program includes research on vertical, slant, and horizontal wells of conventional and slimhole design. The goals of this project are:

- To identify and develop (or assist in the development of) improved theories, strategies, technologies, and equipment to improve the economic, safety and/or environmental impacts of current drilling, completion and recompletion practices
- To develop seminars, workshops, and industry cost-shared field projects for effective technology transfer
- To integrate work with others involved in drilling, completion, and recompletion research, such as the National Advanced Drilling and Energy Technology (NADET), Morgantown Energy Technology Center (METC) Gas Program, Natural Gas & Oil Partnership, and industry and university programs.

91-95 Funding (\$K): **475**      Dates: **1994 - Present**



Technology Transfer: **Reports**

Key Documentation: **1994 Annual Technical Report, Status Report "A Review of Slimhole Drilling".**

Key Personnel: **Tao Zhu (918) 337-4215 Len Volk (918) 337-4466**

Lab Capabilities Applied: **Mechanical Engineering, Chemistry, Chemical Engineering, Fluid Dynamics, Petroleum Engineering, Fatigue Analysis.**



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**Category:** Exploration, Drilling & Completion

**Laboratory:** National Institute for Petroleum and Energy Research

**Contact:** Frank Chung, (918) 337-4274

**Title:** Risk-Based Decision Management

**Description:** The probability of finding oil and the possibility of making profits are difficult to achieve. Under these adverse conditions, risk analysis technology becomes very important for petroleum producers. The technology involves many disciplines such as geoscience, petroleum engineering, environment, business, mathematics, and computer science. Most of the commercially available risk analysis and decision making software are developed for general purposes and do not provide any specific technique for petroleum exploration risk analysis. This project was designed to develop a more reliable risk analysis application specialized for petroleum exploration and development, especially for independent producers.

The risk management research program is a new initiative project (started FY 94). New techniques, especially in the artificial intelligence applications, for exploration, drilling, environment, and EOR-project risk assessment will be developed. A user friendly risk assessment product, which includes both conventional methods and newly developed methods, will be transferred to petroleum industry. The addition of risk-based decision making capabilities should help the independent hydrocarbon producers more effectively evaluate the opportunities in underdeveloped basins and encourage more domestic hydrocarbon exploration.

**91-95 Funding (\$K):** 321

**Dates:** 1994 - Present



**Technology Transfer:** Reports, SPE paper, and workshops will be held in 1995-1996.

**Key Documentation:** DOE reports: 1) State-of-the-art theory and algorithm developments used in the risk-based decision process.  
2) Federal environmental regulations impacting hydrocarbon exploration, drilling, and production operations.

**Key Personnel:** Herb Carroll, (918) 337-4558  
Frank Chung, (918) 337-4274  
Gene Larson, (918) 337-4208  
Bill Johnson, (918) 337-4282  
K.C. Chen, (918) 337-4256

**Lab Capabilities Applied:** Computers-PC, MicroVAX, SUN workstation.



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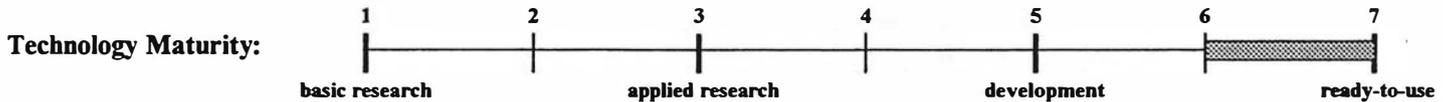
**Category:** Environmental & Regulatory

**Laboratory:** National Institute for Petroleum and Energy Research      **Contact:** Stephen Jones, (918) 337-4528

**Title:** California Pipeline and Gathering Line Assessment

**Description:** An inventory of pipelines and gathering lines in California is required to support development of regulations related to safe operations of those pipelines. The pipelines and gathering lines to be inventoried are those : 1) used for transportation of crude oil that operate by gravity or at a stress level of 20% or less of the specified minimum yield strength of the pipe, and 2) used for transportation of petroleum in onshore gathering lines located in rural areas. The inventory will be coordinated with the California Division of Oil, Gas, and Geothermal Resources.

**91-95 Funding (\$K):** 650      **Dates:** 1994 - Present



**Technology Transfer:** Reports and presentations will be key elements of transfer.

**Key Documentation:**

**Key Personnel:** Stephen Jones and Jerry Simmons  
(918) 337-4528

**Lab Capabilities Applied:** The technical and project management expertise at NIPER in the area of petroleum production make this project possible.



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Category: Oil Processing &amp; Refining

Laboratory: National Institute for Petroleum and Energy Research

Contact: D. L. Ripley, (918) 337-4264

Title: Processing and Utilization Research - Thermodynamic and Thermophysical Property Measurements

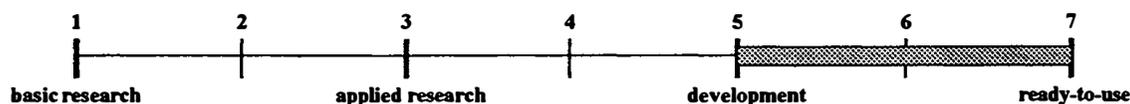
**Description:** The Design Institute for Physical Property Data (DIPPR) now in its 15th year of funded research is the American Institute of Chemical Engineers (AIChE) oldest active sponsored research group. Two DIPPR experimental property measurement projects have been conducted at NIPER for the past several years: Project 821 \_ Pure Component Liquid-phase Vapor Pressure Measurements Project 871 \_ Pure Component Ideal-Gas Enthalpies of Formation. The objectives of this research include measuring thermodynamic and thermophysical property data as directed by the DIPPR Project Steering Committees. The objective of Project 821 is to obtain precise and accurate liquid-phase vapor pressure data for selected pure compounds. The objective of Project 871 is to measure the enthalpies of combustion and derive the enthalpies of formation in both the condensed and ideal-gas phases of "key" compounds that have been chosen to elucidate the enthalpy of particular atomic groupings. These group contributions can then be used to estimate data on large families of related compounds, each containing that particular atomic arrangement.

91-95 Funding (\$K):

500

Dates: 1988 - Present

Technology Maturity:



Technology Transfer: Publications, Reports, Seminars

Key Documentation:

1. Steele, W. V., et. al. "DIPPR Project 871. Determination of Ideal-Gas Enthalpies of Formation for Key Compounds - The 1990 Project Results. Published in Experimental Results for DIPPR" 1990-91 Projects on Phase Equilibria and Pure Component Properties. DIPPR Data Series No. 2, 1994, pp. 188-215 (1994). Cunningham, J. R. and Jones, D. K.; editors.
2. Steele, W. V., et. al. "DIPPR Project 871. Determination of Some Pure Compound Ideal-Gas Enthalpies of Formation. The 1991 Project Results to be published in Experimental Results for Phase Equilibria and Pure Component Properties DIPPR Data Series No. 3." 1995 Cunningham, J. R. & Jones, D. K. editors.

Key Personnel: W. V. Steele, (918) 337-4210

Lab Capabilities Applied: Thermodynamics, Fuels Chemistry



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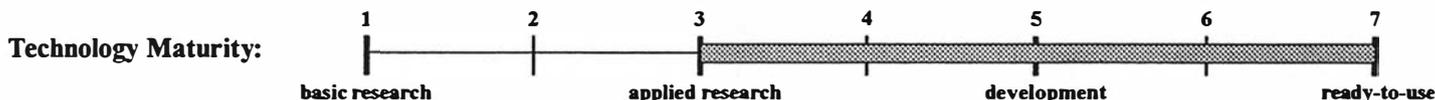
Category: Oil Processing & Refining

Laboratory: National Institute for Petroleum and Energy Research      Contact: Dexter Sutterfield, (918) 337-4251

Title: Conduct Round Robin Tests on Heavy Crude and Bitumen

Description: The Bartlesville Energy Technology Center of the Department of Energy, and subsequently NIPER, have invested considerable resources and effort in the development of methods for the characterization of heavy crude and Cerro Negro crude in particular. From that involvement and interest, NIPER participated in the United Nations Institute for Training and Research (UNITAR) Centre Third and Fourth Round Robin studies on inspection and characterization of Cerro Negro crude. These studies are part of a larger program coordinated by UNITAR "to standardize methods to be used in the evaluation of heavy crude and bitumen and improve the procedures required for the characterization of heavy crude and bitumen samples". This project provides for completion of the Fourth Round Robin Tests on Heavy Crude and Bitumen. The objective of the project is to continue involvement in the development of standardized methods and improved procedures for testing and characterization of heavy crudes and bitumen.

91-95 Funding (\$K): 150      Dates: 1993 - Present



Technology Transfer: Journal Articles, Technical Presentations

Key Documentation:

Key Personnel: Gene Sturm, (918) 337-4314  
 John Green, (918) 337-4255

Lab Capabilities Applied: Petroleum Analysis and Characterization, Instrumentation



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**Category:** Production

**Laboratory:** National Institute for Petroleum and Energy Research

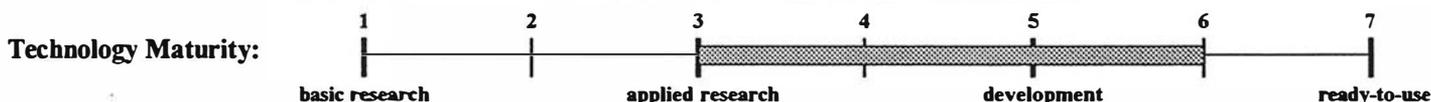
**Contact:** Rebecca S. Bryant, (918) 337-4328

**Title:** Chemical Methods for Improved Oil Recovery

**Description:** Research at NIPER/BDM-Oklahoma, Inc. has been at the forefront of the development efforts in chemical-based improved oil recovery. This has led to the development and testing of several alternative methods of conformance control, including a patented technology based on the surfactant-alcohol treatment system. Similarly, tools such as a PC-based permeability modification simulator have been developed that can be readily utilized by independents for their production operations. NIPER's permeability modification simulator can be used to help independents design and optimize oil production.

Alkaline-surfactant-polymer (ASP) has shown promise to recover oil economically and is very applicable to independent producers. The ASP process has significantly improved economics by reducing front end chemical costs of such treatments. NIPER's ASP project involves field testing and demonstration of this promising process.

**91-95 Funding (\$K):** 2000      **Dates:** 1986 - Present



**Technology Transfer:** PC Gel Simulator, Workshops on Chemical Flooding Technology and Formation Damage Control, Seminars and presentations given at ACS, AIChE, and SPE meetings, Publications in Trade Journals and books, Technology training session given to operators

**Key Documentation:** Patents: 1) Llave, F.M., T.E. Burchfield and D.K. Olsen: Method for Modifying the Permeability of an Underground Formation, U.S. Patent No. 5,101,903, April 7, 1992.  
2) Peru, D.A., Aqueous Flooding Methods for Tertiary Oil Recovery, U.S. Patent No. 4,817,715, April 4, 1989.

**Key Personnel:** F.M. Llave, (918) 337-4359 B.L. Gall, (918) 337-4386 T.R. French, (918) 337-4383 H.W. Gao, (918) 337-4271

**Lab Capabilities Applied:** Petroleum Engineering, Chemical Engineering, Reservoir Engineering, Environmental Engineering, Mechanical Engineering, Field Evaluation and Testing, Process Design/Development and Simulation, Engineering Analysis, Polymer and Gel Chemistry, Micr



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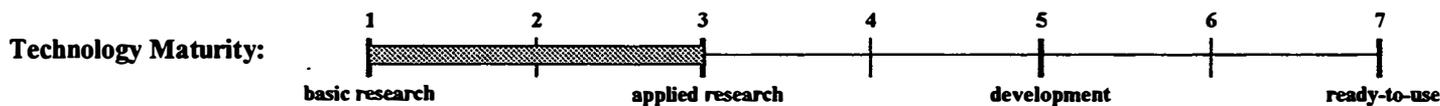
Category: Oil Processing & Refining

Laboratory: National Institute for Petroleum and Energy Research      Contact: D. L. Ripley, (918) 337-4264

Title: Processing and Utilization Research - Analysis and Remediation of Contaminated Soil and Groundwater

Description: This project seeks to develop methods for more rapid and accurate spill characterization, containment, and treatment to keep pace with the evolution of refinery processes and feedstocks. One goal of the study is to shorten identification response time and increase opportunities for the selection of counter measures after a release, and provide strategies for the selection of alternate remedies consistent with local conditions. Because refineries are becoming complex arrangements of physical, chemical, and biological processes, the program seeks to provide a wide spectrum of options to the environmental specialist. These include sampling and analysis techniques, chemical and biological barriers, and treatment processes. The methods are also applicable to general uses in environmental process monitoring of treated streams and for remediation of groundwaters. Contacts with small regional refineries will be made in an effort to apply the evolving system of methods to the problems of the regional refiners.

91-95 Funding (SK): 200      Dates: 1993 - Present



Technology Transfer: Publications, Reports, Seminars

Key Documentation: Interagency Agreement, DFSC

Key Personnel: J. W. Goetzinger, (918) 337-4309

Lab Capabilities Applied: Petroleum Processing, Fuels Chemistry



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**Category:** Environmental & Regulatory

**Laboratory:** National Institute for Petroleum and Energy Research

**Contact:** Stephen Jones, (918) 337-4528

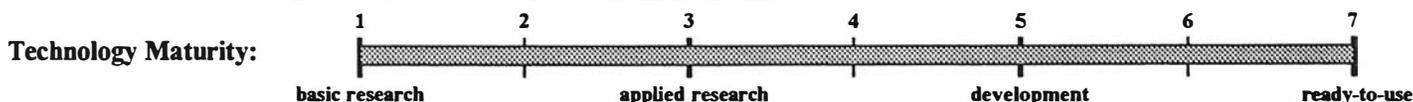
**Title:** Area of Review Variance Program

**Description:** The Safe Drinking Water Act (SDWA) of 1974 required that the Environmental Protection Agency develop minimum requirements to establish effective state programs to protect Underground Sources of Drinking Water (USDW) from contamination resulting from the subsurface emplacement of fluids through injection wells. The SDWA states that these requirements must not impede the reinjection of brine or other fluids resulting from oil and gas production, or the injection of fluids used in secondary or tertiary recovery, unless USDW would be endangered. EPA promulgated rules in 1980 that excluded existing Class II injection wells from Area of Review (AOR) requirements. EPA has recently announced its intent to revise regulations to include the AOR requirement for the previously excluded wells.

A Federal Advisory Committee (FAC) has recommended that AORs for existing wells be performed within five years of any new regulations. The FAC also recognized that conditions could make it possible to exempt wells in a specified region (basin, trend, field, portion of a field, etc.) from individual well AORs through a variance. The proposed rule would require states to establish a variance methodology which would delineate where variances from the proposed requirements would be appropriate.

A variance methodology has been developed under the sponsorship of the American Petroleum Institute. The conditions under which variance can be granted include: 1) the absence of USDWs; 2) the reservoir is underpressured relative to the USDW; 3) local geological conditions preclude upward fluid movement that could endanger USDWs; and 4) other compelling evidence. The methodology requires access to a broad range of data including wellbore related data, reservoir pressure front data, fluid level data to identify under-pressured reservoirs, and locations of major and minor aquifers.

**91-95 Funding (\$K):** 650 **Dates:** 1994 - Present



**Technology Transfer:** Reports and presentations will be key elements of transfer.

**Key Documentation:**

**Key Personnel:** Stephen Jones Jerry Simmons Patrick Navratil (918) 337-4528

**Lab Capabilities Applied:** The technical and project management expertise at NIPER in the area of petroleum production make this project possible.



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Category: Production

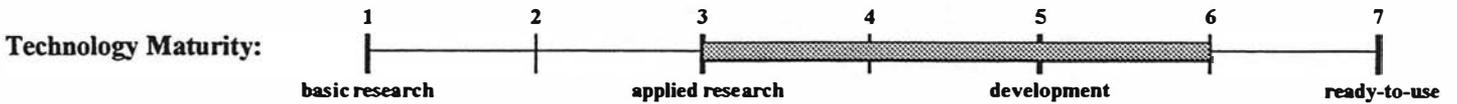
Laboratory: National Institute for Petroleum and Energy Research      Contact: Rebecca S. Bryant, (918) 337-4328

Title: Biotechnology for Improved Oil Recovery

**Description:** The Application of microbial methods for improved oil recovery is one of the cost-effective techniques that DOE has developed for independent producers and Native Americans. Improved oil recovery techniques using microorganisms have the potential to arrest well abandonment and improve oil production significantly in marginal oil fields. As the major oil companies abandon domestic reserves to the independent petroleum producers, technologies must be available to these independents in order to maintain our domestic oil production. Microbial methods for improving oil production are among the very few technologies that are cost-effective and capable of being implemented by the independent oil producing industry.

The current technologies being examined and implemented by the U.S. DOE are cross-cutting and timely. NIPER has demonstrated two successful microbial waterflood pilots and developed a Microbial Transport Simulator. The tasks that are currently being conducted for this project are: 1) Integration of laboratory and field data for microbial process simulation; 2) Assisting independent operators by identifying biological techniques for cost-effective wellbore cleanup; 3) Conducting short courses for independent operators on biotechnology for improved oil production; and 4) Supporting the DOE in sponsoring the International Microbial Enhanced Oil Recovery (EOR) Conference. Technologies being examined for future initiatives include improving cash flow for the independents by coupling improved oil recovery techniques with aquaculture. This program would benefit the environment by creating a closed loop between cleaning up produced water from oil field production, reducing costs of water disposal, and generating cash flow for the operators.

91-95 Funding (\$K): 2417      Dates: 1986 - Present



Technology Transfer: Microbial Transport Simulator, Microbial Technology Short Courses, Seminars, SPE Papers, News Releases on Successful Field Pilots, Trade Journal Articles, INTERNET Home pages

Key Documentation: 1) Bryant, R.S., A.K. Stepp, K.M. Bertus, T.E. Burchfield, and M.D. Dennis, "Microbial Enhanced Waterflooding Field Tests," Proc. of the 1994 SPE/DOE Improved Oil Recovery Symposium, Tulsa, OK, April 17-20, 1994, SPE/DOE Paper No. 27751.  
 2) Buciak, J., A. Vazquez, R. Frydman, J. Mediavilla, and R.S. Bryant, "Enhanced Oil Recovery by Means by Microorganisms: Pilot Test," Proc. of the SPE Latin American and Caribbean Petroleum Engineering Conference, April 22-24, 1994, Buenos Aires, Argentina. SPE Paper No. 27031.

Key Personnel: R.S. Bryant, (918) 337-4328 A.K. Stepp, (918) 337-4290

Lab Capabilities Applied: Microbiological Techniques, Bioremediation Techniques, Petroleum Engineering, Reservoir Engineering, Field Evaluation and Testing, Engineering Analysis, Environmental Engineering, Mechanical Engineering, Process Design/Development and Simulation, Po



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Category: Environmental & Regulatory

Laboratory: National Institute for Petroleum and Energy Research      Contact: Raymond P. Anderson, Manager, Fuels & Engine Testing, (918) 337-4464

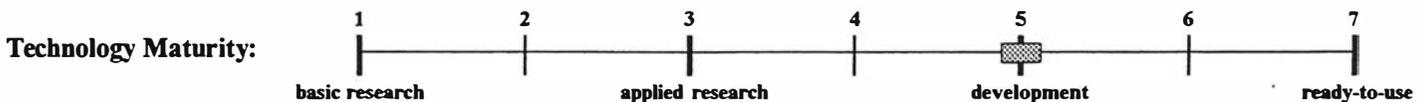
Title: Biodiesel, Commercialization of a Renewable Fuel

**Description:** The objective of this project is the development of the technological base necessary to proliferate the commercialization of biodiesel as a renewable fuel. This effort is in support of the national objectives of decreasing dependence on imported petroleum and improving air quality. Biodiesel is a renewable resource and offers the potential for a reduction of harmful emissions. In this discussion, biodiesel refers to the methyl or ethyl esters of oils of biological origin. Soybean oil is the primary source being developed as a fuel resource. In an unmodified engine, combustion of biodiesel results in a reduction of EPA-regulated emissions except for nitrogen oxides (NOx). Emissions of nitrogen oxides must be decreased, and the acceptance of regulatory agencies, engine manufacturers, and transit users must be gained.

Particular emphasis is placed on the performance of the fuel in a heavy duty diesel engine, the Cummins L-10. Results indicate that biodiesel causes significant reduction in hydrocarbons, carbon monoxide, and particulate emissions but a significant increase in nitrogen oxide emissions.

Perhaps the most significant finding of this project is that the increase in NOx emissions noted with the use of methyl soyate can be counteracted by the addition of a less-expensive blending component (heavy alkylate, a refinery stream), which results in the reductions of all emissions compared to the base diesel fuel. This may provide an attractive market for heavy alkylate as changing refinery product specifications, that are required for the production of reformulated gasoline, will reduce the usefulness of this refinery stream.

91-95 Funding (\$K): 695      Dates: 1993 - Present



Technology Transfer: Publications in open literature, technical presentations

Key Documentation: 1) Marshall, W. F. Improved Control of NOx Emissions with Biodiesel Fuels, Effects of Fuel Additives and Blending Components. Status Report, NIPER/BDM-0044. Prepared for Department of Energy, March 1994  
 2) Marshall, W. F. Improved Control of NOx Emissions with Biodiesel Fuels, Heavy Alkylate Blends. Status Report, NIPER/BDM-0050. Prepared for Department of Energy, August 1994.

Key Personnel: William F. Marshall, (918) 337-4253, Fax (918) 337-4342

Lab Capabilities Applied: Emissions Testing



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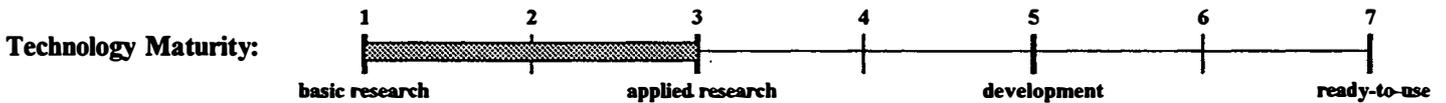
Category: Oil Processing & Refining

Laboratory: National Institute for Petroleum and Energy Research      Contact: D. L. Ripley, (918) 337-4264

Title: Processing and Utilization Research - Analysis of the Refining Industry

**Description:** This program investigates pre-treatment processes with potential applicability in a refinery to convert viscous, high sulfur, high metals heavy oils, such as west coast heavies, into a more transportable, lighter and cleaner material. Since conventional processes are not cost effective for these crudes, modified or novel processes are being investigated. Economics can be improved by optimal incorporation of needed environmental sub-systems and attempting to increase secondary values of the oil product. Since caustic treatment has been found useful in modification of coal, application to heavy oils is being studied, in addition to a series of strong acid treatments. Thermal treatments to reduce viscosity, and sometimes metals content, are in use but are threatened in the marketplace by indifferent demand for the byproduct carbon. The possibility of achieving benefit by short time high temperature thermal shock is investigated in this program. A bench scale carbon black reactor has been designed to be operated in a modified mode to produce lighter products from a heavy crude feed. This program is being coordinated with the refinery of the future project, as it evolves, for processes to be considered and applications of the results to the future refinery concept.

91-95 Funding (\$K): 547      Dates: 1994 - Present



Technology Transfer: Publications, Reports, Seminars

Key Documentation:

Key Personnel: K. Q. Stirling, (918) 337-4283

Lab Capabilities Applied: Petroleum Processing, Thermodynamics, Fuels Chemistry



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**Category:** Oil Processing & Refining

**Laboratory:** National Institute for Petroleum and Energy Research

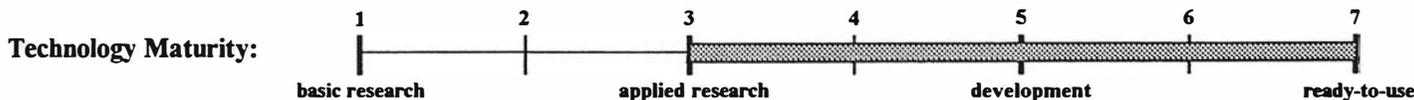
**Contact:** Dexter Sutterfield, (918) 337-4251

**Title:** Development of Analytical Methodology for Analysis of Heavy Crudes: Catalytic Cracking Behavior of Compound Classes in Petroleum Resid

**Description:** Fluid Catalytic Cracking (FCC) is the primary domestic refining process for conversion of heavy distillates (650\_1000øF), and in some cases, atmospheric resids (650øF +) to gasoline and other light products. Because of the substantial FCC capacity, incremental improvements in processing conventional feedstocks and/or extension of FCC to lower quality feedstocks significantly improve refining economics and the ability to process heavy crude. Liquid chromatographic methodology previously developed under the project is being used to fractionate > 650øF resids from conventional and heavy oils into compound class fractions. These fractions are then cracked using a laboratory scale FCC unit. The resulting product distribution is used to define the behavior of a given compound type under FCC conditions. Also, the detailed composition of gasolines produced are related back to the feedstock composition and properties. The results from this program may be used to identify compound types which are detrimental to FCC, to optimize feedstock properties/composition, and to model the FCC process. Particularly with respect to feedstocks derived from heavy oils, optimization of pretreatment processes and blending could significantly improve FCC performance.

**91-95 Funding (\$K):** 1500

**Dates:** 1991 - Present



**Technology Transfer:** Journal Articles, Technical Presentations

**Key Documentation:** 1) Green, J.B., E.J. Zagula, J.W. Reynolds, H.H. Wandke, L.L. Young, and H. Chew. 1994. "Relating Feedstock Composition to Product Slate and Composition in Catalytic Cracking: 1. Bench Scale Experiments with Liquid Chromatographic Fractions from Wilmington, CA, >650øF Resid." Energy and Fuels 8: 856\_67.2) Green, J.B., E.J. Zagula, J.W. Reynolds, L.L. Young, and H. Chew. 1994. "Relating Feedstock Composition to Product Slate and Composition in Catalytic Cracking." NIPER/BDM 0045, July.

**Key Personnel:** Gene Sturm, (918) 337-4314 John Green, (918) 337-4255

**Lab Capabilities Applied:** Petroleum Analysis and Characterization, Petroleum Processing and Engineering, Instrumentation



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Category: Environmental & Regulatory

Laboratory: National Institute for Petroleum and Energy Research

Contact: Raymond P. Anderson, Manager, Fuels & Engine Testing, (918) 337-4464

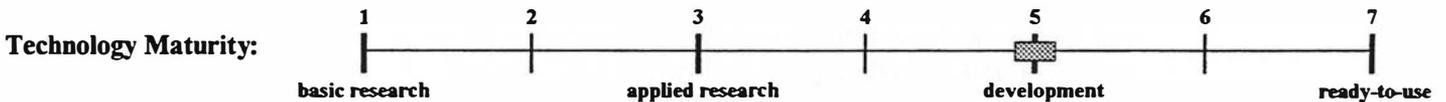
Title: Impacts of Alternative Fuels on Air Quality

Description: The use of alternative fuels has the potential for significant reduction of automotive emissions. Also, the photochemical reactivity of the exhaust from alternative fuel vehicles is typically much lower than that of conventional fuel vehicles. The combined lower emission rates and lower reactivity could have a major impact on ozone formation and air quality. These findings are based on results of tests using standard emissions test procedures and driving cycles. The emissions benefits of alternative fuels might be even greater over driving cycles that are representative of real world driving patterns not included in the standard driving cycle.

Air sampling programs indicate that the inventory of automotive emissions is underestimated by the use of emissions data from the standardized emissions tests. Much of the "excess" emissions could be due to in-use driving patterns being markedly different than the driving cycle used in the standard emissions tests.

Experiments were conducted to generate data relevant to both of these issues. Alternative fuels, Compressed Natural Gas (CNG), liquefied petroleum gas, 85% methanol, and 85% ethanol were compared with reformulated gasoline. A driving cycle patterned after the drivability test was by far the most severe test with respect to mass emissions rates and ozone forming potential. Emission rates of carbon monoxide and volatile organic compounds over this cycle were 4 to 25 times greater than those in the standard emissions test cycle for all fuels other than CNG. The effects of driving cycle on emissions with CNG were relatively minor because fuel enrichment was much less excessive with this fuel. Compared to reformulated gasoline, all of the alternative fuels showed some benefits with respect to emissions of organics, in mass emissions, and in photochemical reactivity

91-95 Funding (\$K): 278 Dates: 1993 - Present



Technology Transfer: Publications in open literature, technical presentations

Key Documentation: 1) Marshall, William F.. Off-Cycle Emissions from Alternate Fuel Vehicles. Presented at the DOE-Transportation Technologies Government Contractors Coordination Meeting (CCM) in Dearborn, MI, October 1994. Published in the CCM proceedings.

Key Personnel: William F. Marshall, (918) 337-4253, Fax (918) 337-4342

Lab Capabilities Applied: Emissions Testing, Analytical Chemistry Laboratories



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Category: Oil Processing & Refining

Laboratory: National Institute for Petroleum and Energy Research      Contact: D. L. Ripley, (918) 337-4264

Title: Processing and Utilization Research - Nuclear Power Training Unit Diesel Fuel Testing

Description: The Department of Navy's Nuclear Power Training Unit utilizes diesel marine fuel (F-76) as an alternate power source for their Moored Training Ships (MTS). Their procedures require periodic analysis OF fuel oil located in both the Port and Starboard fuel oil storage tanks. The analyses required are designated at the time of sampling and usually involve both standard specification testing and accelerated storage testing to estimate the approximate life of the fuel (i.e. before sediment levels in the fuel will reach a critical level). The Navy's Nuclear Power Training Unit has utilized NIPER's unique diesel fuel storage stability testing capability to evaluate diesel fuels stored for emergency use. This project is a continuation of that effort and provides an important link between refinery production processes and commercial utilization.

91-95 Funding (SK): 100      Dates: 1994-Present



Technology Transfer: Publications, Reports

Key Documentation:

Key Personnel: K. Q. Stirling, (918) 337-4283

Lab Capabilities Applied:



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Category: Environmental & Regulatory

Laboratory: National Institute for Petroleum and Energy Research

Contact: Stephen Jones, (918) 337-4528

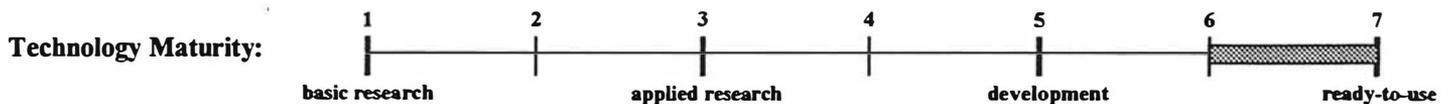
Title: Safety and Environmental Management Program

**Description:** The management of wastes from oil and gas exploration and production is of growing concern for the domestic oil industry. The regulatory requirements for treatment and disposal of those wastes continue to tighten. In addition, there is growing concern over past disposal practices and the resulting impacts to the environment of those practices. Most production and drilling wastes have been dealt with by either reinjection or placement into pits. In some cases, produced brines have been released to the surface as either a disposal method or unintentional release. New methods and technologies are required to remediate previous releases. Lower cost, more effective treatment technologies for sediments, soils, and sludges contaminated by wastes from petroleum exploration and production operations need to be developed and implemented to effectively treat existing contamination from historic operations and to treat/prevent contamination from current operations.

At present, coastal water and open bay oil and gas production operations discharge untreated produced water back to the surrounding waters. Cost effective treatment technologies will enable operators to reduce any toxicity indicated by biomonitoring.

Technologies currently exist and are in use for the treatment of wastewater to remove organic contaminants. The applicability of those technologies needs to be evaluated for highly saline produced water. The technologies to be evaluated will likely come from the following broad categories: thermal destruction, absorption, oxidation, and biological. Information will be developed on the technical performance of the technologies as well as the anticipated costs for implementation in a typical production setting. The technologies that are found to be suitable for treatment of produced water will be readily transferable to the industry. The technologies to be evaluated will be commercially available for other waste streams.

91-95 Funding (\$K): 240      Dates: 1994 - Present



**Technology Transfer:** The technology will be transferred to the industry through field demonstrations at production facilities of small operators. Reports and presentations will be key elements of transfer.

**Key Documentation:**

**Key Personnel:** Stephen Jones and Patrick Navratil (918) 337-4528

**Lab Capabilities Applied:** The technical and project management expertise at NIPER in the area of petroleum production make this project possible.



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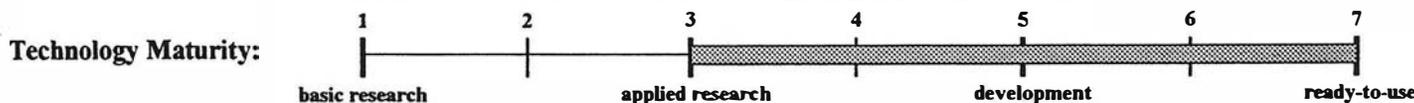
Category: Oil Processing & Refining

Laboratory: National Institute for Petroleum and Energy Research      Contact: Dexter Sutterfield, (918) 337-4251

Title: Processing and Utilization Research - Additives for Coke Reduction during Heavy Oil Processing

**Description:** Delayed and fluid coking are the primary refining processes for upgrading vacuum resids (> 1000øF) to distillate products, particularly resids from low quality crudes. Yields of liquid versus solid (coke) products depend primarily on the H/C atomic ratio of feedstocks. For feeds with low H/C ratios, coke yields can comprise up to 50 wt% of the feed. Coke formation is desirable from the standpoint of providing a sink for metals and other undesirable feedstock elements. However, the optimum situation would be to form a minimum of coke highly enriched in metals and other heteroatoms, thereby providing a maximum yield of liquid product with greatly reduced heteroatom content relative to the feed. Coking processes do not employ catalysts and thus depend solely on thermal cracking for distillate production. Thermal cracking occurs in a free radical chain reaction type of mechanism. In conventional coking units, operating temperatures in excess of 400øC (752øF) are used to provide an initial pool of free radicals and thus an acceptable rate of thermal cracking to form distillates and coke. This project investigates additives for promoting thermal cracking at reduced temperatures. If coking could be carried out at even moderately reduced temperatures, coke formation could be substantially reduced with commensurate increases in liquid yields. The additives under investigation are waste materials containing chemical bonds which may be thermally broken at lower temperatures than required for petroleum. In some cases, distillate production occurs from the additive as well as the petroleum-based feed component. A laboratory scale Delayed Coking Unit (DCU) is used to evaluate each additive's effectiveness.

91-95 Funding (\$K): 445      Dates: 1994 - Present



Technology Transfer: Journal Articles, Technical Presentations

Key Documentation: Green, J.B. 1994. Potential for Improving Thermal Upgrading Processes for Low Quality Petroleum Resids. NIPER/BDM\_0046, July.

Key Personnel: Gene Sturm, (918) 337-4314 John Green, (918) 337-4255

Lab Capabilities Applied: Petroleum Analysis and Characterization, Petroleum Processing and Engineering, Instrumentation



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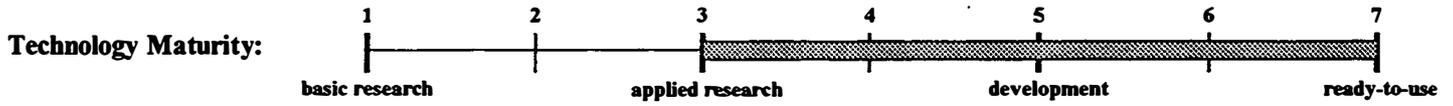
Category: Oil Processing & Refining

Laboratory: National Institute for Petroleum and Energy Research      Contact: Dexter Sutterfield, (918) 337-4251

Title: WFO - Petroleum Product Surveys

**Description:** For over 60 years, NIPER and its predecessors at the Bartlesville research facility have collected, compiled and published chemical and physical property data on petroleum products in use across the United States. The data are provided by the manufacturers (refineries or suppliers) and are presented in a manner which does not reveal the source of particular data. The product survey data are very valuable to the manufacturers and other entities which are interested in the properties of the various products and the trends over time which are presented in the publications. In the past, funding for the project has been provided by the government (Bureau of Mines and later the Department of Energy) and by the American Petroleum Institute. For the last few years the project has been funded by subscription charges. Technical advice and direction are provided by the Fuels Survey Task Force of the Fuels Committee of the American Petroleum Institute to ensure that the product surveys remain responsive to the needs of the petroleum industry and other subscribers across the U.S. and the world. In this project, NIPER will solicit, collect, compile and publish surveys and trends of chemical and physical property data of petroleum fuel products manufactured and sold across the United States with the advice and direction of the Fuels Surveys Task Force of the Fuels Committee of the American Petroleum Institute. Currently, five surveys are published annually covering the following fuel products: 1) Motor Gasolines, Winter; 2) Motor Gasolines, Summer; 3) Diesel Fuel Oils; 4) Aviation Turbine Fuels; and 5) heating oils.

91-95 Funding (\$K): 225      Dates: 1991 - Present



Technology Transfer: Technical Publications

Key Documentation: 1) Dickson, C.L. and G.P. Sturm, Jr. 1994. Diesel Fuel Oils, 1994. NIPER\_187 PPS, December. 2) Dickson, C.L. and G.P. Sturm, Jr. 1995. Motor Gasolines, Summer 1994. NIPER\_188 PPS, February.

Key Personnel: Gene Sturm, (918) 337-4314 Cheryl Dickson, (918) 337-4388

Lab Capabilities Applied: Data Compilation and Analysis



**Index:** 259

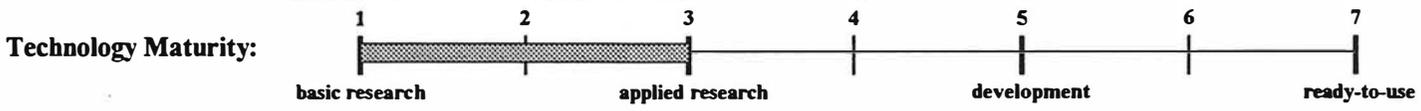
**Category:** Oil Processing & Refining

**Laboratory:** National Institute for Petroleum and Energy Research      **Contact:** D. L. Ripley, (918) 337-4264

**Title:** Processing and Utilization Research - Upgrading and Environmental Concept

**Description:** This research has the goal of integrating optimal environmental process design with existing regulations to relieve the operational and expense burdens of refineries, particularly independent regional facilities. Refinery feedstock availability, product quality constraints, and investment in place must be considered in relation to the operating environment in assessing needs for new technology. A cooperative project will be carried out with one or more small refineries to uncover such needs. Contacts have been made with Lion Oil in El Dorado, Arkansas, and an independent refinery in Kansas. From these first contacts, it is anticipated that a variety of effluent, treatment, and processing problems will be uncovered, many of them unique to this size processing unit. A long term relationship with one or more small refiners, and consequent research studies are expected to be derived from this project.

**91-95 Funding (SK):** 643      **Dates:** 1994 - Present



**Technology Transfer:** Publications, Reports, Seminars

**Key Documentation:**

**Key Personnel:** J. W. Goetzinger, (918) 337-4309

**Lab Capabilities Applied:**



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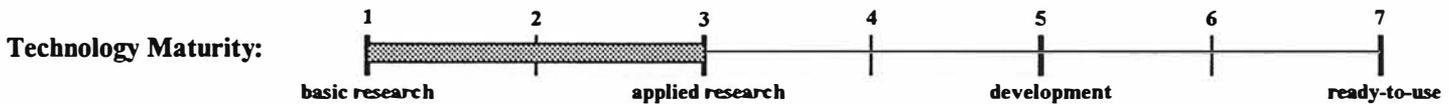
**Category:** Oil Processing & Refining

**Laboratory:** National Institute for Petroleum and Energy Research      **Contact:** D. L. Ripley, (918) 337-4264

**Title:** Processing and Utilization Research - OER and Thermodynamic Properties for Polycyclic Systems by Non-Calorimetric Methods

**Description:** The Thermodynamics Research Group at NIPER has five decades of experience in the determination of the thermodynamic properties of organic compounds. An unique collection of experimental apparatus has been developed for these determinations, and a strong body of expertise has grown for making and interpreting the measurements. The capabilities of the thermodynamics research group were recognized in 1975 by the Basic Energy Sciences Division of the Office of Energy Research, Department of Energy and a continuing research program has developed. This project determine the thermodynamic properties for polycyclic molecules containing five-membered ring (s) via assigned spectra and statistical mechanics. A key goal is attainment of accord between spectroscopic and calorimetrically-derived properties for temperatures ranging from ambient to those approaching the critical region. A consistent theoretical interpretation is sought for the vibrational modes for ring systems understanding of the foundation of estimation techniques such as group-additivity and molecular-mechanics. Parameters derived from this fundamental understanding can then be used to accurately estimate thermodynamic properties for other molecular systems of similar structure (including larger, i.e., four-ring or greater). That would, in turn, facilitate the development of more realistic models of refinery processes such as hydroprocessing of heavy petroleum crudes. At present, when heavy petroleum is refined, a sizable percentage of the barrel ends up as coke due to the lack of a cost-effective method of heteroatom removal.

**91-95 Funding (\$K):** 3000      **Dates:** 1975 - Present



**Technology Transfer:** Publications, Reports, Seminars

**Key Documentation:**

**Key Personnel:** W. V. Steele, (918) 337-4210

**Lab Capabilities Applied:**



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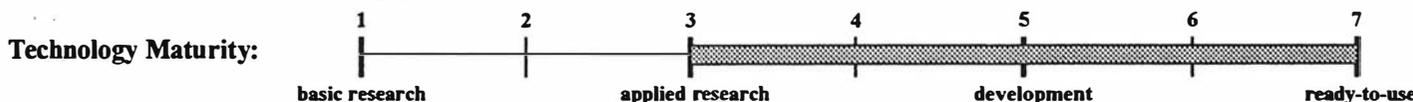
Category: Production

Laboratory: National Institute for Petroleum and Energy Research      Contact: Arden Strycker, (918) 337-4206

Title: Gas Flooding Methods for Advanced Oil Recovery

**Description:** The scope of most activities on these project tasks is divided into two parts: a) improvement of sweep efficiency for injected gases, and b) improvement of predictive tools for multiphase flow. Improving sweep efficiency offers the largest potential for realizing the full benefit of oil recovery by gas injection. Gas flooding is currently successful where a substantial volume of gas is readily available, but recovers far less than optimum as determined in laboratory experiments due to poor sweep efficiencies in the field. Mitigating this problem remains the highest priority for this program. Current activities include developing polymer surfactant systems that generate stable foams in reservoir environments. Foams can retard fluid flow in high permeability zones (gas swept zones) and polymers increase fluid viscosity to reduce liquid drainage and increase foam stability. In addition, improvement of predictive tools reduces project risk by knowing more reliably expected results from multi-million dollar investments often associated with these field projects. Historically, predictive tools have been optimistic in predictions of production performance for gas flooding. A lack of understanding the recovery mechanisms and the use of approximations in predictive tools for practical reasons are considered major causes of poor prediction performance. Current activities include an investigation of the oil-water interfacial tension (IFT) with carbon dioxide and the relationship of IFT to relative permeability with multiphase flow. Many areas of investigation have been studied under this program with a number of improvements benefiting the industry.

91-95 Funding (\$K): 2060      Dates: 1985 - Present



**Technology Transfer:** Trade Journal Articles, Presentations at Professional Meetings (SPE, AIChE), DOE Reports, Private Conferences, Software Distribution, CRADA project, Individualized Training Program, Work For Others Projects, AWU Summer Student Program, INTERNET Ho

**Key Documentation:** Some 30 technical reports and papers resulted from this program.  
 1) Chung, T. H., R.A. Jones, H.T. Nguyen.: "Measurements and Correlations of the Physical Properties of CO<sub>2</sub>/Heavy-Crude-Oil Mixtures." SPE Res. Eng., v.3, No. 3, pp. 822-828, August.  
 2) Hudgins, D.A., F.M. Llave, F.T.H. Chung. "Nitrogen Miscible Displacement of Light Crude Oil: A Laboratory Study." SPE Res. Eng, V. 5, No. 1, pp. 100-106, February.

**Key Personnel:** Frank Chung, 918--337-4274  
 Clarence Raible, 918-337-4287  
 Sonny Llave, 918-337-4359  
 Bharat Jhaveri, 918-337-4257

**Lab Capabilities Applied:** Petroleum Engineering, Reservoir Engineering, Fluid Dynamics, Routine and Specialized Core Analysis, Mechanical Engineering, Corrosion Analysis, CT Imaging, Instrumentation, Simulation, Supercritical Fluid Analysis, Chromatographic Analysis, Chemistry



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Category: Production

Laboratory: National Institute for Petroleum and Energy Research      Contact: Arden Strycker, (918) 337-4206

Title: Thermal Methods for Advanced Oil Recovery

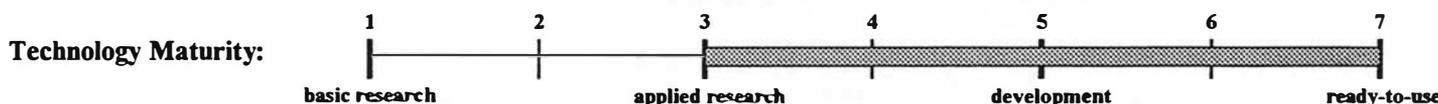
**Description:** The overall purpose is to develop economic and technical improvements in thermal oil production. More domestic oil has already been commercially produced by thermal recovery methods than by all other advanced recovery methods combined. One of the primary resource targets for thermal recovery is heavy crude oil (API gravity between 10\_ and 20\_). Heavy oil makes up between 10 and 20 percent of the total U.S. crude oil resource; estimates are 80 to 100 billion bbl. Advanced recovery methods are required to produce this oil, because the in situ viscosities are usually too high for primary recovery techniques. The goal of this program is to modify a proven economic process (thermal recovery) to effectively recover domestic oil resource targets not currently being produced.

The focus for all tasks have been to develop thermal methods for recovering otherwise unrecoverable domestic oil and to increase the effectiveness of existing operations. These include the following:

- Design effective steamflood foam processes to increase sweep efficiency
- Minimize steam gravity override effects
- Establish methods and maximize thermal recovery in oil-wet reservoirs
- Develop recovery methods for high paraffin oils in sucrosic reservoirs
- Develop thermal recovery methods for thin low-permeability heavy oil reservoirs

The national energy policy, whose purpose is to minimize the economic and political impact of importing crude oil, must further develop advanced recovery processes for the U.S. domestic heavy oil resource. This program builds on already successful technologies in thermal recovery.

91-95 Funding (\$K): 833      Dates: 1985 - Present



**Technology Transfer:** International Heavy Oil Conference, Symposia on Focused Subjects (Foam, In Situ Combustion), Trade Journal Articles, Presentations at Professional Meetings (SPE, ACS, OGS, NCPI, OAS, UNITAR), DOE Reports, Private Conferences, Software Distribution

**Key Documentation:** Over 90 technical reports and papers resulted from this program. 1) Strycker, A. R., M. P. Madden and P. S. Sarathi: "Effectiveness of Screening Tests as Predictive Models for Steamflood Additives", SPERE, pp. 543-548, November 1987. 2) Mahmood, S., D. K. Olsen and C. P. Thomas: "Heavy Oil Production from Alaska," Proc. of Sixth UNITAR International Conference on Heavy Crude and Tar Sands (Houston, Feb. 13-17, 1995).

**Key Personnel:** Arden Strycker, 918-337-4206 David Olsen, 918-337-4479 Partha Sarathi, 918-337-4304 Amit Sarkar, 918-337-4490 Syed Mahmood, 918-337-4429

**Lab Capabilities Applied:** Petroleum Engineering, Reservoir Engineering, Fluid Dynamics, Modeling, Mechanical Engineering, Instrumentation, Simulation, Chromatographic Analysis, Chemistry, Chemical Engineering, Database Development, Instrumentation Networking, Routine and



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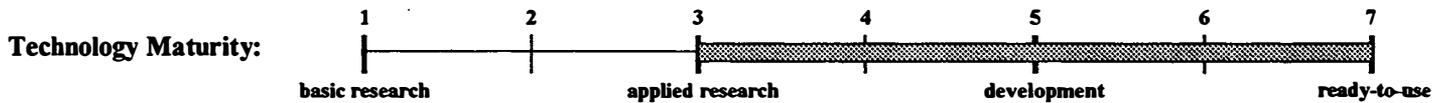
Category: Development

Laboratory: National Institute for Petroleum and Energy Research      Contact: Daniel Maloney, (918) 337-4364

Title: Relative Permeability - Development of Relative Permeability measurement Methodology and Correlations of Pore Characteristics with Multiphase Relative Permeability and Capillary Pressure Functions

Description: Relative permeability data is critical for designing petroleum recovery processes and for reservoir management. Objectives of this project include advancing the state-of-the-art in characterizing multiphase flow through rock under reservoir conditions. The current direction of relative permeability research at NIPER is to develop methods for estimating relative permeability and capillary pressure functions from measurements on drill cuttings or rock fragments. Tasks include performing tests on water-wet and intermediate wet rocks to examine relationships among rock pore size distribution, coordination number, pore structure and oil/brine steady-state relative permeability. The ultimate goal is to develop a relative permeability model relating fluid flow to pore structure, pore size distribution, and other parameters that can be determined from drill cuttings or core fragments. Successful development of this technology will provide a means for modeling fluid flow and predicting recovery efficiency in petroleum reservoirs where only rock fragments are available for analyses. This technology will be directly transferred to the domestic petroleum industry.

91-95 Funding (\$K): 1507      Dates: 1991 - Present



Technology Transfer: Society of Petroleum Engineers meetings, technical presentations at Society of Core Analysts meetings, work-for-others projects, laboratory tours, communications with research staff at other facilities.

Key Documentation: 1) Gilland, R. and D. Maloney: "Apparatus and Method for Measuring Relative Permeability and Capillary Pressure of Porous Rock," U.S. patent no. 5,297,420 (Mar. 29, 1994).  
2) Maloney, D., K. Doggett, and R. Gilliland: "New Procedure and Apparatus for Combined Reservoir Condition Gas-Brine Relative permeability, Capillary Pressure, and Electrical property Measurements," presented at the 1994 International Symposium of the Society of Core Analysts, Stavanger, Norway (Sept. 12-14, 1994).

Key Personnel: Min Tham, (918) 337-4387 Daniel Maloney, (918) 337-436 Kevin Doggett, (918) 337-4298

Lab Capabilities Applied: Flow through porous media laboratory including about \$300,000 in equipment for routine and special core analyses (2-D linear X-ray scanner for saturation measurements, pumps, transducers, computers, specialized coreholders, explosion-proof ovens,



**Index:** 264

**Category:** Oil Processing & Refining

**Laboratory:** National Institute for Petroleum and Energy Research

**Contact:** D. L. Ripley, (918) 337-4264

**Title:** Processing and Utilization Research - Naval Air Warfare Center - Jet Fuel Support

**Description:** The Naval Air Warfare Center (NAWC) responds to problems or concerns of all types at Naval Air Stations located all over the world. This is especially true of problems related to fuels, fuel related components, or fuel testing. NAWC utilizes the unique capabilities at NIPER to help solve problems, to better understand the fundamental properties of fuels, and to help develop new procedures and equipment for fuel testing. This project is a continuation of this cooperative effort. The incidence of fuels becoming unacceptable between production and use is rapidly increasing. The first sectors to see the effects of a combination of deterioration in quality of refinery feedstocks and increased processing severity have been the public utility companies and the military. The former have experienced problems early because they procure the heaviest fuels, which are often used as repositories for resids and by-products from high severity treatment. The military experience problems because of their strict specifications and the need for long-term storage capability.

**91-95 Funding (\$K):** 250

**Dates:** 1988 - Present

**Technology Maturity:**

1	2	3	4	5	6	7
basic research	applied research		development		ready-to-use	

**Technology Transfer:** Publications, Reports, Symposia

**Key Documentation:**

**Key Personnel:** K. Q. Stirling, (918) 337-4283

**Lab Capabilities Applied:**



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Category: Oil Processing & Refining

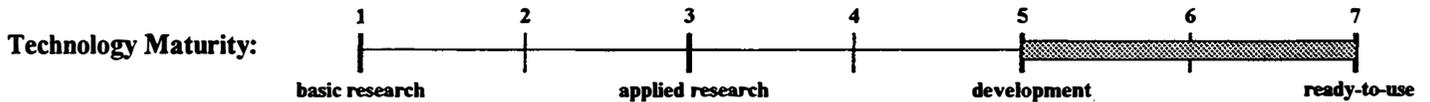
Laboratory: National Institute for Petroleum and Energy Research

Contact: D. L. Ripley, (918) 337-4264

Title: Processing and Utilization Research - Navy Petroleum Office - Fuel Reclaiming

**Description:** In the mid 1980s, NIPER conducted an analysis for the Navy to determine whether it was technically and economically feasible to process reclaimed product into Navy distillate. The analysis concluded that it was technically feasible to produce Navy distillate in this way, but the results of the economical analysis were inconclusive. This project involves an analysis to determine whether it is economically feasible to recover Navy distillate from reclaimed product. The analysis will be conducted using the latest Navy economic analysis standards and premises established jointly by NIPER and the Navy. Sensitivity analyses will be performed to evaluate the economic impact of changes in critical premises. Cost factors will be based on typical commercial refinery capital costs and escalation factors.

91-95 Funding (\$K): 100      Dates: 1994-1995



Technology Transfer: Publications, Reports

Key Documentation: Goetzinger, J. W.; D. L. Ripley. 1994. Recovery of Navy Distillate Fuel From Reclaimed Product, Updated Economic Analysis - 1994. NIPER/BDM-0096, December.

Key Personnel: J. W. Goetzinger, (918) 337-4309

Lab Capabilities Applied: Petroleum Processing, Fuels Chemistry



Index: 266

Category: Environmental & Regulatory

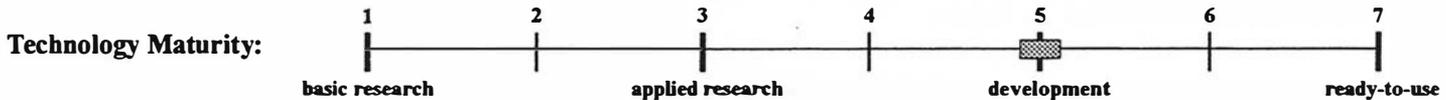
Laboratory: National Institute for Petroleum and Energy Research      Contact: Raymond P. Anderson, Manager, Fuels & Engine Testing, (918) 337-4464

Title: Monitoring Tulsa Public Schools Alternative Fuel Fleet

**Description:** There has been a recent emphasis on the use of alternative fuels for transportation applications. The Clean Air Act and other regulatory actions have caused fuel producers and automotive manufacturers to consider different fuels. The use of Compressed Natural Gas (CNG) is one alternative that holds promise of providing an ample supply while reducing combustion emissions. The use of CNG is finding growing acceptance in fleet applications where the fleet vehicles return to a central refueling facility where large commercially available compression equipment is maintained. The largest single fleet of dedicated CNG school buses (50) in the United States is operated by the Tulsa Schools transportation system, which also has a fleet of approximately 60 dual fuel (gasoline/CNG) buses.

Monitoring this fleet included emissions measurements, fuel economy measurement, and engine performance. Emissions measurements were made using a transient duty light/medium duty chassis dynamometer which was transported to the Tulsa maintenance facility. A number of dedicated CNG engine problems were experienced. The engine problems generally included burned exhaust valves which is most likely due to oil combustion. The oil could originate either from the fuel (compressor oil from the natural gas compression system) or from engine lubricating oil. Analysis of cylinder deposits indicated that their primary source was engine lubricating oil.

91-95 Funding (\$K): 315      Dates: 1991 - 1994



Technology Transfer: Publications in open literature

**Key Documentation:** 1)Anderson, Raymond P., W. F. Marshall, M. J. Robertson. Monitoring Dedicated CNG Vehicles (Tulsa School Bus Fleet), Technical Progress Report No. 3. NIPER-BO6853. Prepared for DOE-Office of Alternative Fuels, April 22, 1993.  
2)Anderson, Raymond P., W. F. Marshall, and M. J. Robertson. Monitoring Dedicated Natural Gas Vehicles (Tulsa School Bus Fleet). Technical Progress Report No. 2, February 15, 1992 - July 31, 1992. Prepared for DOE-Office of Alternative Fuels and State of Oklahoma, Office of the Secretary of Energy. August 31, 1992.

**Key Personnel:** Raymond P. Anderson, (918) 337-4464, Fax (918) 337-4342  
William F. Marshall, (918) 337-4253, Fax (918) 337-4342  
M. Daniel Gurney, (918) 337-4379, Fax (918) 337-4342

Lab Capabilities Applied: Emissions Testing



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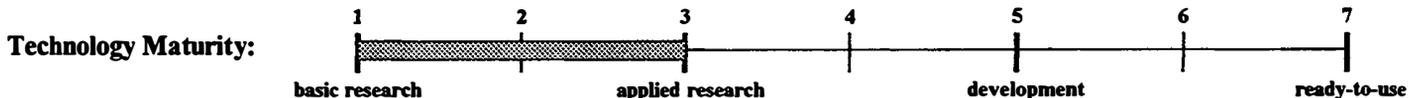
Category: Oil Processing & Refining

Laboratory: National Institute for Petroleum and Energy Research      Contact: D. L. Ripley, (918) 337-4264

Title: Processing and Utilization Research - Process Engineering Property Measurements on Heavy Oils

Description: This series of studies provides thermal, chemical and physical property data on pure components and fractions of heavy oil. Because of industrial interest in lower quality feedstocks, priority is given to compounds of oxygen, sulfur, nitrogen and metals that increase operating problems and expense for refiners. The project utilizes many unique property measurement instruments designed and constructed at the NIPER facility. Established group-additivity correlation methods will be used to incorporate data obtained from "key" functional groups in pure compounds into an engineering design property system for a broad range of compounds and mixtures, essential for the investigation of novel methods of processing atypical feedstocks of the future. The database is expected to allow estimates of thermodynamic feasibility to support speculative engineering design proposals including refinery re-configuration or the addition of units for processing difficult feedstock fractions.

91-95 Funding (\$K): 10000      Dates: 1944 - Present



Technology Transfer: Publications, Reports, Seminars

Key Documentation: 1. 50 Years of Thermodynamics Research at Bartlesville. The Hugh M. Huffman Legacy. The 42nd Huffman Memorial Lecture. by W. V. Steele. Accepted for publication in J. Chemical Thermodynamics, August, 1994.

Key Personnel: W. V. Steele, (918) 337-4210

Lab Capabilities Applied:



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**Category:** Environmental & Regulatory

**Laboratory:** National Institute for Petroleum and Energy Research      **Contact:** Raymond P. Anderson, Manager, Fuels & Engine Testing, (918) 337-4464

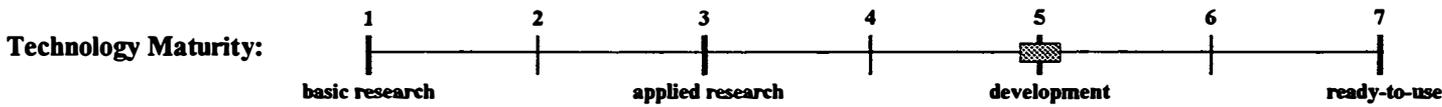
**Title:** Monitoring of Tinker Air Force Base Alternative Fuel Fleet

**Description:** In response to the Clean Air Act Amendments of 1990 and the 1992 Energy Policy Act, Tinker Air Force Base (TAFB) is utilizing NIPER capabilities in a major commitment to an alternative fuels program for its fleet vehicles. In the first stage of the TAFB program, 186 vehicles were converted to a dual fuel gasoline/Compressed Natural Gas (CNG) configuration. Converted vehicles were tested with both CNG and gasoline. The test results of the converted vehicles when fueled with CNG generally show benefit with respect to emissions of Non Methane Hydrocarbons (NMHC) and Carbon Monoxide (CO) but marked increases in Nitrogen Oxides (NOx) emissions.

Improved emission results were obtained for additional conversion using several different state-of-the-art conversion technologies. Following these conversion, TAFB had approximately 60 additional vehicles converted to dual fuel operation using improved conversion technology. Emissions of these conversions are currently being monitored.

NIPER has constructed a mobile dynamometer capable of performing emissions tests on light/medium duty vehicles operated over a transient duty cycle (either the FTP or IM240). The mobile dynamometer will be transported to TAFB to allow emissions testing of a larger number of vehicles and may allow simple on-site modifications to the conversion systems resulting in improved emissions performance. Monitoring is being extended to a new alternative-fuel fleet at Vance Air Force Base.

**91-95 Funding (\$K):** 900      **Dates:** 1991 - Present



**Technology Transfer:** Publications in open literature, technical presentations

**Key Documentation:**

- 1) Anderson, Raymond P., W. F. Marshall, and M. J. Robertson. Tinker Air Force Base, Alternative Fuel Program. PER/BDM-0018, Proceedings of the Annual Automotive Technology Development Contractors' Coordination Meeting. (CCM Paper) Prepared for the U.S. Air Force, Tinker Air Force Base, and the Department of Energy. April 1994.
- 2) Anderson, Raymond P., W.F. Marshall, and M. J. Robertson. Monitoring the Tinker Air Force Base Alternative Fuel Fleet, Technical Progress Report No. 4. Prepared for DOE-Office of Alternative Fuels. June 15, 1993.

**Key Personnel:** Raymond P. Anderson, (918) 337-4464, Fax (918) 337-4342  
 William F. Marshall, (918) 337-4253, Fax (918) 337-4342  
 Brent S. Morrison, (918) 337-4350, Fax (918) 337-4342

**Lab Capabilities Applied:** Emissions Testing



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Category: Environmental & Regulatory

Laboratory: National Institute for Petroleum and Energy Research

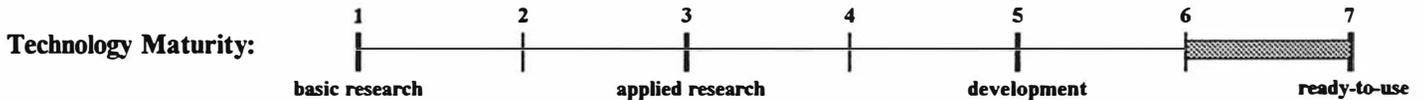
Contact: Stephen Jones, (918) 337-4528

Title: Safety and Environmental Management Demonstration Program

**Description:** This project is a joint DOE/MMS/industry demonstration of the feasibility of a Safety and Environmental Management Program (SEMP) for small operators on the Outer Continental Shelf. This project is designed to provide technical advice and assistance to DOE and MMS in assessing and implementing environmental and safety requirements for small and midsize operators. SEMP is a voluntary standard developed by the API and Offshore Operators Committee to promote safety and environmental protection for oil and gas and sulfur operations on the Outer Continental Shelf. The basis for SEMP is found in API RP 75, "Recommended Practices for Development of a Safety and Environmental Management Program for Outer Continental Shelf (OCS) Operations and facilities", published in May, 1993.

Information will be collected on the costs and effort required of a small to medium owner and operator on Outer Continental Shelf oil and gas facilities on federal leases to implement SEMP. The operator will own and operate one or more production platforms on federal leases and have no affiliation with a major oil or gas producer. Measures of effectiveness will be developed and to determine tangible or intangible improvement or regression related to resource recovery, profitability, facility and personnel safety, environmental protection as a result of implementing API RP 75.

91-95 Funding (\$K): 660      Dates: 1994 - Present



**Technology Transfer:** This is a demonstration project for an existing operator. This technology is being transferred and implemented now. The project will result in a joint NIPER/DOE-MSO/MMS conference on the implementation of SEMP.

**Key Documentation:**

**Key Personnel:** Stephen Jones and Patrick Navratil  
(918) 337-4528

**Lab Capabilities Applied:** The technical and project management expertise at NIPER make this project possible.



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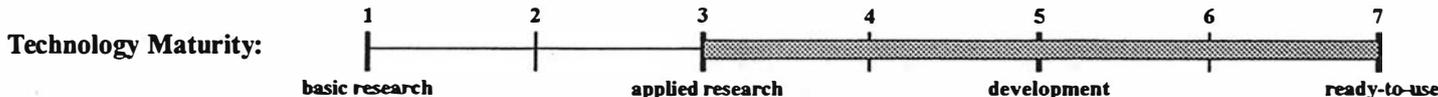
Category: Oil Processing & Refining

Laboratory: National Institute for Petroleum and Energy Research      Contact: Dexter Sutterfield, (918) 337-4251

Title: Strategic Petroleum Reserve Supporting Research

**Description:** The Strategic Petroleum Reserve (SPR) was established in December 1975 by the Energy Policy and Conservation Act (Public Law 94-163). This law and subsequent amendments declared it to be the policy of the United States to purchase and store up to 750 million barrels of crude oil to reduce the impact of disruptions in supply. Crude oil purchase specifications as well as an analytical research and quality control program were established by SPR Headquarters (HQ) to ensure the marketability of petroleum stored in the reserve. NIPER/BDM-Oklahoma and its predecessors have served as the analytical and technical support laboratory for the SPR HQ of the United States Department of Energy since 1978. The work covered is a continuation of these support activities to assist the SPR in fulfilling its mandated task of providing and maintaining a viable stockpile of crude oil. In this project, chemical and physical property data will be determined for crude oil streams and for SPR crude oil cargoes and for crude oil, sludge, and brine samples from selected caverns using a wide variety of standard methods, including ASTM. Stable isotope ratios and biological properties will be determined for selected samples. SPR crude oils will also be screened for possible contaminants. PVT measurements will be performed on selected SPR crude oil samples and detailed composition of the gas phase samples will be determined. Other technical support will be provided as requested. The level of effort in each of the above areas will depend on priorities established by SPR HQ.

91-95 Funding (\$K): 3750      Dates: 1991 - Present



Technology Transfer: Journal Articles, Technical Presentations

**Key Documentation:**  
 1) Green, J.B., T.B. McWilliams, S.K.-T. Yu, and R.P. Vrana. "GC/MS Determination of Polyglycols in SPR Crudes/Sludges." NIPER/BDM\_0024, March 1994.  
 2) Green, J.B., S.K.-T. Yu, J.A. Green, J.W. Reynolds, D.A. Doughty and J.Y. Shay. "Sludge Formation in SPR Caverns Final Technical Report Section 3 Origin, Composition and Physical Properties of Sludge-Entrained Brines." NIPER/BDM 0032, July 1994.

**Key Personnel:** Gene Sturm, (918) 337-4314 Johanna Shay, (918) 337-4437

**Lab Capabilities Applied:** Petroleum Analysis and Characterization, Petroleum Engineering, Instrumentation



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Category: Development

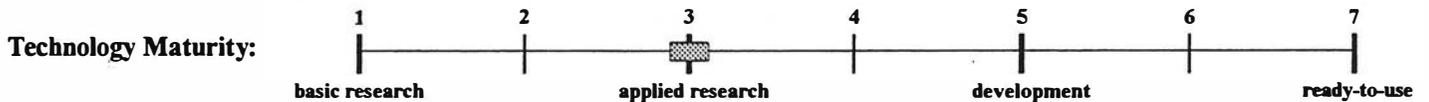
Laboratory: National Institute for Petroleum and Energy Research      Contact: Liviu Tomatsu, (918) 337-4364

Title: Imaging Techniques Applied to the Study of Fluids in Porous Media

**Description:** Imaging techniques using X-ray Computed Tomography (CT), Nuclear Magnetic Resonance (NMR) microscopy, minipermeametry, and Petrographic Image Analysis (PIA) are being developed to study oil recovery mechanisms and the effect of small scale rock heterogeneity on oil entrapment. The current work is applying imaging technology to calculate effective permeability and relative permeability in large samples containing ripple laminations. Simulation-based procedures are being used to investigate improved scale-up of permeability and relative permeability from small core plugs to the large block containing ripple laminations.

Low magnetic field NMR logging is more sensitive for calculating reservoir engineering parameters such as porosity, pore size distribution, permeability, residual water and oil saturation. Currently, high resolution MRI microscopy is being developed for multi-nuclear imaging and will be applied to imaging chemical Improved Oil Recovery (IOR) systems in fractured cores to study effects of fracture systems on chemical trapping.

91-95 Funding (\$K): 2163      Dates: 1991 - Present



Technology Transfer: Society of Petroleum Engineers meetings, Society of Core Analysts meetings, work-for-others projects, new technology for Independent Producers Workshop.

Key Documentation: 1) D.A. Doughty and L. Tomutsa: "NMR Microscopy for Fluid Imaging at Pore Scale in Reservoir Rock," presented at the 6th Annual Technical SCA & SPWLA Symposium, Oklahoma City, OK, June 1992.  
 2) French, T., R. Schatzinger and L. Tomutsa: "CT Imaging of Sandstone Core to Help Define Reservoir Properties: an Example From Tucker Sandstone, Southeast Kansas," published in the Proceedings of the Joint TGS/GST/SPE/SPWLA Multidisciplinary Approaches to Reservoir Characterization, May 10-11, 1994.

Key Personnel: Liviu Tomutsa, (918) 337-4472 Daryl Doughty, (918) 337-4296

Lab Capabilities Applied: X-ray Compute Tomography, Low Magnetic Field (NMR), NMR Microscopy, Minipermeametry, Petrographic Image Analysis and Reservoir Simulation.



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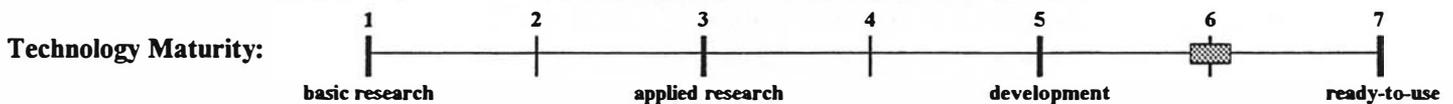
**Category:** Environmental & Regulatory

**Laboratory:** National Institute for Petroleum and Energy Research      **Contact:** Stephen Jones, (918) 337-4528

**Title:** Regulatory Streamlining

**Description:** Oil and gas producers face regulatory oversight of their operations by an increasing number of agencies( both Federal and State ) and under an increasing number of laws. The growing complexity of the regulatory process increases the cost of oil production, without necessarily improving environmental protection. A unified, streamlined approach to compliance would benefit the industry and results in more cost effective environmental compliance. This type of approach also has the potential for more effective, rational regulations. The feasibility of streamlining regulations that apply to natural gas and oil exploration and production should be investigated and improved regulatory approaches and systems developed. The priority states for this task will include Wyoming, Colorado, California, and New Mexico. Activities that result in actual streamlined regulatory processes are the key element of this task, not the production of studies. A collaborative effort should be conducted to streamline the regulatory process while working with State governments at the highest level and with regular communication at the Federal level on oil and gas regulatory processes. A working group which represents all appropriate agencies and offices ( State, Federal, Tribal ) which regulate gas and oil production on Federal lands in the priority states will be organized. The working group will include representatives from the petroleum exploration and production industry ( both majors and independents ). An appropriate environmental organization of national stature will be included as a participant in the working group.

**91-95 Funding (\$K):** 1000      **Dates:** 1994 - Present



**Technology Transfer:** Applicable within the near term The results will be transferred through reports, working groups, and the development of improved procedures.

**Key Documentation:**

**Key Personnel:** Stephen Jones and Deborah Pratt  
(918) 337-4528

**Lab Capabilities Applied:** The technical and project management expertise at NIPER in the area of petroleum production make this project possible.



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Category: Oil Processing & Refining

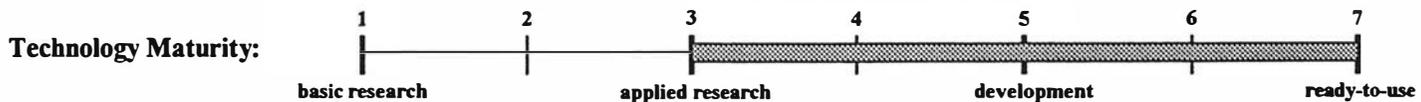
Laboratory: National Institute for Petroleum and Energy Research

Contact: Dexter Sutterfield, (918) 337-4251

Title: Crude Oil Analysis Database

**Description:** Crude oil analyses by a routine method have been conducted at NIPER since the 1920s when the facility was part of the United States Department of the Interior, Bureau of Mines. By 1965, more than 7,000 crude oils had been analyzed which created one of the largest collections of such information in the world. The data were digitized by the late seventies and a custom software application (COASYS) was implemented in 1980. The Crude Oil Analysis Data Base (COADB) has been used extensively within the government, academia, and industry. This important source of information on 9,100 crude oils is publicly available through a telephone modem on NIPER's Microvax\_ computer. In the current project, a new system for storing and retrieving data has been beta tested. The new system has the same data elements and reports as the previous system with the addition of new data fields for trace metals and hydrocarbon types. The new system has on-line help to make it more user friendly than the previous version but it has maintained the same general keyword approach for searching the data bank. A commercial relational data base management system has been used as the engine for storage and retrievals. The beta version will replace the current on-line version when it has been approved by DOE for operation\_timing depends on the dissemination of a new user's guide and other preparatory announcements. There have been many new oil field discoveries around the world in the past ten or so years for which data are not available in the database. In response to numerous requests by users of the COADB for information not presently available from the database, a program to solicit new crude oil samples and to update the analyses including measurement of metals by Inductively Coupled Plasma-Atomic Emission Spectrometry (ICP-AES), as well as determination of Benzene, Ethylbenzene, Toluene, Xylenes (BETX), and hydrocarbon types by a Gas Chromatographic (GC) method has been initiated in this project.

91-95 Funding (\$K): 225 Dates: 1993 - Present



Technology Transfer: Journal Articles, Technical Presentations, Computer Accessed Database

Key Documentation:

Key Personnel: Gene Sturm, (918) 337-4314  
Johanna Shay, (918) 337-4437

Lab Capabilities Applied: Petroleum Analysis and Characterization, Instrumentation



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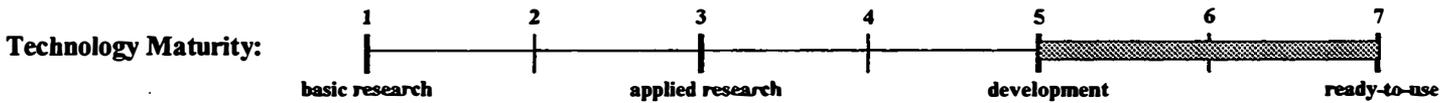
Category: Oil Processing & Refining

Laboratory: National Institute for Petroleum and Energy Research      Contact: D. L. Ripley, (918) 337-4264

Title: Processing and Utilization Research - Defense Fuel Supply Center Problem Fuel Chemistry

Description: The Defense Fuel Supply Center, in the course of supplying military fuels, experiences fuel quality problems whose causes cannot be identified through routine specification testing. It is suspected that these problems likely related to changes in the petroleum and refining industry. New crude sources, heavier crude and feedstocks, increased severity of refining conditions and wide-spread use of hydro and catalytic cracking systems are among those reasons thought to be underlying these quality problems. Specific examples of problems currently facing us include filtration time, long-term storage stability and thermal stability. Until such time as research efforts yield specification requirements that reflect these changes, the need exists for laboratory testing services which provide the capability to perform detailed investigations and analyses of the chemical properties of specific fuel samples using state-of-the-art methods of analysis. The goal of this testing program is to identify the causes of problems as indicated to determine methods of correction, the product's suitability for use, and/or possible disposition.

91-95 Funding (\$K): 750      Dates: 1988 - Present



Technology Transfer: Publications, Reports, Seminars

Key Documentation: Interagency Agreement, DFSC

Key Personnel: J. W. Goetzinger, (918) 337-4309

Lab Capabilities Applied: Petroleum Processing, Fuels Chemistry



**Index:** 275

**Category:** Exploration

**Laboratory:** National Institute for Petroleum and Energy Research      **Contact:** Herb Carroll, (918) 337-4558

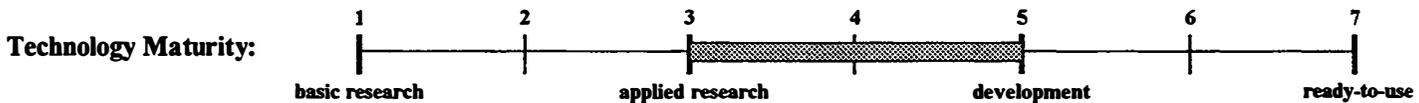
**Title:** Exploration Keys Used to Reduce Risk in Exploration Prospect Generation in Selected U.S. Basins

**Description:** The exploration program was initiated at NIPER in FY 94 and advanced in FY 95 under a Management and Operating (M&O) Contract with DOE, No. DE-AC22-94PC91008. The project addresses methodology of assessing a hydrocarbon potential in selected geologic provinces of the continental United States. The objective is to facilitate the development and deployment of improved and advanced technology to expand the efficient finding and assessing of undiscovered, producible oil resources in underexplored areas. Computer-assisted modeling of basin evolution and resulting present-day rock and fluid system is employed for identification of the areas where risk of successful exploratory drilling will be low. The modeling is supported by geological, geochemical, geophysical, and hydrologic databases as well as the air-image analysis of structural features.

The exploration effort in FY 94-95 meets the DOE's goals with respect to the Native Tribes Initiative by focusing on the Osage, Hopi, and Navajo Nation lands in Oklahoma and Arizona. A Memorandum Of Understanding (MOU) with the Osage Tribe on Joint Energy R&D was signed by the DOE and BDM representatives in Pawhuska, OK at the beginning of FY 95. Work is ongoing on preparation of similar MOU's with the Hopi and the Navajo Nations in northeastern Arizona.

Exploration for new hydrocarbon reserves has also been initiated within the Central Mid-Continent Rift System and associated structural units. If results of the current exploration analyses are encouraging, the scope of work will be expanded to minimize drilling risk for new hydrocarbon reserves in the best documented prospective areas.

**91-95 Funding (\$K):** 1500      **Dates:** 1994 - Present



**Technology Transfer:** Exchange of technologies and exploration results with the Indian tribes on tribal lands and with independent producers on lands under state jurisdiction, staff exchange with interested parties, technology transfer seminars, DOE reports, profession

**Key Documentation:** 1. Status Report on Exploration Methodologies and Prioritization of Basins for Study, Aug. 1994.  
2. Status Report on Geological Analysis of the Priority Basins, Aug.

**Key Personnel:** Herb Carroll, 918-337-4558  
K.C. Chen, 918-337-4256 Genliang Guo, 918-337-4467  
T.K. Reeves, 918-337-4468  
Bijon Sharma, 918-337-4399  
Michael Szpakiewicz, 918-337-4456  
Len Volk, 918-337-4466  
Bill Johnson, 918-337-4282

**Lab Capabilities Applied:** Basin Analysis and Modeling, Field Geology, Core Analysis, Advanced Geological-Geophysical-Geochemical Prospecting for Hydrocarbons, Fluid Dynamics, Basinal Petroleum Hydrogeology, Air-Image Analysis, Petroleum Engineering.



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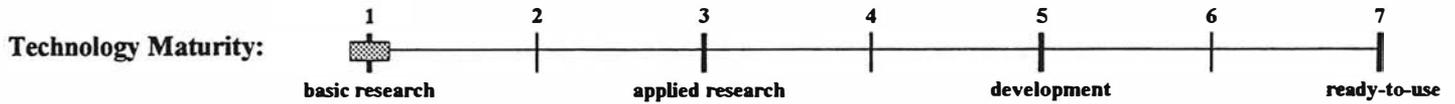
Category: Oil Processing & Refining (2, 16, 18, 4)

Laboratory: Oak Ridge National Laboratory      Contact: Elias Greenbaum

Title: Renewable Hydrogen Production for Fossil Fuel Processing

Description: Renewable hydrogen and oxygen production by microalgal water splitting. The key objective of this project is to develop a chemical engineering process system that can be used to product hydrogen from water. Hydrogen is a valuable chemical feedstock in the petrochemical industry.

91-95 Funding (\$K): 500      Dates: 1993-1995



Technology Transfer: DOE/EE Hydrogen Program

Key Documentation:

Key Personnel: E. Greenbaum, (615)574-6835, exg@ornl.gov

Lab Capabilities Applied: Design of original experimental instrumentation. Energy production, biosciences and biotechnology.



Index: 277

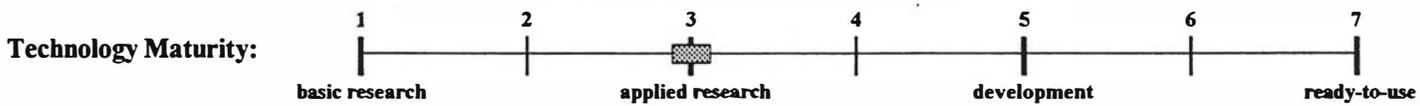
Category: Oil Processing & Refining (16, 18, 4)

Laboratory: Oak Ridge National Laboratory      Contact: E. Kaufman

Title: Separations Concepts

**Description:** Chemical and/or physical separations are usually a necessary part of any bioprocessing concept. This will certainly be true for processes in which biocatalysts interact with coal and oil. Of particular interest will be the separation of product components or fractions from an organic liquid mixture and the recovery and recycle of dissolved biocatalysts (e.g., chemically-modified enzymes or whole cells). Conventional separation of coal derived liquids is through distillation. This process is highly energy intensive and the temperatures required would not be compatible with biocatalyst viability. Enzymes or whole cells when used in aqueous systems may be separated by means of filtration. We will investigate the compatibility of various membrane systems with the range of solvents that would be present in our organic coal derived liquid product. An alternative approach will be to study adsorption systems in which solid particulates are used in appropriate contactors to first recover the used biocatalyst and then to fractionate the resulting product into classes of compounds. Inorganic adsorbents will be the first material tested for the fractionation of the organics. Weak ion exchange materials will be the adsorbents of choice for enzyme isolation. Such solid phase adsorption systems are already in commercial operation for the separation of mixed aromatics, branched cycloalkanes, olefins and paraffins. They may be utilized for thousands of adsorptive/regeneration cycles and may be reprocessed at the end of their useful lifetime. Additionally, solid sorbents pose an advantage over liquid extraction since there is no loss of reagent due to solubility in other liquid phases or through evaporation. Regeneration is also less energy intensive.

91-95 Funding (SK): 300      Dates: 1994-present



Technology Transfer: Publications

Key Documentation:

Key Personnel: Dr. Eric N. Kaufman, (615) 574-6624, ekn@ornl.gov  
 Dr. Costas Tsouris, (615) 241-3246, tsourisc@ornl.gov

Lab Capabilities Applied: Energy production, bioscience and biotechnology, environmental science



Index: 278

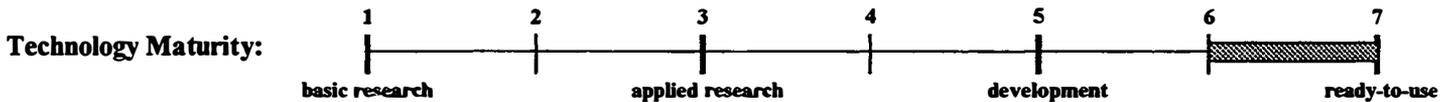
Category: Environmental & Regulatory (1, 2, 3, 4, 9)

Laboratory: Oak Ridge National Laboratory Contact: M. T. Naney

Title: In Situ Vitrification

**Description:** In situ technologies for vitrification of contaminated soils and hazardous waste have been patented and developed by (1) Pacific Northwest Laboratory (PNL) for the U. S. Department of Energy (technology is licensed to Geosafe, Inc. for commercial application), and (2) Plasma Technology Corporation (PTC) and the Georgia Institute of Technology (GIT). The technology developed by PNL has been tested at Oak Ridge National Laboratory (ORNL) for environmental remediation of contaminated soils and radioactive waste seepage pits and trenches. ORNL research has focused on vitrification of contaminated soils and waste slug containing 137Cs and 90Sr, physical and chemical characteristics of the melt, solidification products, and volatilized gases. The successful completion of these tests has resulted in the current treatability study (1993-present) that will demonstrate the technology at a inactive radioactive liquid waste seepage pit. Results of this research are reported in ORNL/TM-10992 and 12201, as well as journal articles. Collaboration between ORNL, PTC, and GIT is in progress to develop the PRISM concept (plasma remediation of in situ materials) for applications that are at present beyond capabilities of the in situ vitrification (ISV) technology developed by PNL. The PRISM concept has potential application to problems defined by the NPC. Specifically advanced recovery and refining processes in which thermal extraction or reservoir stimulation have potential benefit to enhance resource recovery.

91-95 Funding (SK): 2000 Dates: 1989-1993



Technology Transfer: Publications in open literature, staff exchange, licensed technology.

**Key Documentation:** Spalding, B. P., Jacobs, G. K., Dunbar, N. W., Naney, M. T., Tixier, J. S., Powell, T. D. (1992) Tracer-level radioactive pilot-scale test of in situ vitrification for the stabilization of contaminated soil sites at ORNL, ORNL/TM-12201, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 184 pp.  
 Spalding, B. P., and Jacobs, G. K. (1989) Evaluation of an in situ vitrification field demonstration of a simulated radioactive liquid waste disposal trench, ORNL/TM-10992, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

**Key Personnel:** M. T. Naney, 615-576-2049, lvp@ornl.gov  
 G. K. Jacobs, 615-576-0567, gkj@ornl.gov  
 B. P. Spalding, 615-576-7265, bps@ornl.gov

**Lab Capabilities Applied:** Environmental Scienc and Technology, Adv. Materials, Syn. Characterization and Processing, Advanced computing, modeling and simulation.



Index: 279

Category: Gas Processing (2, 3, 8), Oil Processing &amp; Refining (1, 4, 16)

Laboratory: Oak Ridge National Laboratory

Contact: Steve H. Overbury

Title: Heterogeneous Catalysts Related to Energy Systems

**Description:** The objective of this program is to understand fundamentals of catalytic reactions of organosulfur molecules occurring at metallic and bi-metallic surfaces and to understand how these molecules affect and are affected by the surface structure and composition. The approach is experimental but is complemented by theoretical modeling used as an interpretive tool. Three dedicated ultra-high vacuum systems are used to identify and monitor molecular and atomic adsorbates as a function of environmental variables such as coverage and temperature, to monitor reactions and determine their mechanisms and kinetics, and to analyze surface structure. An associated aspect is the development synchrotron based techniques for this purpose. Adsorbates chosen for study include thiols, substituted thiophenes, bi-functional molecules such as benzenethiol and mercapto-ethanol, related organic molecules and partially deuterated derivatives of these molecules. Substrates are metallic and bi-metallic single crystals, ultra-thin films grown on metal single crystals, and these surfaces following sulfidation or oxidation. Current research directions include studies of adsorbate geometry by photoelectron diffraction and x-ray standing waves, adsorption and reaction of methanethiol on ultra-thin Ni films on W, reactions of substituted thiophenic compounds on Ni surfaces, effects of O, H and S on reaction selectivity in thiophene hydro-desulfurization, and structure of clean and metal dosed bulk oxide surfaces.

91-95 Funding (\$K): 3520

Dates: 1981-present

1

2

3

4

5

6

7

Technology Maturity:

basic research

applied research

development

ready-to-use

Technology Transfer: Publications in open literature

**Key Documentation:** T.S. Rufael, D.R. Huntley, D.R. Mullins, and J.L. Gland, "Adsorption and Reaction of Benzenethiol on Ni(111)", J.Phys. Chem., 98 (1994), 13022. D.R. Huntley "Patterns of Reactivity for Ni(110) with Organosulfur Compounds", Preprints of the Division of Petroleum Chemistry< 38, (1993), 684.

**Key Personnel:** Steven H. Overbury, (615)574-5040, overburysh@ornl.gov, D.R. Huntley, (615)576-2638, huntleydr@ornl.gov, D.R. Mullins, (615)574-2796, mullins@ornl.gov

**Lab Capabilities Applied:** UHV techniques applied to surface science including Auger electron spectroscopy, high resolution electron energy loss spectroscopy, x-ray photoemission electron spectroscopy, low energy ion scattering, temperature programmed reaction/desorption spectro.



Index: 280

Category: Exploration (15), Arctic Region Activities (2, 3, 5, 7)

Laboratory: Oak Ridge National Laboratory Contact: P. Papadopoulos

Title: Joint High-Performance, High-Resolution Ocean Circulation Modeling for Enhancing Offshore Oil and Gas Exploration and Production

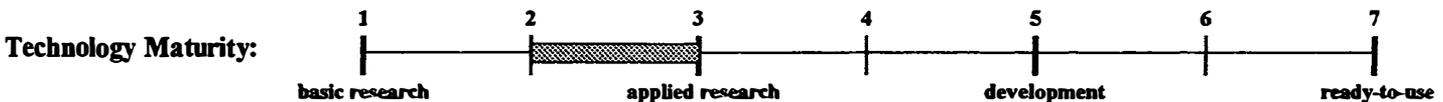
**Description:** Operators of deep water leases have long realized that simple extensions of technologies employed in shallow water exploration and production either simply do not work or are cost prohibitive in deep water. Among the critical concerns in deep water exploration and production are characterizations of ocean currents and eddies so that drilling equipment can be designed for and operated in the hostile deep water environment. The only practical solution for characterizing the ocean's physical behavior is to rapidly develop sophisticated regional ocean models.

The objective is to model ocean currents in selected geographic areas, with concentration on the Gulf of Mexico, using high-resolution, high-performance computational techniques. A suite of software tools will be produced to facilitate the characterization of ocean basin surface-to-sea-floor dynamics. The Modeling tools will help in the design of exploration and production facilities for deeper water.

This project has been developed in cooperation with oil and gas companies who are members of the Eddy Joint Industry Project (EJIP) and includes inter-laboratory cooperation with Sandia, Oak Ridge and Los Alamos National Laboratories. The involvement with EJIP assures that the technology developed will help meet the needs of deep water exploration companies. EJIP has provided extensive real-world measurement data to calibrate the models. Future funding would enable the development of new analysis tools and the transfer of technology to the oil and gas companies.

Several ocean models have been developed that can provide the desired data. These include the POP (parallel ocean program), a parallel version of MICOM (Miami Community Ocean Model) and a new overlapping grids model from Sandia. Future work would involve making these complex programs easy to use by our industry partners.

91-95 Funding (\$K): 350 Dates: 1993-1994



Technology Transfer: Publication, data exchange, industry/laboratory meetings

Key Documentation: LDRD-Program Development funds (Los Alamos), GO-NII project funding.

Key Personnel: James G. Sanderson, (505) 665-6605, jgsander@lanl.gov  
 Daniel W. Barnette, (505) 845-7874, dwbarne@sandia.gov  
 Philip M. Papadopoulos, (615) 241-3972, pqx@ornl.gov

Lab Capabilities Applied: Mathematical modeling, parallel computing, scientific computation, graphics.



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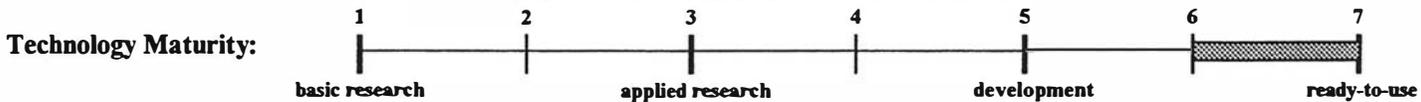
Category: Environmental & Regulatory (14)

Laboratory: Oak Ridge National Laboratory      Contact: R. Miller

Title: Programmatic Environmental Assessment for the Oil Research Program

**Description:** In 1991-1992, ORNL staff prepared a programmatic environmental assessment (PEA) for DOE, as part of addressing the National Environmental Policy Act (NEPA) for the Oil Research Program. The PEA evaluated programmatic environmental issues associated with alternatives related to achieving the program's goals and objectives. The PEA focused on assessing the overall environmental consequences of widespread commercialization by the petroleum industry of technologies emanating from successful demonstration of cost-shared projects resulting from DOE solicitations. In addition to the proposed action, the PEA evaluated the potential consequences of the no-action alternative. The analyses performed for the PEA found no major environmental impacts associated with commercialization of the technologies. The level of impacts resulting from widespread commercialization in the year 2010, in which U.S. oil production could increase by about 4% over present levels, would be very similar to the level of existing impacts. Overall, the expected increase is so small that the level of impacts would be indistinguishable from the existing level. Short-term impacts would not be expected to differ appreciably from the impacts evaluated for 2010. In comparison with the proposed action, impacts would generally be less at existing oil fields with abandoned wells under the no-action alternative, in which oil production would decrease by about 40% in the year 2010 compared with present levels. However, this decrease in impacts would be offset by an increase in impacts in other geographical areas resulting from additional ocean tanker traffic transporting imported oil.

91-95 Funding (\$K): 250      Dates: 1991-1992



Technology Transfer: DOE-ORNL-industrial partner interactions

Key Documentation: Programmatic Environmental Assessment

Key Personnel: R. L. Miller, 615-576-0751, met@ornl.gov

Lab Capabilities Applied: Technical expertise in geology, air quality, water quality, and ecology.



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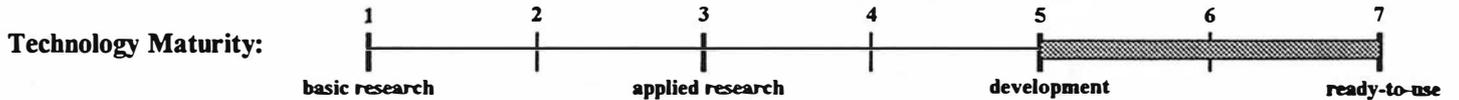
Category: Environmental & Regulatory (4, 10, 12, 14), Gas Processing (6)

Laboratory: Oak Ridge National Laboratory Contact: Steve Lindberg

Title: Mercury Air/Surface Exchange in the Environment

**Description:** The existence of extensive soil contamination by elemental mercury (Hg) around natural gas pipelines is widely known. Mercury is an important human toxin designated in the Clean Air Act Amendments for possible emission control. Methods are needed to assess the rate of Hg loss from such sites, and the primary pathway is expected to be through the air by volatilization, since soil Hg leaching is generally small. With support from the electric utility industry (Electric Power Research Institute) we have developed and tested several methods for directly measuring emission rates of mercury vapor from environmental surfaces. We use multiple independent methods for the purpose of reducing uncertainties in emission flux measurements. The most unique methods involve state-of-the-art micrometeorological approaches (e.g. the modified Bowen ratio gradient method) which have been modified for application to Hg for the first time. We have also made other advances in measuring the speciation of airborne Hg, which is needed to model its fate once emitted. Currently, we have 11 papers published or in press in the open literature describing the development and testing of these new methods for Hg. We have extensively tested these methods by measuring Hg emissions from both background and contaminated soils. Our results suggest that Hg in soils is readily mobilized into the air by volatilization. Emission rates from contaminated soils (total Hg = 5-50 ppm) exceed those from background soils by orders of magnitude, indicating the importance of quantifying fluxes from such sites.

91-95 Funding (\$K): 1100 Dates: 1992-1995



Technology Transfer: Open literature publications, hands-on training

**Key Documentation:** Lindberg, S.E., K-H. Kim, T.P. Meyers, and J.G. Owens. 1995. A micrometeorological gradient approach for quantifying air/surface exchange of mercury vapor: Tests over contaminated soils. *Envir. Sci. Technol.* 29:126-135.  
Kim, K.-H., Lindberg, S. E., and Meyers, T. P. 1995 Micrometeorological measurements of mercury fluxes over background forest soils in eastern Tennessee. *Atmos. Envir.* 27:267-282.

**Key Personnel:** S. E. Lindberg, (615) 574-7857, SLL@ORNL.GOV, J. G. Owens, (615)576-8544, OGJ@ORNL.GOV

**Lab Capabilities Applied:** Environmental Sciences, National Environmental Research Park User Facility



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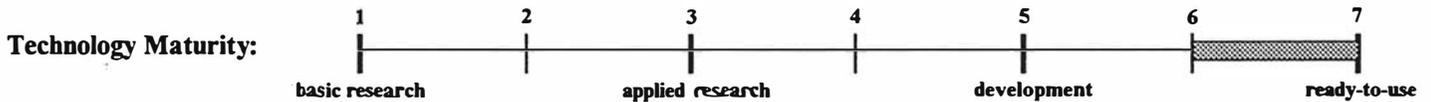
**Category:** Production (3, 4, 6, 9, 12, 15), Arctic Region Activities (5, 7), Deepwater Offshore (1, 2, 4, 5, 6, 8, 15), Gas Gathering (2, 3, 4, 5), Oil Processing & Refining (14, 15), Environmental & Regulatory (8, 10, 14)

**Laboratory:** Oak Ridge National Laboratory      **Contact:** A. L. Wright

**Title:** Pipeline Safety

**Description:** The Oak Ridge Complex will provide technical and engineering support for regulatory compliance and to program activities of the Office of Pipeline Safety (OPS) for calendar years 1995 through 1998. This assistance will include 1) responding to designated pipeline accidents in determining or confirming accident cause(s), identifying circumstances influencing the accident and its consequences to public safety, property, and the environment, and developing findings and recommendations for corrective actions to mitigate the possibility of future accidents and evaluate the condition of pipeline systems to ensure future safe operation; 2) assisting in the inspection of pipeline operating units, recording evidence and findings, and preparing reports; 3) conducting audits of pipeline operators to ensure compliance with remedial actions resulting from inspections and compliance actions; 4) inspecting pipeline construction projects to ensure the design and installation conform to pipeline safety regulations; and 5) providing specialized consultation and laboratory services.

**91-95 Funding (\$K):** 4500      **Dates:** 1995-present



**Technology Transfer:** Work for Others with Department of Transportation

**Key Documentation:**

**Key Personnel:** R. B. Honea, (615)574-5932, bbh@ornl.gov, R. R. Rawl, (615)574-4713, rur@ornl.gov, A. L. Wright, (615)574-6878, alw@ornl.gov

**Lab Capabilities Applied:** Energy Production & Use, Advanced Materials, Advanced Computing



Index: 284

Category: Gas Processing (2, 3, 8), Oil Processing & Refining (4, 6, 21)

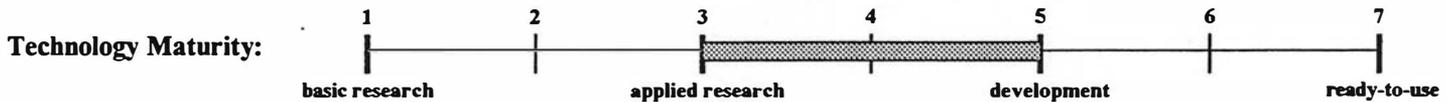
Laboratory: Oak Ridge National Laboratory      Contact: E. Kaufman

Title: Advanced Bioreactor Systems for Gaseous Substrates

**Description:** Current methodologies for the removal of acid rain forming flue gas emissions either produce large quantities of solid waste or require expensive downstream reduction processes after SO<sub>2</sub> capture. ORNL research has focused upon the reduction of SO<sub>2</sub> from regenerable flue gas sorbents. We are utilizing a mixed culture of heterotrophs and sulfate reducing bacteria (SRB) to reduce SO<sub>2</sub> into H<sub>2</sub>S which may then be further reduced either chemically or biologically to elemental sulfur and sold as a chemical feedstock. The mixed culture eliminates the need for the strict anaerobic environment required by SRB and also decreases process nutrient costs. We are currently operating the process using municipal waste as a feed source, with the potential for a negative cost process feed. Initial economic assessment has demonstrated that our microbial process may be competitive with conventional hydrotreating of SO<sub>2</sub>. Additional cost savings are realizable with the high biocatalyst density afforded by cell immobilization.

We are also investigating and demonstrating the conversion of waste gases (CO and CO<sub>2</sub>) into ethanol in this research program through a Cooperative Research and Development Agreement (CRADA) with Bioengineering Resources, Inc.

91-95 Funding (\$K): 300      Dates: 1994-present



Technology Transfer: Staff exchange, licensed product, publications, CRADA agreement

Key Documentation:

Key Personnel: Dr. Eric N. Kaufman, (615)574-6624, ekn@ornl.gov

Lab Capabilities Applied: Energy production, Biosciences and Biotechnology



Index: 285

Category: Exploration (8, 15), Environmental & Regulatory (5, 7, 8, 14)

Laboratory: Oak Ridge National Laboratory Contact: Bill Doll

Title: Airborne Geophysical Surveying

Description: Airborne magnetic, electromagnetic, and radiometric surveying techniques that were originally developed for the mineral prospecting industry have been adapted for investigation of environmental sites in the largest and most thorough application of airborne geophysics to a hazardous waste site which has been conducted to date. Tests have been conducted to determine the sensitivity of these systems over known waste sites and representative environmental targets. Techniques for managing and evaluating these large data sets have been developed, as well as methods for integrating geophysical data with aerial photographic images, multispectral scanner data, and other site information. Data acquisition and baseline processing were conducted by Geonex Aerodat Ltd. Data processing methods are being developed for our data set by our group, as well as the U.S. Geological Survey and the University of Utah. High resolution data were acquired over the entire 35,000-acre Oak Ridge Reservation, and very high resolution data were acquired over selected areas. Magnetic data are effective for defining the boundaries of waste areas, combing large areas for unreported waste areas, and mapping certain geologic and soil features. Electromagnetic data acquired with a horizontal coplanar coil configuration are useful for mapping geologic contacts and waste areas which have been placed in poor conductors. Vertical coaxial coils provide higher resolution at the expense of some noise. Radiometric data are useful not only for mapping man-made radionuclides, but for mapping geology with the potassium channel.

91-95 Funding (\$K): 2405 Dates: 1992-present

	1	2	3	4	5	6	7
Technology Maturity:	basic research		applied research		development		ready-to-use

Technology Transfer: Publications in open literature, interactions with Goenex Aerodat, the contractor

Key Documentation: Doll, W.E. J.E. Nyquist, J.S. Holladay, V.F. Labson, and L. Pellerin, Preliminary results of a helicopter electromagnetic survey of the Oak Ridge Reservation, Tennessee for environmental and geologic site characterization, Symposium on the Application of Geophysics to Engineering and Environmental Problems, 1993 Proceedings, p. 281-295.  
  
Nyquist, J.E. and W.E. Doll, Comparison of surface and aerial techniques for characterizing a hazardous waste site: A case study, Expanded abstracts, 1993 Society of Exploration Geophysicists Annual Meeting, p. 468-471.

Key Personnel: W.E. Doll, (615)-576-9930, d8e@ornl.gov  
J.E. Nyquist, (615)-574-4646, nyq@ornl.gov  
A.D. King, (615)-576-1509, alk@ornl.gov ("a-one-k")

Lab Capabilities Applied: Energy production, advanced computing



**Index:** 286

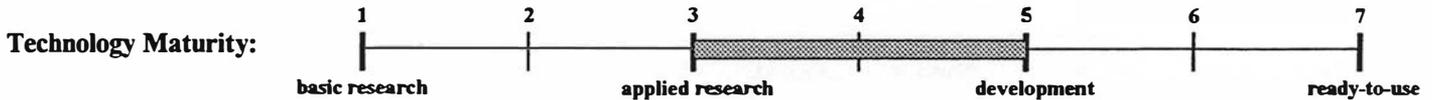
**Category:** Oil Processing & Refining (15, 5), Deepwater Offshore (1, 4, 5, 6, 7)

**Laboratory:** Oak Ridge National Laboratory      **Contact:** G. Yoder

**Title:** ANS Flow blockage Computational Fluid Analysis and Experimentation

**Description:** This project was a portion of the Advanced Neutron Source (ANS) Safety and R&D programs. The objective of the project was to develop benchmarked Computational Fluid Dynamics (CFD) models for use in thermal hydraulic design and safety analysis of high velocity, recirculating heavy water flows. The project was divided into two major tasks, one analytical and one experimental. The analytical portion of the project included a survey of potential codes to perform the analysis, a down select <Adjective> of these codes, benchmark testing of the down selected codes using existing data, comparison of the selected code predictions to data specifically developed for the ANS, and design analysis of the ANS geometry. Initial benchmark testing included evaluating various turbulence models for specific geometries, evaluation of solution algorithms for solution speed, and direct comparison of calculated results to experimental data in similar geometries. The code finally selected to use in the analysis (FLUENT) was then benchmarked against data taken in an experiment specifically designed to simulate the geometry and fluid conditions of interest. Once benchmarked, the code was used to help resolve various design issues, and was used in combination with structural analysis to determine fluids induced structural loads on core components. The experimental portion of the project was aimed at simulating the thermal and hydraulic characteristics of ANS fuel plates under conditions where the inlet of the coolant channel was partially blocked. A technique was developed which used thermochromic liquid crystals combined with image processing techniques to make continuous (spatially) temperature measurements. Local heat transfer coefficients determined using this method were used to benchmark the CFD code. In addition, laser Doppler velocimetry measurements were made using a state-of-the art system to determine the local velocity profiles downstream of the flow blockage. Applications of this work include problems which require general CFD computational capabilities and specifically, problems which require analysis which has been benchmarked under recirculating conditions (this could include areas such as erosion, material deposition due to thermal or velocity gradients in the flow, chemical reactions, etc.).

**91-95 Funding (\$K):** 1300      **Dates:** 1993-1995



**Technology Transfer:** 3 publications in open literature

**Key Documentation:** D. K. Felde, T. K. Stovall, and J. A. Crabtree, "Experimental Investigation of Flow Blockage Phenomena in the ANS Core," accepted for publication in American Nuclear Society 1995 Annual Meeting, Philadelphia, PA, June 25-29, 1995.  
 T. K. Stovall, J. A. Crabtree, and D. K. Felde, "A Computational Fluid Dynamics Model of Separated Flow in a Thin Rectangular Channel was Benchmarked for Use in Predictive Design Analysis," accepted for publication in International Heat Transfer Conference, Portland, OR, August 6-9, 1995.

**Key Personnel:** J. A. Crabtree, (615) 576-5298, Internet j8c@ornl.gov  
 D. K. Felde, (615) 574-4555, Internet dvd@ornl.gov  
 G. L. Yoder, (615) 574-5282, Internet gly@ornl.gov

# NPC LAB CAPABILITIES STUDY

May 1, 1995

# PROJECT SUMMARY



**Lab Capabilities Applied:** Heat transfer and fluid flow analysis, thermal-hydraulic experimentation

**Index:** 287

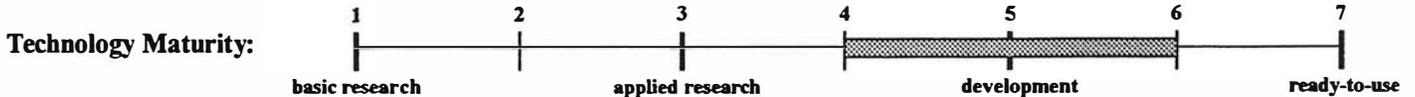
**Category:** Oil Processing & Refining (3, 15, 19, 25), Production (3, 4)

**Laboratory:** Oak Ridge National Laboratory      **Contact:** G. Yoder

**Title:** ANS and HFIR Thermal and Hydraulic Analysis and Experimentation

**Description:** This program included tasks aimed at developing the design and quantifying the safety of the Advanced Neutron Source (ANS) reactor system. Thermal and hydraulic analysis ranged from such areas as detailed conduction analysis and two phase forced convective heat transfer to CFD analysis analyzing natural circulation within piping systems. In addition, a significant thermal hydraulic data base developed from world data was used to execute statistical uncertainty analysis. Both steady state and transient thermal hydraulic calculations were performed including pressure wave propagation studies. Codes used in this program included TRUMP, HEATING7, RELAP5, TASHA, P THERMAL, PTA2 and software developed specifically for this application, as well as many others. An experimental program complimented the analysis by providing heat transfer data at ANS specific coolant conditions. This data included heat transfer coefficients, as well as critical heat flux and flow excursion limits. Detailed modeling of the test section was used to account for experimental variables such as axial and spanwise conduction, variable joule heating, and corrosion of the aluminum test article. High speed instrumentation and data acquisition systems allowed measurement of phenomena which occurred on a few millisecond time scales. Applications of this work include thermal analysis of both fluid and solid systems, energy inventory analysis to improve energy efficiency or control, and transient design and accident analysis.

**91-95 Funding (\$K):** 12000      **Dates:** 1991-1995



**Technology Transfer:** 30+ publications in open literature

**Key Documentation:** G. L. Yoder, et. al, Steady State Thermal-Hydraulic Design Analysis of the Advanced Neutron Source Reactor, ORNL/TM-12398, May 1994.  
 N. C. J. Chen, M. W. Wendel and G. L. Yoder, "Conceptual Design Loss-of-Coolant Accident Analyses for the Advanced Neutron Source Reactor," Nuclear Technology, Vol. 105, No. 1, pp 104-122, January 1994.

**Key Personnel:** N. C. J. Chen, (615) 574-0753, Internet ncj@ornl.gov, D. K. Felde, (615) 574-4555, Internet dvd@ornl.gov, M. W. Wendel, (615) 574-2825, Internet mwq@ornl.gov, G. L. Yoder, (615) 574-5282, Internet gly@ornl.gov

**Lab Capabilities Applied:** Thermal and hydraulic analysis, thermal and hydraulic experimentation.



Index: 288

Category: Environmental & Regulatory (7, 8, 10, 14)

Laboratory: Oak Ridge National Laboratory      Contact: G. Yoder

Title: METER and AENEC Programs

**Description:** The Atmospheric Effects of Nuclear Energy Centers (AENEC) Program was managed and coordinated by ORNL with participants from other laboratories and universities: Atmospheric Turbulence and Diffusion Laboratory (NOAA), Battelle Pacific Northwest Laboratories, Pennsylvania State University, and Rand Corporation. The objective of the program was to develop and verify methods (analytical or experimental) for predicting the maximum amount of energy that can be dissipated to the atmosphere through cooling towers or cooling ponds from proposed nuclear energy centers without affecting (adversely or beneficially) the local and regional environment (weather). The findings were summarized in ORNL reports (ORNL/TM-5778).  
 Meteorological Effects of Thermal Energy Releases (METER) Program was a continuation of the AENEC. The initial program scope (mathematical modeling, laboratory and field experimentation, and societal impact assessment) had narrowed to emphasis on the field data acquisition from a network of rain gauges installed at the Bowen Plant in Georgia. The primary objectives were, through airborne sampling and ground measurements, to determine (1) plume aerosol characteristics and precipitation chemistry, (2) temperature/humidity profiles, (3) drift-drop concentration as a function of plume height. Some results were documented in ORNL reports (ORNL/TM-7286).  
 Although these programs are not presently active at ORNL, similar activities are being pursued under the umbrella of EIS analyses. Techniques developed under these various programs could be applied directly to air pollutant dispersion and transformation.

91-95 Funding (\$K): 600      Dates: 1991

	1	2	3	4	5	6	7
<b>Technology Maturity:</b>	basic research		applied research		development		ready-to-use

Technology Transfer:

**Key Documentation:** N. C. J. Chen and L. Jung, "A Mathematical Model of Drift Deposition from a Bifurcated Cooling Tower Plume," Atmospheric Environment, Vol. 12, 1969-1980.  
 A. A. N. Patrinos, N. C. J. Chen and R. L. Miller, "Spatial Correlations of Monthly Rainfall: Applications in Climatology and Weather Modification Experiments," Journal of Applied Meteorology, Vol. 18, No. 6, June 1979.

**Key Personnel:** N. C. J. Chen, (615) 574-0753, Internet ncj@ornl.gov, R. L. Miller, (615) 574-0751, Internet met@ornl.gov

**Lab Capabilities Applied:** Atmospheric aerosol dispersion, Plume modeling



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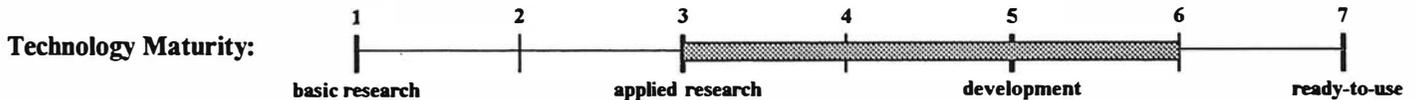
Category: Environmental & Regulatory (7, 8, 10, 14)

Laboratory: Oak Ridge National Laboratory Contact: R. L. Miller

Title: Prediction of Air Pollution Dispersion/Transformation/Fate

Description: Atmospheric scientists at ORNL have been involved in a variety of projects related to applied research in air pollution meteorology and atmospheric chemistry. Much of the effort has been associated with environmental impact assessment for the National Environmental Policy Act. Frequently, staff members characterize the existing climatology and air quality at the sites of proposed projects, and perform air dispersion modeling to predict downwind concentrations resulting from proposed emissions. The concentrations are compared with standards to evaluate the potential impacts expected from the proposed projects. The concentrations often are used as input for human health studies. Analyses have also been performed for odorous emissions, visibility impairment, and photochemical transformation. Studies have been conducted of potential impacts resulting from deposition of mercury emissions. Source characterization based on receptor modeling has been performed.

91-95 Funding (\$K): 3000 Dates: 1991-1995



Technology Transfer: Federal agencies-ORNL interactions

Key Documentation: Journal articles, conference proceedings, ORNL reports, environmental impact statements and assessments.

Key Personnel: R. L. Miller, 615-576-0751, met@ornl.gov, T. J. Blasing, 615-574-7368, bla@ornl.gov, D. A. Lombardi, 615-576-9231, d76@ornl.gov, M. D. Cheng, 615-576-5042, ucn@ornl.gov

Lab Capabilities Applied: Technical expertise in meteorology, climatology, air quality, and atmospheric chemistry



**Index:** 290

**Category:** Oil Processing & Refining (24, 27, 28, 20, 21)

**Laboratory:** Oak Ridge National Laboratory      **Contact:** A. L. Compere

**Title:** Low Emmissions Diesel Fuels

**Description:** Microemulsion technology can be used to incorporate a wide variety of oil-insoluble materials into clear, transparent, stable diesel fuels. The oil-insolubles are contained in dispersed-phase aggregates, typically in around 4 nm in diameter. Fuels which have conventional performance in terms of ignition delay, but markedly lower emissions, can be formulated using this technology. Compounds which reduce NOx and particulate emissions when incorporated into the fuels include water, alkyl and aromatic alcohols, urea, and ketones. Submicron solid materials, including conventional catalysts, can also be incorporated into diesel fuels. The surfactants are typically vegetable or tree oil fatty acids partially neutralized with alkyl amines. Microemulsion fuels typically contain 10 to 30% of the aqueous, or discontinuous, phase. Thus, this technology permits incorporation of a wide variety of renewables into low-emissions diesel fuels.

**91-95 Funding (\$K):** 1050      **Dates:** 1991-1995

	1	2	3	4	5	6	7
<b>Technology Maturity:</b>	basic research	applied research			development	ready-to-use	

**Technology Transfer:** CRADA

**Key Documentation:** West, B. H.; Compere, A. L.; and Griffith, W. L. 1990. High alcohol microemulsion fuel performance in a diesel engine. Society of Automotive Engineers pape

Caponetti, E.; Lizzio, A.; Triolo, R.; Griffith, W. L.; and Johnson, J. S., Jr. 1992. Alcohol partition in a water-in-oil microemulsion from small-angle neutron scattering. Langmuir 8: 1554-1562.

**Key Personnel:** A. L. Compere, (615) 574-4970, cal@ornl.gov

**Lab Capabilities Applied:** Formulation, physical and chemical properties, small-angle neutron scattering, engine testing with emissions monitoring, combustion modeling, and model combustion systems.



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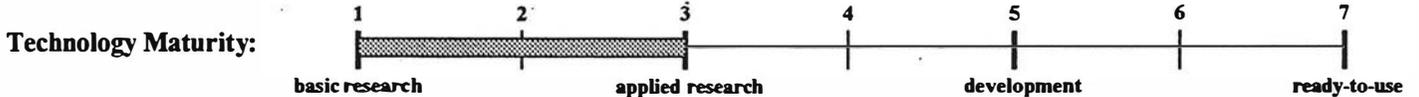
Category: Exploration (8, 10), Environmental & Regulatory (5, 7, 8, 14), Gas Gathering (2)

Laboratory: Oak Ridge National Laboratory      Contact: T. W. Schmidt

Title: Airborne Remote Sensing of Natural Gas Leaks

**Description:** The program is to develop an airborne laser sensor system designed to detect gas leaks associated with pipelines. The system is designed to operate from a small fixed wing or helicopter platform at speeds which provide economical ground coverage. The system is a continuous mapper and can detect leaks as small as 3 SCFH. In order to avoid false positives, the system detects both methane and ethane, ethane being present in natural gas at concentrations of 0.5-2.0%. At speeds of 120-150 miles per hour (160-250 km/hr) the system can inspect and document hundreds of miles of pipeline per day. The initial goal of the program is to construct a light weight airborne laser sensor package which can be flown economically to inspect natural gas pipelines for leaks. Once this equipment is in hand it will be used to survey natural gas pipelines for leaks in Russia and the United States. Operating at an altitude of 300-500 meters and at an air speed of 200 km/hr, the system will provide continuous ground coverage, and by using frequency agile mid-infrared laser techniques to identify both methane and ethane, false positive reports will be eliminated. Because of the need for leak verification and continuous coverage from an altitude of 300 meters, laser specifications require the use of current state of the art, diode laser pumping of optical parametric oscillators in conjunction with optical amplifier receivers in order to increase sensitivity and to provide safe laser exposure limits to personnel on the ground.

91-95 Funding (\$K): 1065      Dates: 1995



Technology Transfer: NIS/IPP Project with Russia and Belarus, CRADA with LaSen, Inc.

Key Documentation:

Key Personnel: T. W. Schmidt, (615)574-4977, t3w@ornl.gov

Lab Capabilities Applied: Advanced materials, environmental science, energy production



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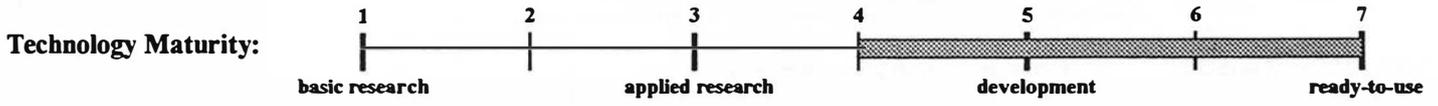
Category: Environmental & Regulatory (3, 6, 9, 14), Exploration (4)

Laboratory: Oak Ridge National Laboratory      Contact: Bill Doll

Title: Seismic Reflection Acquisition, Processing and Source Comparison

**Description:** Shallow seismic reflection methods have been applied at sites on and off of the Oak Ridge Reservation, and a thorough test of eight non-invasive sources has been conducted. The testing was in response to two needs: 1) environmental regulations require that non-explosive and non-penetrating sources be used at hazardous sites, and 2) High-frequency swept sources are becoming available for environmental applications and need to be tested against more conventional sources. Sources tested at our site ranged from a Failing vibrator and Bolt Land Air Gun to a sledge hammer. The goal was to optimize imaging in the 1000' depth range. Data from swept sources were stored in uncorrelated format. Shots were recorded by 95 surface geophones, 48 hydrophones, and one vertical component geophone at 1000 ft depth. High frequency vibrators (e.g. Mini- vib) performed favorably when appropriate pre-correlation processing was done, using routines appended to Cogniseis FOCUS workstation processing software. Shear sources were also evaluated. A full suite of geophysical well logs was collected at two 1000' deep wells at the site. The data suggest that shallow seismic techniques, using a Minivib source and 96-channel engineering seismograph could be adapted for high resolution imaging of shallow petroleum targets, particularly in areas like East Tennessee, where the mobilization cost of acquiring data with conventional systems is prohibitive.

91-95 Funding (\$K): 575      Dates: 1992-present



Technology Transfer: Publications in open literature

Key Documentation: Doll, W.E., R.D. Miller, and J. Xia, Noninvasive shallow seismic source comparison for hazardous waste site investigations, Abstracts, 1994 Society of Exploration Geophysicists Annual Meeting, p. 591-594.

Key Personnel: W.E. Doll, (615)-576-9930, d8e@ornl.gov

Lab Capabilities Applied: Environmental science, energy production



Index: 293

Category: Environmental & Regulatory (3, 6, 9, 12, 14)

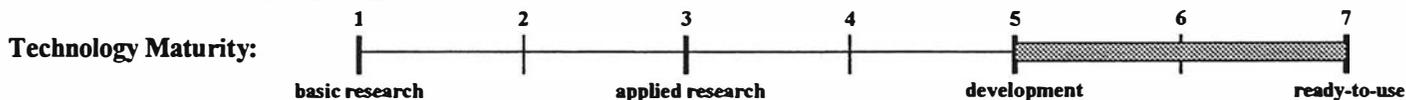
Laboratory: Oak Ridge National Laboratory      Contact: David M. Hetrick

Title: The Seasonal SOIL Compartment Model (SESOIL) and Computational Fluid Dynamics Modeling

**Description:** SESOIL is an acronym for SEasonal SOIL compartment model and is a zone-dimensional vertical transport code for the unsaturated soil zone. It is an integrated screening-level soil compartment model and is designed to simultaneously model water transport, sediment transport, and pollutant fate. The program was developed for EPA's Office of Water and Office of Toxic Substances in 1984 by Marcos Bonazountas and Janet Wagner of Arthur D. Little, Inc. and was modified extensively in 1986 by David Hetrick of Oak Ridge National Laboratory (ORNL) to enhance its capabilities.

SESOIL was developed as a screening-level model, utilizing less soil, chemical, and meteorological values as input than most other similar models. SESOIL was designed to perform long-term simulations of chemical transport and transformations in soil. Climatic data, compartment geometry, and soil and chemical property data are the major components used in the equations. Output of SESOIL includes time-varying pollutant concentrations at various soil depths and pollutant loss from the unsaturated zone in terms of surface runoff, percolation to the groundwater, volatilization, and degradation. A three-dimensional hydrological model of the Clinch River was developed using a state-of-the-art commercial fluid-dynamics program, CFDS-FLOW3D. The purpose of the model is to track dispersion of low-level waste entering the river from a side stream in order to predict contaminant concentration levels downstream.

91-95 Funding (\$K): 135      Dates: 1991-1995



Technology Transfer: Environmental Computer Workshops, Seminars, Publications in open literature.

Key Documentation: 1) Hetrick, D.M., and Scott, S.J.: "The New SESOIL User's Guide," PUBL-SW-200-93, Wisconsin Department of Natural Resources, May 1993.  
 2) Hetrick, D.M., Travis, C.C., Leonard, S.K., and Kinerson, R.S.: "Qualitative Validation of Pollutant Transport Components of an Unsaturated Soil Zone Model (SESOIL)," ORNL/TM-10672, Oak Ridge National Laboratory, Oak Ridge, TN, 42 pp., 1989.

Key Personnel: David M. Hetrick, 615-576-7556, dmh@ornl.gov, Ronald M. Widgeon, 615-574-8672, wid@ornl.gov M. W. Wendel, 615-576-2825, mwq@ornl.gov, P. T. Williams, 615-576-2111, ptw@ornl.gov

Lab Capabilities Applied: Computational Engineering, Contaminant Transport Modeling, Soil Physics, Latin Hypercube Sampling Methods.



Index: 294

Category: Gas Processing (3), Oil Processing &amp; Refining (16, 18, 4)

Laboratory: Oak Ridge National Laboratory

Contact: E. Kaufman

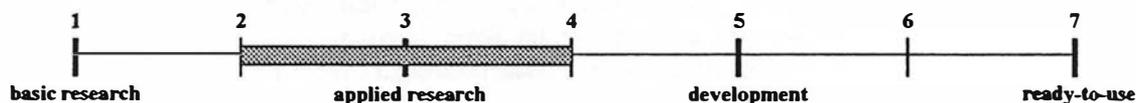
Title: Removal of Heteroatoms form Crude Oil

**Description:** To reduce its sulfur content, petroleum is currently treated thermochemically, a process that is energy intensive. Our goal is to develop a cost-effective and environmentally acceptable biological process for the removal of organic sulfur from hydrocarbon feedstocks. Our approach has been to use a microbial system where organic sulfur is anaerobically reduced to H<sub>2</sub>S by sulfate-reducing bacteria (SRB). These bacteria are being used as a biocatalyst in an aqueous-hydrocarbon liquid-liquid biphasic system. Initial work investigating the model compound dibenzothiophene in kerosene by the bacteria *D. desulfuricans*, demonstrated a promising sulfur reduction rate of 10-14 moles DBT per second per cell. We are currently developing advanced electric field driven reactors to allow for low cost aqueous/hydrocarbon mixing of the biocatalyst and substrate, and will be demonstrating this technology using actual crude oil feed.

91-95 Funding (\$K): 900

Dates: 1994-present

Technology Maturity:



Technology Transfer: Licensed product, CRADA agreement

**Key Documentation:** Lizama, H.M., Wilkins, L.A., and Scott, T.C., "Dibenzothiophene Sulfur Can Serve as the Sole Electron Acceptor During Growth by Sulfate-reducing Bacteria," *Biotechnol. Lett.* 17, 113-116, (1995).

**Key Personnel:** Dr. Timothy C. Scott, (615) 574-5962, tcs@ornl.gov  
Dr. Eric N. Kaufman, (615) 574-6624, ekn@ornl.gov

**Lab Capabilities Applied:** Biosciences and Biotechnology, Energy Production



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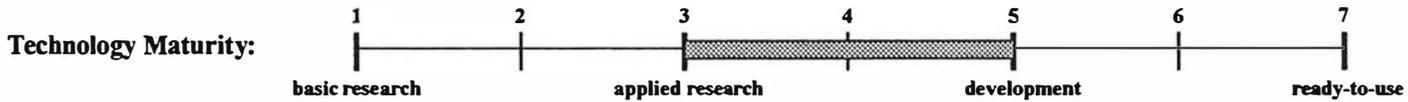
Category: Oil Processing & Refining (16, 18, 1, 2, 4, 6, 21)

Laboratory: Oak Ridge National Laboratory      Contact: E. Kaufman

Title: Advanced Bioreactor Concepts and Development

Description: In order to be economically feasible, all of the potential applications of biotechnology to coal and oil processing will require efficient and inexpensive bioreactors and contactors. The aim of this program is to develop advanced bioreactor concepts that are compatible with continuous operation and maximum throughput. Three reactor configurations are being considered: (1) a fluidized-bed bioreactor that allows the direct contacting of coal particles with the biocatalyst (microorganisms or enzymes) in an aqueous or organic liquid; (2) columnar bioreactors, either fixed-bed or fluidized-bed that can operated with a continuous gas phase or at least with a high gas loading; and (3) a liquid-liquid contacting system in which the biocatalyst in an aqueous liquid contacts an immiscible organic liquid such as a coal-derived liquid or oil. In all cases, a predictive model of the bioreactor system will be developed during the course of the research for future design and scale-up and a specific coal application will be chosen to experimentally confirm the model.

91-95 Funding (\$K): 1400      Dates: 1991-present



Technology Transfer: Publications, licensed product

Key Documentation: 1. □ Kaufman, E. N. and C. D. Scott (1994). "Liquefy Coal with Enzyme Catalysts." CHEMTECH 24(4):27-32.  
2. □ Asif, M., J. N. Petersen, E. N. Kaufman, J. M. Cosgrove, and T. C. Scott (1994). "A Dynamic Model of the Hydrodynamics of a Liquid Fluidized Bed." Ind. Eng. Chem. Res. 33:2151-2156.

Key Personnel: Dr. Eric N. Kaufman, (615)574-6624, ekn@ornl.gov

Lab Capabilities Applied: Energy production, bioscience and biotechnology





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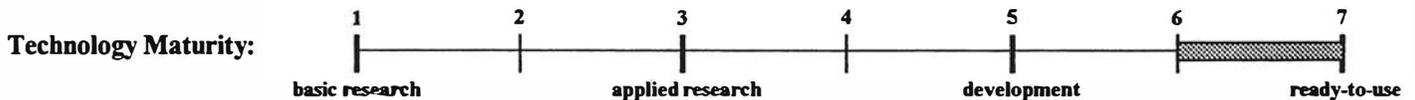
**Category:** Environmental & Regulatory (7, 8, 10)

**Laboratory:** Oak Ridge National Laboratory      **Contact:** Mary Francis

**Title:** Environmental Regulations and Compliance Requirements for Clean Air Act and Other Regulations

**Description:** Oak Ridge National Laboratory (ORNL) has 15-30 staff involved in developing information resources and regulatory expertise to assist various sponsors in efforts to comply with federal and state environmental laws and regulations. The staff track, monitor and report new environmental laws and regulatory initiatives; provide up-to-date reference materials on all major federal environmental laws; and uses scientific, engineering, legal and regulatory expertise to analyze regulatory issues, develop environmental compliance methodologies and assist the Department of Energy (DOE) or other sponsors in creating and implementing environmental policy and guidance. This expertise is used to develop and conduct training courses on environmental laws and regulations as well as produce newsletters for a broad audience. ORNL also has more than 25 years of experience in preparing Environmental Impact Statements for federal agencies. The staff are currently supporting 10 federal agencies in the preparation of 30 NEPA documents, involving integrated assessments of complex environmental issues over a wide spectrum of geographic areas.

**91-95 Funding (\$K):** 4500      **Dates:** 1970-present



**Technology Transfer:** Newsletters, journal publications, public documents, publically available databases, environmental impact statements, environmental assessments.

**Key Documentation:** (1) Saylor, R. E., and L. N. McCold, "Bounding Analyses in NEPA Documents: When Are They Appropriate?" The Environmental Professional, 16(4) 285-291, 1994. (2) Houlberg, L.M., G. T. Hawkins, R. E. Bock, S. J. Mayer, and M. S. Salk, Environmental Regulatory Update Table, Published bi-monthly by Oak Ridge National Laboratory. (3) Francis, M. W. and A. M. Vance, ESHNEWS 95, Published weekly, newsletter of announcements of current events, decisions, and trends in environmental issues and regulations.

**Key Personnel:** J. T. Ensminger, 615-574-5657, etj@ornl.gov,  
L. M. Houlberg, 615-574-7763, houlberglm@ornl.gov  
R. L. Miller, 615-576-0751, millerri@ornl.gov,  
S. E. Arnold, 615-576-1753, arnoldse@ornl.gov

**Lab Capabilities Applied:** Toxicology, human health effects, environmental engineering, geology, surface/ground water, hydrology, socioeconomics, environmental justice, public involvement, cultural resources. Regulatory environmental and regulations.



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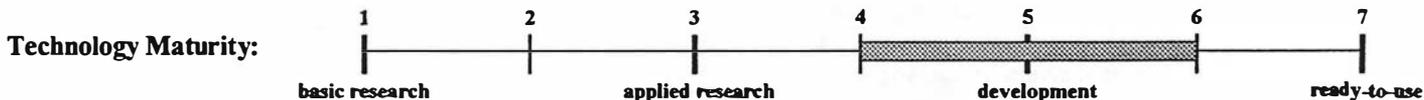
Category: Environmental & Regulatory (1, 2, 10, 12, 14)

Laboratory: Oak Ridge National Laboratory      Contact: Dianne D. Gates

Title: In Situ Chemical Oxidation of Organic Contaminants in Soil and Groundwater

**Description:** In situ chemical oxidation offers several advantages over other in situ and ex situ remediation technologies. In addition to the benefits associated with most in situ treatment processes (less worker exposure to hazardous compounds, reduced cost, and applicability to inaccessible sites), in situ chemical oxidation uses inexpensive, readily available reagents, is easily controlled, and is applicable to a wide variety of volatile and non-volatile contaminants. In situ chemical oxidation utilizes the hydroxyl radicals (OH) formed by hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) and potassium permanganate (KMnO<sub>4</sub>) to oxidatively degrade organic contaminants of interest. Hydroxyl radicals are known to be very powerful, non-specific oxidizers that react very rapidly with many compounds, including volatile and semi-volatile contaminants of environmental interest. With this technology, organic compounds are oxidized with low-strength chemical oxidants, resulting in the formation of simple inorganic compounds (i.e., HCl), water, carbon dioxide (with H<sub>2</sub>O<sub>2</sub>) or manganese oxide (with KMnO<sub>4</sub>). Both H<sub>2</sub>O<sub>2</sub> and KMnO<sub>4</sub> were evaluated as potential in situ chemical oxidants in laboratory studies. These studies were designed to evaluate the applicability of the proposed technology to several soil types (low permeability clayey and high permeability sandy) that are representative of the soils found at contaminated sites. The model contaminants for the screening studies included TCE, PCE, TCA, naphthalene, phenanthrene, and pyrene. With 5% KMnO<sub>4</sub> solutions, >95% removal of TCE, PCE, naphthalene, pyrene and phenanthrene was observed in both the clay and sandy soils. The greatest removals of TCE and PCE observed with 8.5% H<sub>2</sub>O<sub>2</sub> in the clay soils were 86 and 68% respectively. Lower TCE and PCE removals (61 and 32%) were observed in the sandy soil treated with H<sub>2</sub>O<sub>2</sub>. In the clay soil, H<sub>2</sub>O<sub>2</sub> was able to remove over 95% of the three SVOCs while in the sandy soil considerably lower SVOC removals (avg = 24%) were observed. Two field demonstrations including of in situ chemical oxidation have been successfully completed and a third demonstration is being planned.

91-95 Funding (\$K): 555      Dates: 1992-present



Technology Transfer: Open literature publications, presentations at national/international conferences

Key Documentation:

Key Personnel: Dianne D. Gates, (615)576-4027, gatesdd@ornl.gov, Robert L. Siegrist, (303)273-3490, siegrist@ornl.gov, Steven R. Cline, (615)231-3957, clinesr@ornl.gov

Lab Capabilities Applied: Bench- and pilot-scale treatment studies, field demonstration capabilities.



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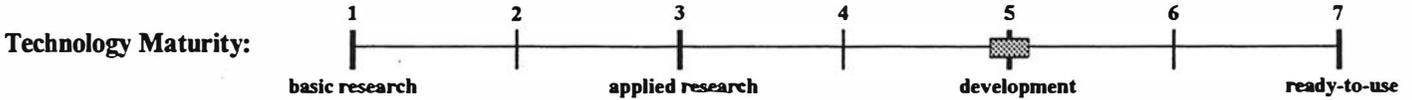
Category: Oil Processing & Refining (16, 17, 6, 23)

Laboratory: Oak Ridge National Laboratory      Contact: J. R. Keiser

Title: Development of Materials for Black Liquor Recovery Boilers for Pulp and Paper Mills

Description: This project involves pulp and paper companies, boiler manufacturers, boiler tube fabricator, the U.S. and Canadian paper institutes and Oak Ridge National Laboratory in a project to identify better materials, in particular boiler tubes, to improve the safety of recovery boilers. The paper institutes and ORNL are surveying the paper industry to define the extent of recovery boiler problems and to better define the operating conditions in boilers. Laboratory tests will be conducted to define the corrosion mechanisms that are operative in boilers, and residual stress measurements will be made and computer modeling done to define the stresses in composite tubes at elevated temperatures. The stresses around openings like smelt spout openings and air ports will also be calculated. Based on these studies, alternate materials will be identified and tests conducted to determine the suitability of these materials.

91-95 Funding (SK): 550      Dates: 1995-present



Technology Transfer: Open literature publications, letter reports, staff exchanges

Key Documentation:

Key Personnel: James R. Keiser, 615-574-4453, keiserjr@ornl.gov  
 Camden R. Hubbard, 615-574-4472, hubbardcr@ornl.gov  
 Thomas Zacharia, 615-574-4897, zachariat@ornl.gov  
 Robert W. Swindeman, 615-574-5108, bozemanjb@ornl.gov

Lab Capabilities Applied: Residual stress measurements using neutron and x-ray diffraction, finite element analysis using massive parallel computers, mechanical property measurements of metals, thermal fatigue experiments, microstructural analysis of samples using microscopic tech



Index: 300

**Category:** Oil Processing & Refining ((16, 18, 1, 6, 21, 23), Production (1, 2, 3, 4, 16, 21))

**Laboratory:** Oak Ridge National Laboratory

**Contact:** E. Kaufman

**Title:** Biological Catalysts in Organic Media

**Description:** There are several potential bioprocessing concepts that could use an organic solvent or produce liquid organic products, for example, the bioconversion of coal to liquids in an organic solvent or the bioprocessing of coal-derived liquids and crude oil. For such a process, the biocatalyst (microorganism or enzyme) must be compatible with the organic medium. Reducing enzymes such as hydrogenase have been modified to accept non-polar groups which render the otherwise hydrophilic proteins soluble and active in organic media. We investigate enzymes capable of operating at extreme conditions such as high temperatures and harsh chemical environments. As organisms are to possess specific biocatalytic activities, we will attempt to purify the enzymatic mechanisms responsible for the biological conversion of interest. The purified enzymes will enable higher yields, and reactor throughput with decreased operating costs and may also allow reactions to occur in environments where the whole organism would not survive.

**91-95 Funding (\$K):** 1100

**Dates:** 1991-present

1

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3

4

5

6

7

**Technology Maturity:**

basic research

applied research

development

ready-to-use

**Technology Transfer:** Publications

**Key Documentation:** 1. Kaufman, E. N. and C. D. Scott (1994). "Liquefy Coal with Enzyme Catalysts." CHEMTECH 24(4):27-32.

2. Scott, C. D., C. A. Woodward, and T. C. Scott (1994). "Mechanisms and Effects of Using Chemically Modified Reducing Enzymes to Enhance the Conversion of Coal to Liquids." Fuel Process. Technol. 40: 319-329.

**Key Personnel:** Dr. Eric N. Kaufman, (615) 574-6624, ekn@ornl.gov  
 Charlene A. Woodward, (615) 574-6786, caw@ornl.gov

**Lab Capabilities Applied:** Energy Production, Biosciences and biotechnology



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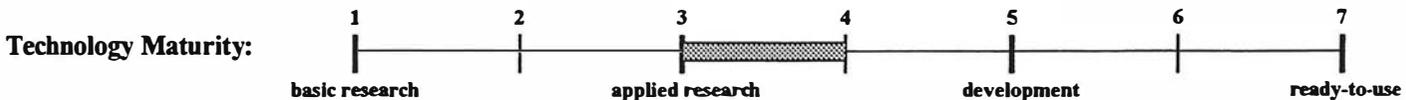
Category: Environmental & Regulatory (3, 6, 9, 12, 14)

Laboratory: Oak Ridge National Laboratory Contact: Bob Siegrist

Title: Remediation of DNAPL Compounds in Low Permeability Media

**Description:** The purpose of this work is to research and demonstrate in situ remediation technologies for dense, non-aqueous, phase liquid compounds (DNAPLs) (e.g., trichloroethylene (TCE) and tetrachloroethylene (PCE)) in low permeability media (e.g., silt and clay deposits). These compounds and physical settings are prevalent at many DOE sites and acceptable environmental restoration technologies are currently unavailable. The proposed work represents a joint initiative between DOE and the American Petroleum Institute (API). It is a logical extension of ongoing work within both organizations and represents a synergy of resources involving a consortium of nationally recognized scientists and engineers affiliated with universities (e.g., Oregon Graduate Institute, Colorado State University, University of Cincinnati, New Jersey Institute of Technology, University of California-Berkeley), federal laboratories (ORNL), and private industry (BP Oil, CH2M-Hill, Freeze Engineering, Hayward Baker Environmental). The project includes technology evaluation and screening, and laboratory and field-scale testing at both clean and contaminated test sites in the U.S. and Canada. Progress to date has included technical team meetings, preparation of state-of-the-art review papers, and initiation of laboratory and field experiments in support of work at three test sites. Technologies being evaluated include: fracture-enhanced soil vapor extraction (Sarnia, Canada), hydraulic fracturing and steam injection (Aber Road, Ohio), and multi-port reagent injection (DOE Portsmouth Site, Portsmouth, Ohio). The end result of this task will be identification of technologies suitable for further testing or for direct infusion into the DOE environmental restoration program.

91-95 Funding (\$K): 1000 Dates: 1993-present



Technology Transfer: Publications in open literature, staff exchange

Key Documentation: In Situ Remediation of DNAPL Compounds in Low Permeability Media: Transport/Fate, Treatment, and Risk Reduction. 1994. U.S. Department of Energy, Office of Technology Development, In Situ Remediation Integrated Program. (In review).

Key Personnel: Robert L. Siegrist, 303-273-3490, bs7@ornl.gov  
 Olivia R. West, 615-576-0505, qm5@ornl.gov  
 Nic E. Korte, 303-248-6210, nek@ornl.gov

Lab Capabilities Applied: Environmental science and technology



**Index:** 302

**Category:** Development (4, 21, 23, 24), Environmental & Regulatory (5, 8, 9)

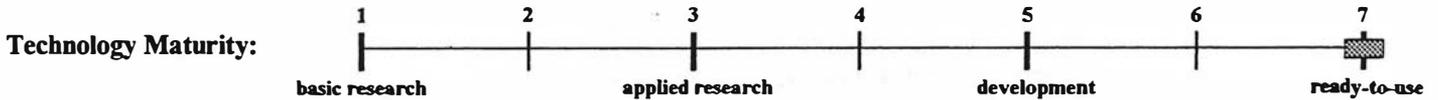
**Laboratory:** Oak Ridge National Laboratory      **Contact:** Jack Collins

**Title:** Tracer Technology

**Description:** Radioisotopes are available for a large number of elements. Because they are readily measurable in small amounts, and in most cases behave identically to the corresponding nonradioactive isotopes of the same element, they can be used to "trace" the behavior of specific elements in a variety of environments.

Tracer technology can be used in many applications. These applications include studies on efficiencies of separation processes, determination of chemical reaction mechanisms, studies of diffusion processes, and metabolism in plants and animals. Radioisotope tracers can also be used in medicinal treatments and diagnosis, measurement of metal wear and corrosion, and rate of uptake of specific elements in the environment. The extreme sensitivity of detection methods make these applications possible.

**91-95 Funding (\$K):** 8000      **Dates:** 1946-present



**Technology Transfer:** Medical diagnosis, well logging, chemistry research, isotope production and separation

**Key Documentation:**

**Key Personnel:** J. L. Collins, (615)574-6689, [Ins@ornl.gov](mailto:Ins@ornl.gov), B. Z. Egan, (615)574-6868, [ega@ornl.gov](mailto:ega@ornl.gov)

**Lab Capabilities Applied:** Energy production, environmental science, manufacturing technology, bioscience and biotechnology



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Category: Oil Processing & Refining (15, 20, 27, 28)

Laboratory: Oak Ridge National Laboratory Contact: R. Rawl

Title: Fuel Models

Description: The fuels modeling capability addresses availability, quality and use. The forecasting system consists of a world petroleum distribution model and the Oak Ridge National Laboratory Refinery Yield Model (regional petroleum refinery linear programs). This system has been used to study world oil disruptions; fuel specifications; jet fuel conversion; ultra low sulfur diesel fuel; gasoline reformulation and fuel effects on jet engine performance. Model applications include determination of conservation opportunities, the effects of fuel use policies and measuring progress in meeting energy use targets. Oak Ridge National Laboratory scientists have developed computer models to assist in several issues regarding the Strategic Petroleum Reserve (SPR). Issues addressed include optimal size of inventory, draw down and distribution capabilities, regional product reserves versus centralized crude storage, crude oil mix, financing and the economic effects of market disruptions.

91-95 Funding (\$K): 500 Dates: 1990-1994



Technology Transfer: Work for Others with the Department of Defense.

Key Documentation:

Key Personnel: R. R. Rawl, (615(574-4713, rur@ornl.gov)

Lab Capabilities Applied: Energy production and end use, advanced computing modeling



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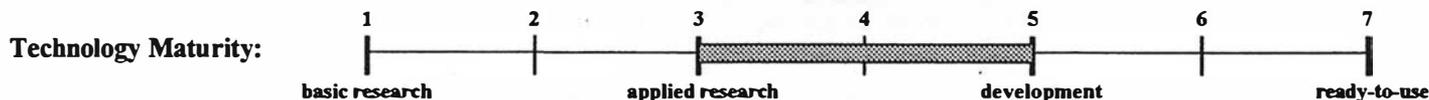
Category: Production (25, 26), Development (26)

Laboratory: Oak Ridge National Laboratory      Contact: Leonard Gray

Title: Computational Simulation of Hydrofracturing

**Description:** The hydraulic fracturing process is widely used to stimulate reservoirs, but often fails for non-vertical wellbores. Nevertheless, due to their significant advantages (reduced drilling, environmental impact, cost, and enhanced recovery) the percentage of directionally-drilled wells continues to increase. Consequently, it is imperative to develop a better understanding of the fracturing process for these wells. The purpose of this project is to develop a next generation continuum-based simulator for predicting crack initiation and near-wellbore propagation from cased, perforated, deviated wellbores. This work is in collaboration with Schlumberger, Cornell University, and the University of Minnesota. Development of this simulator will be based upon recent technical advances achieved by the project team in the areas of (a) crack-tip physics, (b) hypersingular boundary integral methods for fracture analysis, (c) computer tools for crack representation and propagation, and (d) parallel computing. The simulator will be capable of modeling multiple, arbitrary, non-planar, three-dimensional, fluid-driven crack initiation and propagation. It will include sophisticated computational geometry capabilities and efficient software tools for visualization and interpretation of results (FRANC3D). Finally, it will function in a distributed-workstation parallel computing environment (PVM). Schlumberger will provide experimental and field data for validating the computational model, and they will apply it to develop optimal fracturing treatments from inclined wellbores. This project is currently not funded.

91-95 Funding (SK): 155      Dates: 1994-present



Technology Transfer: Open literature publications, software

Key Documentation: "A Posteriori Pointwise Error Estimates for the Boundary Integral Method", ORNL/TM-12820, "Crack Tip Interpolation, Revisited", SIAM Journal of Applied Mathematics, submitted.

Key Personnel: Leonard Gray, (615)574-8189, ljg@ornl.gov

Lab Capabilities Applied: Applied Mathematics, Numerical Analysis, Parallel Computing



Index: 305

Category: Environmental & Regulatory (3, 4, 7, 14)

Laboratory: Oak Ridge National Laboratory Contact: Lawrence Barnthouse

Title: Quantitative Assessment of Environmental Risks

**Description:** In 1981 ORNL staff initiated the first formally-designated ecological risk assessment research program. Risk assessment methodologies have since been developed for DOE, EPA, NOAA, and DOD. Work has involved innovative applications of data bases, quantitative statistical techniques, and simulation models to environmental problems at the local, regional and global scale. Applications have included technology assessment, standard-setting, hazardous chemical evaluation, and environmental restoration. For example, codes have been developed to integrate laboratory toxicological data with aquatic ecosystem models to calculate risks to biota. Extensive site testing and computer modeling at a DOE facility demonstrated that alternatives to RCRA concentration limits could be justified, leading to preparation of a petition for cessation of groundwater pump-and-treat operations to be submitted to EPA. Ecological benchmarks have been developed for aquatic biota, sediment-associated biota, wildlife, and terrestrial plants. In 1983 another ORNL group was charged by DOE's Synthetic Fuels Program to "justify the need to monitor specific unregulated substances and to provide threshold values above which these substances must be monitored" In response the group has developed a Rapid Screening of Hazard (RASH) methodology, usable by either experts or non-experts, for the scoring of relative hazard of unregulated substances. In a recent international workshop held to predict the carcinogenicity of chemical compounds using only short-term assay data and chemical structures, the RASH method was judged superior to methods developed by a dozen other research groups. Both ORNL Groups collaborated in the development of a site screening method being used by the Department of Defense to set remedial action priorities. These two groups frequently cooperate on risk assessment projects and both are called upon to provide regulatory agencies with guidance on the use of environmental risk data.

91-95 Funding (\$K): 5000 Dates: 1981-present



**Technology Transfer:** Books, Journal articles, PC-compatible ecological effects database, CRADA with a hazardous waste clean-up company, work with the National Toxicology Program

**Key Documentation:** Bartell, S. M., R. H. Gardner, and R.V. O'Neill. 1992. Ecological Risk Estimation. Lewis Publishers, Ann Arbor, Michigan, 252pp.  
 C. E. Easterly, T. D. Jones, L. R. Glass, B. A. Owen, and P. J. Walsh. "Biotesting Waste Water for Hazard Evaluation", Water Research 27(7):1145-1152(1993).

**Key Personnel:** Glen W. Suter, 615,574-7306,sutergw@ornl.gov, Robert V. O'Neill, 615-574-7846,oneillrv@ornl.gov, Annetta P. Watson, 615-576-2125,watsonap@ornl.gov, Troyie D. Jones, 615-574-6257, jonestd@ornl.gov

**Lab Capabilities Applied:** Ecological Risk Assessment, Theoretical Ecology, Ecotoxicology, Microbiology, Bioremediation, Statistics, Modeling, Analytical Chemistry



**Index:** 306

**Category:** Production (11, 16, 18, 23)

**Laboratory:** Oak Ridge National Laboratory      **Contact:** Peter Kearl

**Title:** Enhanced Recovery of Petroleum Using High-Power Microwaves

**Description:** The high-power microwave remediation program developed by California Applied Physics (CAP) in cooperation with Oak Ridge National laboratory (ORNL) has the potential to remove 99 plus percent of the DNAPL in the subsurface. Unlike conventional methods used by the Oil Industry and DOE, which rely on a hydrodynamic pathway to remove organic compounds, microwaves utilize an electromagnetic (EM) pathway which is dependent on reservoir heterogeneities of multiphase limitations. An antenna, capable of producing a directional beam, is lowered into a specially designed well. Electromagnetic energy is propagated into the subsurface where dielectric properties of the oil results in the enhanced heating, vaporization, and removal. It is important to note that this microwave technology is different than other EM approaches because it uses a high power and high frequency technology developed by the defense industry.

Another important facet of this microwave technology is the permeability enhancement observed in fine grained materials. Under controlled laboratory conditions, clay soils placed under the same energy density that will occur in the field, have shown a 4 orders of magnitude increase in permeability. The result is that microwaved clay has a permeability that is similar to dry coarse sand. This effect will greatly enhance the removal of oil from the fine grained reservoirs.

Using a 0.5 MW CW klystron tube that will be used in the field demonstration, a 6 meter radius can be cleaned. For full-scale field operations using a 2 MW system, the radius will increase to 25 to 30 meters. Modeling and laboratory measurements of the egress rate indicate that regions in the subsurface can be treated in minutes resulting in relatively low power consumption.

**91-95 Funding (\$K):** 2300      **Dates:** 1993-1995



**Technology Transfer:**

**Key Documentation:** Patent #5299887

**Key Personnel:** Peter Kearl, (303) 248-6211, PMK@ORNL.GOV, Nic Korte, (303) 248-6210, NEK@ORNL.GOV

**Lab Capabilities Applied:** Site characterization, modeling, petrology laboratory



Index: 307

**Category:** Environmental & Regulatory (7, 14), Oil Processing & Refining (8)

**Laboratory:** Oak Ridge National Laboratory      **Contact:** Russ Lee

**Title:** Estimating the Externalities of Fuel Cycles Associated with Electric Power Production

**Description:** This study, the most comprehensive of its kind, was jointly funded by DOE and the Commission of the European Communities. The study provides a scientific basis for environmental and other regulations. Its primary objective was to develop methods to estimate costs (and benefits) that are not reflected in market decisions, i.e. externalities. The study addressed those externalities on a life cycle or fuel cycle basis. The electric power fuel cycles include mining, transportation, power production and waste disposal. The fuel cycles addressed included the use of coal, biomass, oil, small hydropower, natural gas, and nuclear technologies to generate electric power. The major products of the study were a methodological framework and a set of analytical tools. The study emphasized that externalities were very site specific, depending on the design of the power plant, its location, and on extant regulation that may have some damages already reflected in the price of the power. Numerical examples in the study suggested some of the more important externalities. For example, for coal the more important externalities are health effects from particulate matter, except, where baseline concentration are very low; morbidity from exposure to ozone in areas already high in ozone concentration; crop damage from ozone; road damage if trucks are used for fuel transport; and injuries and fatalities from transportation accidents. For nuclear, the externalities include remediation costs from a severe accident, should one occur; expected effects to public health from releases of radioactive materials during transport; and occupational and public fatalities from exposure to radon from uranium mines. For oil and natural gas the primary externalities were health effects from ozone and particulate matter. Damages from oil spills are largely internalized.

**91-95 Funding (\$K):** 4000      **Dates:** 1990-1994



**Technology Transfer:** Publication of report, workshops and conferences, new releases

**Key Documentation:** Lee, R., (ORNL/Resources For the Future ) (1995) External Costs and Benefits of Fuel Cycles, 7 Volumes, Washington, DC: McGraw-Hill/Utility Data Institute.

**Key Personnel:** Randy Curlee, 615-574-5151, curleetr@ornl.gov; Clay Easterly, 615-574-6254, easterlyce@ornl.gov; Bob Perlack, 615-574-5186, perlackrd@ornl.gov; Carolyn Hunsaker, 615-574-7365, hunsakerct@ornl.gov

**Lab Capabilities Applied:** Life cycle analysis, economics and regulatory analysis, process engineering, modeling dispersion of pollutants, risk assessment, ecological analysis, epidemiological analysis.



Index: 308

**Category:** Oil Processing & Refining (20, 24, 28), Development (5, 18, 30), Environmental & Regulatory (4, 14)

**Laboratory:** Oak Ridge National Laboratory

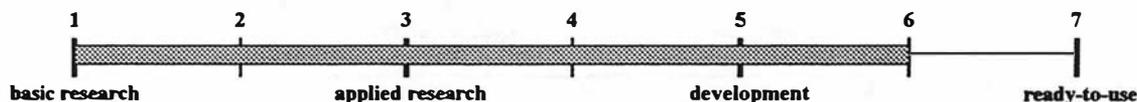
**Contact:** Scott A. McLuckey

**Title:** Advanced Mass Spectrometry for the Characterization and Quantitative Analysis of High Molecular Weight Materials

**Description:** The U.S. petroleum industry is placing increasing emphasis on quantitative and qualitative characterization of complex high boiling hydrocarbon mixtures. Mass spectrometry, a mainstay analytical technique in the petroleum industry, is typically used to characterize hydrocarbon mixtures. However, current techniques that work well for lower boiling fractions do not provide useful information from higher boiling fractions now being used as feedstocks. New mass spectrometric techniques for production and detection of ions from lower volatility (higher mass and/or polar) compounds are being developed in our laboratory. These techniques may lead to significant improvement in the ability to characterize these high molecular weight compounds. Work is being performed in the area of field ionization/field desorption, the technique currently used to ionize high boiling petroleum materials, to define and control critical parameters affecting long term precision of quantitative measurements. New ionization methods are also being developed to enhance the analysis of high molecular weight compounds, including novel electrospray ionization techniques for the selective ionization of targeted constituents (including high molecular weight aromatic hydrocarbons, geoporhins, and others), supersonic expansion cooling of analytes in conjunction with post-ionization for enhanced reproducibility in quantitative measurements, laser ionization of intractable materials in sludges and wastes, and others. Improvements in mass analyzers for detection and characterization of high mass materials are also being pursued using quadrupole ion trap, Fourier transform ion cyclotron resonance, and magnetic sector instruments. Applications of these techniques include low-volatility materials found in petroleum, geological, environmental and biological samples (including DNA and proteins with masses far in excess of 10,000 Daltons).

**91-95 Funding (\$K):** 3500

**Dates:** 1986-present

**Technology Maturity:**

**Technology Transfer:** Publications in open literature, presentations at technical conferences, training, 2 licensed products, current CRADA with automotive industry.

**Key Documentation:**

1. "Ion Trap Mass spectrometry of Externally Generated Ions", S.A. McLuckey, G.J. Van Berkel, D. E. Goeringer, and G.L. Glish, *Analytical Chemistry*, 1994, 66, 737A-743A.
2. "Fourier Transform Mass Spectrometry of High-Mass Biomolecules," M.V. Buchanan and R.L. Hettich, *Analytical Chemistry*, 1993, 65, 245A-259A.

**Key Personnel:** Scott A. McLuckey, (615)574-2848, mcluckey@ornl.gov  
Michelle V. Buchanan, (615)574-4868, buchananmv@ornl.gov  
Peter J. Todd, (615)574-2455, toddpj@ornl.gov

**Lab Capabilities Applied:** Mass Spectrometry, Advanced Instrumentation Development, Structural Characterization, Analytical Chemistry, Gas Phase Ion Chemistry, Biomolecule/Biopolymer Analysis, Environmental Analysis, Geochemistry, Fullerene Chemistry



**Index:** 309

**Category:** Oil Processing & Refining (17, 5, 15), Arctic Region Activities (4, 5, 6), Deepwater Offshore (4, 5, 7, 8)

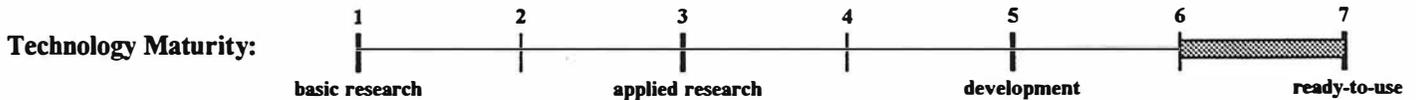
**Laboratory:** Oak Ridge National Laboratory      **Contact:** Randy K. Nanstad

**Title:** Heavy-Section Steel Technology and Irradiation Programs

**Description:** The petroleum industry utilizes various engineering materials for construction of components which are variously subjected to high temperatures, high pressures, and corrosive environments. Some of these high pressure components are constructed of thick-section steels, both ferritic and austenitic alloys. Various programs at ORNL have, over the years, investigated the behavior of materials for such applications, to include the development of improved alloys for fossil energy applications. The programs listed above have been the progenitor of many of the advances in the technology of engineering fracture mechanics, especially that associated with heavy-section pressure vessels and piping. Through the combined efforts of the Metals and Ceramics Division and the Engineering Technology Division, significant advances have been effected in the areas of experimental fracture mechanics, both on the laboratory and component scales, and analytical fracture mechanics. For example, elastic-plastic fracture mechanics is routinely used in laboratory experiments and in component analyses to predict the fracture behavior of thick-section vessels and piping.

Capabilities include facilities for the conduct of laboratory-scale fracture mechanics and fatigue crack-growth experiments (as well as other mechanical properties) from liquid nitrogen to 1500 C, facilities for testing of thick-section vessel and piping components, laboratories for welding and non-destructive testing, and world-class computational facilities for analytical and modeling studies.

**91-95 Funding (\$K):** 5000      **Dates:** 1967-present



**Technology Transfer:** DOE/Fossil Energy

**Key Documentation:**

**Key Personnel:** Randy K. Nanstad, (615) 574-4471, nkr@ornl.gov

**Lab Capabilities Applied:** Energy Production and End Use Technology, Advanced Materials



**Index:** 310

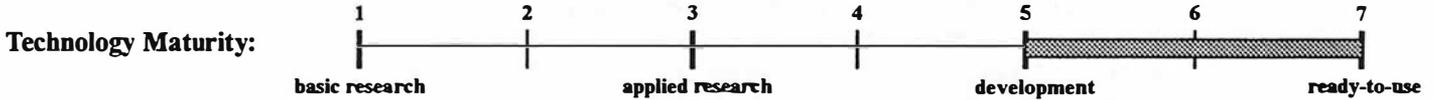
**Category:** Development (5, 7, 8, 9, 17, 23), Drilling & Completions (3), Production (25)

**Laboratory:** Oak Ridge National Laboratory      **Contact:** Bill Doll

**Title:** Borehole Geophysical Logging

**Description:** ORNL's borehole geophysical program has, over the last four years, been assigned three primary tasks:  
 1) identification of fractures or zones of water flow within the borehole for use in locating multipoint sampling intervals.  
 2) evaluation of well construction to support the design of plugging and abandonment plans, and cement bond log evaluation to aid in the selection of wells for plugging and abandonment.  
 3) evaluation of new monitoring well installations for compliance with construction design criteria, and cement bond quality evaluation to assure that the screened interval is isolated.

**91-95 Funding (\$K):** 975      **Dates:** 1991-present



**Technology Transfer:** Publications in open literature, interactions with logging contractors such as COLOG, MOUNT SOPRIS INSTRUMENT COMPANY, COMPROBE, OWL TECHNICAL ASSOCIATES.

**Key Documentation:** "Additional Borehole Geophysical Logging at WAG 1, Technical Memorandum 01-04, Oak Ridge National Laboratory, Remedial Investigation/Feasibility Study", ORNL/ER/Sub-87/99053/54, June 1992  
  
 "Multizone Well Installation at WAG 5 ORNL RI/FS Project Technical Bulletin 05-TB-033" Vol. I & Vol. II, ORNL/ER/Sub/87-99053/68, November 1994  
 "WAG 10 OU3 Phase I Well Evaluation Technical Bulletin", 10-TB-001, January 1995  
  
 "Site Characterization Summary Report for WAG 10 Wells at the Old Hydrofracture Facility at Oak Ridge National Laboratory, Oak Ridge, Tennessee", ORNL/ER/Sub/87-99053/78, March 1995

**Key Personnel:** R. K. Davis, (615) 574-4558, d1x@ornl.gov  
 R. O. Kennard, (615) 574-4558, aok@ornl.gov

**Lab Capabilities Applied:** Energy production, advanced computing, environmental science



**Index:** 311

**Category:** Exploration (7), Development (4, 5, 6, 14, 18, 21, 22, 23, 24, 28), Production (4, 5)

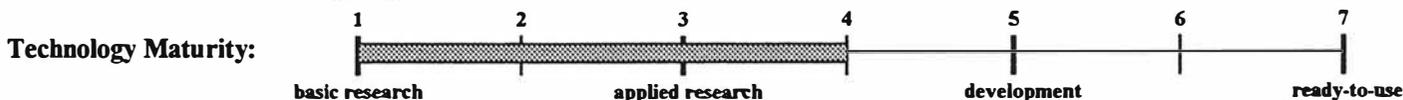
**Laboratory:** Oak Ridge National Laboratory      **Contact:** M. R. Guerin

**Title:** Experimental and Analytical Geochemistry

**Description:** A focussed effort is funded by DOE's Geoscience Research Program, Office of Basic Energy Sciences, to address fluid-rock interactions in the Earth's crust as related to hydrocarbon and geothermal energy resources, contaminant transport and remediation, and the sustainability and environmental impact of energy production. Currently, this project consists of six tasks: 1.) Ion Microprobe Studies of Diagenesis; 2.) Geochemistry of Geothermal Systems; 3.) Thermodynamic Properties of C-O-H-N Gases; 4.) Potentiometric Studies of Geochemical Processes; 5.) Fundamental Stable Isotope Exchange Reactions; and 6.) Mechanisms and Rates of Isotope Exchange Reactions. Also, a Laboratory-Directed R&D effort seeks to develop an ion microprobe specifically designed to obtain information related to fluid-rock interactions in hydrocarbon and geothermal reservoir rocks.

Of specific interest are: a.) Studies of the stable isotope signatures of fluid flow and sour-gas production in major oil fields, in collaboration with R. J. Pottorf of Exxon Production Research Co.; b.) examination of the time-temperature-hydrodynamic history of U.S. sedimentary basins; c.) detailed investigations of common reservoir minerals (solubility, dissolution kinetics, sorption) and fluids (pressure-volume-temperature relations of natural gases, metal speciation and pH-control in oil field brines, thermal stabilities of organics; d.) development of an organic ion microprobe applicable to kerogen maturation and enhanced oil recovery; e.) corrosion in production wells and fossil power plant steam cycles; and f.) environmental impacts of acid rain.

**91-95 Funding (\$K):** 1890      **Dates:** 1995-present



**Technology Transfer:** Direct interactions with oil company geologists and chemists. Numerous publications in the scientific literature.

**Key Documentation:**

**Key Personnel:** David J. Wesolowski, (615)574-6903, dqw@ornl.gov

**Lab Capabilities Applied:** Experimental Geochemistry, Analytical Chemistry, Reservoir Hydrogeochemistry, Organic Geochemistry, Instrumentation, Corrosion Processes



Index: 312

Category: Environmental &amp; Regulatory (5, 7, 8, 10, 14)

Laboratory: Oak Ridge National Laboratory

Contact: M. R. Guerin

Title: Applied Analytical Mass Spectrometry (Emissions/Process Monitoring, Field Instrumentation, Residuum/Product Characterization)

## Description:

A collection of projects are under way which seek to take advantage of advanced mass spectrometry technologies for rapid chemical analyses, the characterization of intractable materials, and continuous real-time monitoring. The most immediate applications to petroleum industry interests are for emissions monitoring and environmental analyses. Applications to feedstock and product characterization, process monitoring, and exploration are very likely. A unique aspect of the program is its focus on trapped ion mass spectrometry: quadrupole ion trap (ITMS) and Fourier transform mass spectrometry (FTMS). Other forms of mass spectrometry are in use for the measurement of metals and of surface constituents.

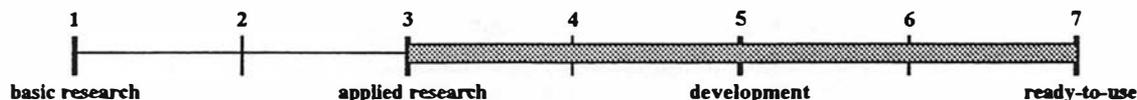
Direct Sampling Ion Trap Mass Spectrometry (DSITMS) instrumentation developed as part of this program has been shown to be especially promising for the rapid measurement and/or continuous monitoring of petroleum hydrocarbons in air, water, and soil. Discrete samples can be analyzed for volatile organic chemicals (VOC's) to USEPA specifications in three minutes or less. VOC's can be monitored continuously in aqueous and air streams at concentrations as low as 50 ppb with the promise of a 10-100 fold increase in sensitivity being possible. Both laboratory-based and field-transportable instrumentation are available. Field instruments have been demonstrated at several sites for rapid analyses of groundwater, groundwater well headspace, and soil. Laboratory instruments have been successfully used to rapidly fingerprint petroleum crude oils. Methods for semivolatile organics are currently being developed. The instrumentation is being commercialized through an ARPA-TRP led by Teledyne Electronics and involving Phillips Petroleum and Monsanto as major industrial partners. Air emissions and process monitoring are receiving particular attention.

91-95 Funding (\$K):

3500

Dates: 1991-present

Technology Maturity:



Technology Transfer:

Licensed DSITM inlet system, ARPA-TRP Cooperative Agreement, Cooperative Demonstrations and Testing, Publications and Presentations, Training and Support

Key Documentation:

- 1) Thompson, C.V., and Wise, M.B., "Sample Introducing Apparatus and Sample Modules for Mass Spectrometer," Patent No. 5,272,337, December 21, 1993.
- 2) Wise, M.B., Thompson, C.V., Buchanan, M.V., Merriweather, R., and Guerin, M.R., "Direct Sampling Ion Trap Mass Spectrometry," Spectroscopy, 8(5) 14-22 (1993).

Key Personnel:

Marcus B. Wise, 615-574-4867, wisemb@ornl.gov  
 Scott A. McLuckey, 615-574-2848, mcluckeysa@ornl.gov  
 Cyril V. Thompson, 615-574-4861, thompsoncv@ornl.gov  
 Michelle V. Buchanan, 615-574-4868, buchananmv@ornl.gov

Lab Capabilities Applied:

Analytical Instrumentation, Analytical Methods, Mass Spectrometry, Chemistry, Software and Computing, Environmental Sampling, Statistics, Field Studies



Index: 313

Category: Gas Processing (4), Oil Processing & Refining (16, 17, 2, 6, 23)

Laboratory: Oak Ridge National Laboratory      Contact: J. R. Keiser

Title: High Pressure Heat Exchange System - Advanced Materials for Steam-Methane Reforming

Description: The conversion efficiency of steam-methane reformers could be improved by operating at higher temperatures. In order to achieve operating temperatures several hundred degrees higher than currently achievable with metal tubes, the use of ceramic tubes is being investigated. We are providing technical assistance to Stone & Webster Engineering Corporation in that we are conducting experiments to assess the compatibility of various ceramic materials in the relevant environments. The results of our studies will be data on the oxidation rates, extent of strength degradation, and microstructural changes that occur as a result of exposure of ceramics to steam-hydrogen-carbon monoxide-carbon atmospheres at 13.6 atmospheres pressure.

91-95 Funding (SK): 1600      Dates: 1991-1995

1	2	3	4	5	6	7
basic research	applied research		development		ready-to-use	

Technology Transfer: Open literature publications, letter reports, staff exchanges

Key Documentation: CORROSION/93 paper 93-239

Key Personnel: J. R. Keiser, 615-574-4453, keiserjr@ornl.gov

Lab Capabilities Applied: Utilizing high temperature furnaces that are equipped with system for supplying high pressure steam and mixed gases to experiment.



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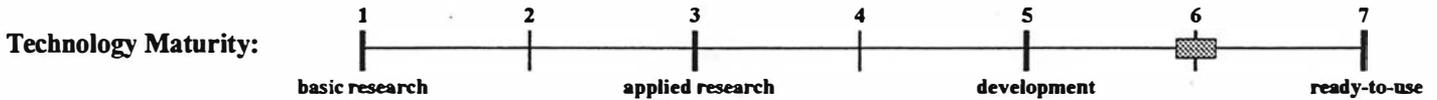
Category: Environmental & Regulatory (5, 6)

Laboratory: Pacific Northwest Laboratory      Contact: Brian Shaw, 509-372-6157, BR\_SHAW@PNL.GOV

Title: The Effects of the Exxon Valdez Oil Spill on Pacific Herring

Description: Based on previous research involving herring, MSL scientists developed a combination of field, laboratory, and analysis tasks to address the occurrence and extent of injury to the herring resource in the Sound. These tasks were structured by the time course of reproductive and other life history events. First, field surveys were performed to assess injury to prespawning adult herring through histopathological examination and chemical analysis of the herring roe for petroleum hydrocarbons. Second, eggs fertilized in the field and eggs-on-kelp were incubated in the laboratory to measure the viability of eggs from herring captured in Prince William Sound. Third, the hatching success and frequency of abnormal larvae for herring spawn drawn from control and assessed areas were determined through examination and statistical analysis. The results of these field and laboratory studies are presently being used to estimate damages to the herring fishery through the use of resource valuation models. Battelle also compiled fishery statistics, reviewed age-structure models for herring populations, and analyzed oceanographic data in relation to herring population dynamics.

91-95 Funding (\$K): 3500      Dates: 1991 - Present



Technology Transfer: Private contract

Key Documentation: Pearson, WH, E Moksness, and JR Skalski. 1994. "A Field and Laboratory assessment of Oil Spill Effects on Survival and Reproduction of Pacific Herring (*Clupea harengus pallasi*). IN: Proceedings of the Third Symposium on Environmental Toxicology and Risk Assessment, ASTM Special Technical Publication STP. American Society for Testing and Materials, Philadelphia. In Press.

Key Personnel: RM Ecker, 360-683-4151, RM\_ECKER@PNL.GOV; WH Pearson, 360-681-3610, WH\_PEARSON@PNL.GOV; JQ Word, Jr., 360-681-3668, JQ\_WORD@PNL.GOV; EA Crecelius, 360-681-3604, EA\_CRECELIUS@PNL.GOV

Lab Capabilities Applied: Live animal toxicology



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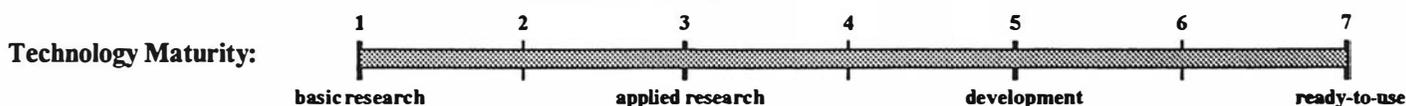
Category: Environmental & Regulatory (4, 5)

Laboratory: Pacific Northwest Laboratory      Contact: Brian Shaw, 509-372-6157, BR\_SHAW@PNL.GOV

Title: Effects of Petroleum Products on Bull Kelp; Perform Field Assessment of Possible Damages to Eelgrass in Faadalgo Bay, WA; Investiagte Effects of Oil on Kelp Nereocystis Leutkeana; Analyses Using Seimpermeable Membrane Devices

Description: DNR initiated this study to investigate the effects of the Tenyo Maru oil spill on kelp as part of the assessment of damage to these resources. The study consisted of investigating, in experimental tanks, the effects of weathered and unweathered crude oil, bunker-C, intremediate fuel oil (IFO), and diesel fuel on kelp tissue health, gorwth rate, and photosynthesis. Based on photosynthetic rate studies, whole-plant experiments, and blade growth-rate measurements, the relative ranking of petroleum-treatment effects to kelp were weathered diesel>unweathered IFO>unweathered diesel>weathered IFO>unweathered crude>weathered crude. This study was the first of its kind to demonstrate effects of these types of petroleum products on kelp. Three study sites were selected within Fidalgo Bay. One site received oil, one site was not oiled (reference site), and one site was not oiled, but may have been affected by skimmer activity. All three sites contained eelgrass. Transects were set up within each area, and density measurements made at 10 meter intervals using a 0.25 m2 quadrat. The transect lines were surveyed at low tide, which was from 7 p.m. - 1 a.m. in December, 1991. Impacts to the eelgrass were inferred following a statistical analysis of the density and percent cover data taken along the transects. The key issue investigated was the effect of various product type and level of weathering on the survival and productivity of kelp. There was no industry involvement, other than ARCO supplied crude oil used in the experiments. The results showed that weathered diesel was most toxic. There was a final report. These results changed the way the state assessed damages from spills. The purpose of this work was to provide Chevron with a scientifically sound, yet fast and inexpensive testing, to estimate the potential for bioaccumulation of oil additives in aquatic life. Semipermeable membrane devices (SPMDs) similar to those that have been developed by the United States Fish and Wildlife Service will be used for this work because they function as "model fish" with selective membranes and lipid reservoirs that can concentrate organic compounds from water.

91-95 Funding (\$K): 201      Dates: 1991 to present



Technology Transfer: Private contract. The results were published in "Marine Biology." NRDA analysis pursuant to CERCLA; report submitted to Texaco,, Anacortes, WA. Work probably proprietary since it involves damage assessment by Wash St Natural Resource Trustees.

Key Documentation: Antrim, LD, RM Thom, WW Gardiner, VI Cullinan, DK Shreffler, and R.W. Bienert. 1994. "Effects of Petroleum Products on Bull Kelp (Nereocystis leutkeana P.et R)." Marine Biology (in press). Report to Texaco Inc, Anacortes, WA.

Key Personnel: RM Ecker, 360-683-4151, RM\_ECKER@PNL.GOV; WH Pearson, 360-681-3610, WH\_PEARSON@PNL.GOV; JQ Word, Jr., 360-681-3668, JQ\_WORD@PNL.GOV; EA Crecelius, 360-681-3604, EA\_CRECELIUS@PNL.GOV; RM Thom, 360-681-3657, RM\_THOM@PNL.GOV; RC Phillips, 509-372-3691.

Lab Capabilities Applied: Large flaming seawater systems with state of the art treatment system was essential to this project. Paper Study, Report, Computer Model (designed by CA Brandt). Trace contaminant analysis, semipermeable membrane devices.



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Category: Environmental & Regulatory (7, 8)

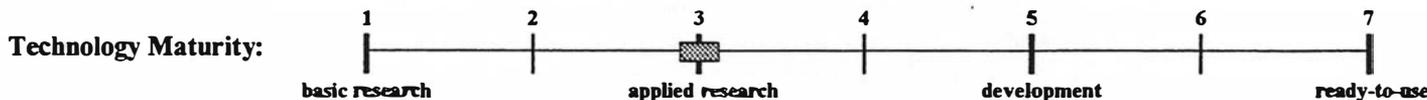
Laboratory: Pacific Northwest Laboratory

Contact: Brian Shaw, 509-372-6157,  
BR\_SHAW@PNL.GOV

Title: Low-Temperature Catalytic Gasification of Wet Wastes

**Description:** The goal of this cooperative research project is to facilitate the commercialization of Thermochemical Environmental Energy System (TEES) through the operation of an Industrial Onsite Demonstration Unit at the plants of potential customers and the continued laboratory development of catalyst systems. TEES is a high-pressure, aqueous--phase, catalytic process which recovers organics from wastewater, slops, or wet sludge as a med-Btu fuel gas. The project requires a two-pronged effort of onsite testing managed by Onsite\*Ofsite and laboratory support at PNL. The Industrial Onsite Demonstration Unit was built based on designs from PNL bench-scale processing systems. It is a DOE resource being used within the CRADA as part of the DOE contribution. The balance of the DOE contribution is the laboratory support provided to the onsite demonstrations including preliminary feedstock analysis and testing, onsite startup support, and specialized analytical and problem-solving support during the demonstrations. In addition, a catalyst development research program continues at PNL to improve the TEES catalyst and to prove the extended lifetime of the catalyst through the use of high-pressure processing systems and specialized analytical equipment in the laboratory. For their part, Onsite\*Ofsite is responsible to market TEES, to make arrangements to fund the onsite demonstrations, and to manage the onsite operations. The expected outcome of the research is the commercialization of an innovative wet waste treatment process which eliminates solid and chemical waste and efficiently recovers otherwise wasted energy.

91-95 Funding (\$K): 1905      Dates: 1994 - Present



Technology Transfer: Publication

Key Documentation: CRADA and license with Onsite\*Ofsite

Key Personnel: DC Elliott, 509-375-2248, DC\_ELLIOTT@CCMAIL.PNL.GOV

Lab Capabilities Applied: Hydrothermal processing



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Category: Environmental & Regulatory

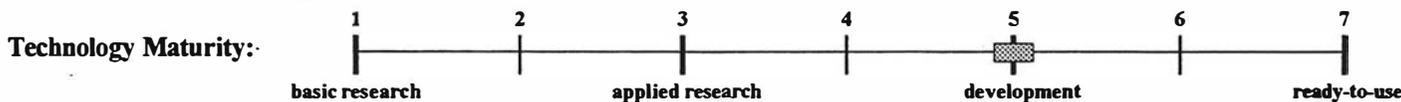
Laboratory: Pacific Northwest Laboratory

Contact: Brian Shaw, 509-372-6157, BR\_SHAW@PNL.GOV

Title: Investigation of Self-Help Oil-Spill Response Techniques and Equipment and Effects of Petroleum Contaminated Waterways on the Spawning Migration of Pacific Salmon

Description: This study considered the hypothetical outflow of oil in the case of side damage and bottom damage to single-hull designs. The results were considered by the Coast Guard in drafting regulations pertaining to the requirement for tanker vessels to carry oil pollution response equipment (i.e., in response to the Oil Pollution Act of 1990). Based on the findings of this investigation, it was recommended that research pertaining to onboard self-help countermeasures focus on the pumping-containment category of concepts. Other recommendations included further developing the model used in this study to obtain more realistic oil outflow times, especially in the case of grounding; combining the simulation models used in this study into one global model; and making a more in-depth investigation of the environmental data. The purpose of the salmon study was to determine how petroleum contamination might impair chemoreception and migratory behaviors in salmon. Laboratory experiments determined the chemosensory detection threshold for oil and the effects of oil exposure on detection of biologically relevant cues.

91-95 Funding (\$K): 173 Dates: 1991 - Present



Technology Transfer: Publications

Key Documentation: Enderlin, WI, JP Downing, CW Enderlin, TF Sanquist, and WS Pope. 1992. "Investigation of Self-Help Oil-Spill Response Techniques and Equipment." Prepared for U. S. Department of Transportation, U.S. Coast Guard. Pacific Northwest Laboratory, Richland, WA. PNL-8096; Pearson, WH, DL Woodruff, and PB Johnson. 1990. Effects of Petroleum Contaminated Waterways on Spawning Migration of Pacific Salmon. Phase I. Laboratory Studies. OCSEAP Final Rep 66:203-279. Prepared for U.S. Department of Commerce, NOAA, by Battelle/Marine Sciences Laboratory, Sequim, Washington and Battelle, Pacific Northwest Laboratories, Richland, Washington

Key Personnel: RM Ecker, 360-683-4151, RM\_ECKER@PNL.GOV; WH Pearson, 360-681-3610, WH\_PEARSON@PNL.GOV; JQ Word, Jr., 360-681-3668, JQ\_WORD@PNL.GOV; EA Crecelius, 360-681-3604, EA\_CRECELIUS@PNL.GOV

Lab Capabilities Applied:



Index: 318

Category: Oil Processing & Refining (11)

Laboratory: Pacific Northwest Laboratory

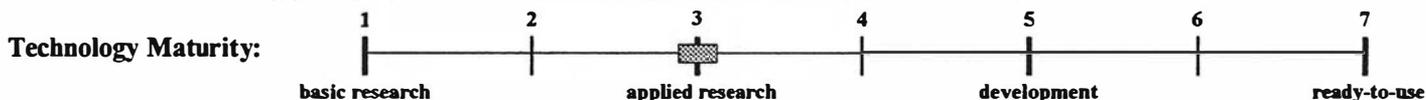
Contact: Brian Shaw, 509-372-6157,  
BR\_SHAW@PNL.GOV

Title: Catalytic Hydrotreating of Biomass Pyrolysis Oils

Description: The goal of this research project is to develop methods for hydrotreating biomass fast pyrolysis oils to produce clean, stable hydrocarbons which are useful as turbine fuels or as refinery blending stock. The research is an extension of an earlier 7-year program of process development within DOE's Biofuels Program for production of gasoline from biomass. The current emphasis of the research is on low-severity processing to reduce costs while producing less-refined products. Batch and continuous-feed bench-scale reactors are used in the research. Adaptation of existing hydrotreating technology, both conditions and catalysts, is being undertaken to accomplish the goal. Collaboration with European biomass oil hydrotreating researchers has been a continual effort beginning in 1986.

91-95 Funding (\$K): 160

Dates: 1994 - Present



Technology Transfer: Publications

Key Documentation:

Key Personnel: DC Elliott, 509-375-2248, DC\_ELLIOTT@CC:MAIL.PNL.GOV

Lab Capabilities Applied: Catalysis, thermal processing



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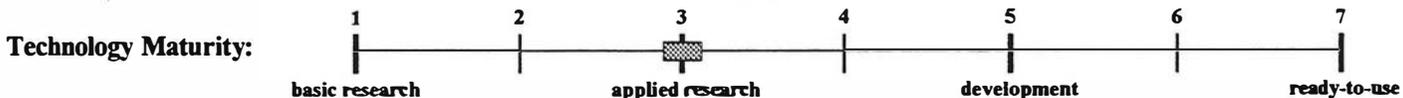
Category: Oil Processing & Refining (11)

Laboratory: Pacific Northwest Laboratory      Contact: Brian Shaw, 509-372-6157, BR\_SHAW@PNL.GOV

Title: Nanophase Catalyst Synthesis and Reaction Mechanisms

**Description:** The goal of this program is two-fold. First, new synthetic mehtods of nanophase catalyst production at industrially useful rates are being developed. The successful methods developed at PNL include Rapid Expansion of Supercritical Solutions (RESS) (US Patent), Rapid Thermal Decomposition of precursors in Solutions (RTDS) (US Patent pending), and Modified Reverse Micelles (MRM) (US Patent pending). These unique methods allow production of nanocrystalline metal oxides, metal sulfides, metals, and mixed systems at rates of up to 1 lb/h per unit. These nanophase materials have been demonstrated as exceptional hydrocracking catalysts and have shown promise for other catalytic applications as well as for the production of advanced materials. The second goal is the understanding of the reaction mechanisms which are applicable to these nanophase catalysts and for reactions under extreme conditions can lead to better, more economic methods of fuel and chemical processing from natural materials as well as from recycled materials. This program has developed unique high pressure, high temperature analytical capabilities with in situ RAMAN, IR and NMR observation of reaction under supercritical conditions. In total, these programs have developed new techniques and methods for the production of nanocrystalline materials and studies of reactions under extreme conditions. These advances may lead to more cost effective processes for fuel and chemical production.

91-95 Funding (\$K): 1585      Dates: 1994 - Present



Technology Transfer: Publications

Key Documentation:

Key Personnel: JC Linehan, 509-375-3983, JC\_LINEHAN@PNL.GOV

Lab Capabilities Applied: Materials Synthesis



Index: 320

Category: Environmental & Regulatory (9, 10)

Laboratory: Pacific Northwest Laboratory

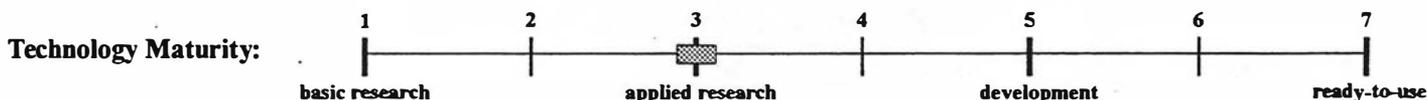
Contact: Brian Shaw, 509-372-6157,  
BR\_SHAW@PNL.GOV

Title: Conduct Literature Review on Polychlorinated Biphenyl (PCB) Sorption from Gas Line Condensates into Soils

Description: The focus of this research was to determine how PCB congeners introduced into natural soil-water systems in an immiscible condensate phase migrate through soils and subsoils at condensate spill sites. Volatilization of the PCB and condensate was not considered in this research. Partitioning of PCB between the condensate-soil-water system was investigated as was the movement of PCB-condensate and dissolved aqueous PCB plumes.

91-95 Funding (\$K): 106

Dates: 1990 - 1993



Technology Transfer: Open literature publications, syposiums, and exchange between staff (PNL and Weston, Inc.)

Key Documentation: Only a year end progress report exists for this research

Key Personnel: CC Ainsworth, 509-375-2670, CC\_AINSWORTH@PNL.GOV

Lab Capabilities Applied: Radiotracers, solubility determinations, determination of liquid (condensate) physical characteristics, multiphase, subsurface-transport simulator STOMP (i.e., subsurface transport over multiple phases)



**Index:** 321

**Category:** Environmental & Regulatory (4, 5)

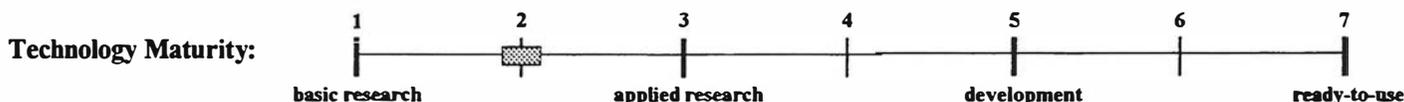
**Laboratory:** Pacific Northwest Laboratory      **Contact:** Brian Shaw, 509-372-6157, BR\_SHAW@PNL.GOV

**Title:** Predicting TPH Biodegradation & Leaching in Contam. Soils Using State-of-the-Art Hydrocarbon Charact. Evaluate Chem. & Phys.Properties in Solids, Water, & Oil Samples Great Lakes; Evaluate Environmental Monitoring Program for Legovan Amuay Oil Refinery

**Description:** The objective of this R&D effort is to develop a methodology for predicting the biodegradation and leaching potential of TPH (total petroleum hydrocarbon) contaminated soils. Since the extent of TPH biodegradation is strongly influenced by the hydrocarbon type composition of the soil contaminant (e.g., diesel fuel contains a larger fraction of biodegradable hydrocarbon types than heavy crude oil), it should be possible to predict the TPH biodegradation potential if the molecular composition of the spilled petroleum source is known. Initial and residual TPH extracts are subjected to a state-of-the-art hydrocarbon characterization procedure involving group type separation, boiling point distribution, and field desorption mass spectroscopy (FDMS). The overall extent of TPH biodegradation is correlated to the hydrocarbon type composition of the initial TPH. This information is subsequently used to develop a predictive model for estimating the bioremediation potential of hydrocarbon contaminated soils.

The objective of the Toxicity and Chemistry Work Group was to assess the current nature and extent of contaminated sediment problems by studying the chemical, physical, and biological characteristics of contaminated sediments and their biotic communities, and to demonstrate cost-effective assessment techniques at the priority consideration areas that can be used at Marine Sciences Laboratory (MSL) project was to assess chemical contamination of sediments, pore waters, sediment elutriates, and tissues at selected U.S. Great Lakes AOC. It was the objective of this study to evaluate and analyze the design and sampling procedures of Lagoven's monitoring program and to determine their adequacy to detect impacts in chemical and biological systems of Amuay Bay. This was accomplished by a site visit to Lagoven's oil refinery and coking plant in late January 1990, and by subsequent review and evaluation of sampling and analytical protocols, as well as data generated during environmental surveys conducted by Lagoven and others.

**91-95 Funding (SK):** 117      **Dates:** 1991 - Present



**Technology Transfer:** Technical Reports

**Key Documentation:** Crecelius, E., B. Lasorsa, L. Lefkowitz, P. Landrum, and B. Barrick, 1994, "Chemical Analysis." In Assessment and Remediation of Contaminated Sediments (ARCS) Program. Assessment Guidance Document, pp. 69-85. Great Lakes National Program Office, U.S. Environmental Protection Agency, Chicago, Illinois. Cullinan, V. I., E. A. Crecelius, and J. A. Strand, 1991. Evaluation of Lagoven, S. A. Refinery Environmental Monitoring Program of Amuay Bay, Venezuela. Prepared for Bariven Corporation by Pacific Northwest Laboratories, Battelle Marine Sciences Laboratory.

**Key Personnel:** MH Huesemann, 509-373-2261, MH\_HUESEMANN@PNL.GOV; EA Crecelius, 360-681-3604, EA\_CRECELIUS@PNL.GOV

**Lab Capabilities Applied:** Trace contaminant analysis; Fate and effects of contaminants on the marine environment



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Category: Oil Processing & Refining (7)

Laboratory: Pacific Northwest Laboratory

Contact: Brian Shaw, 509-372-6157,  
BR\_SHAW@PNL.GOV

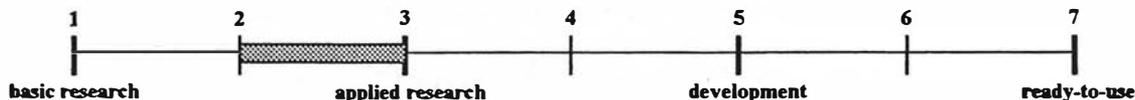
Title: Superacidic Solid Acid Catalysts

**Description:** This research program is aimed at developing solid superacidic catalysts based upon a comprehensive, molecular-level understanding of acidic materials. In particular, we are studying the synthetic variables which increase the acidity of inorganic metal oxide materials, characterizing the resulting physicochemical properties, and measuring the performance of these catalysts under realistic conditions. Catalyst optimization is being guided through an understanding of dissimilar acid sites; including strength, distribution, number, and type, as well as their relationship to catalytic performance using model isomerization and alkylation reactions. In addition, regeneration of deactivated catalysts is a subject of study with emphasis on the restoration of activity and selectivity without any detrimental changes in the physical properties of the catalyst. Pacific Northwest Laboratory is utilizing a state of the art catalyst characterization system and laboratory scale reactors, while Unocal is providing technical guidance, extrudate studies, and further catalyst testing using realistic feeds at the pilot or advanced bench scale. Washington State University is also providing additional characterization and analytical studies. The expected outcome of this project is the development of commercially applicable solid superacid catalytic materials which can replace corrosive liquid acid catalysts used in the petroleum and petrochemical industries.

91-95 Funding (\$K): 680

Dates: 1994 - Present

Technology Maturity:



Technology Transfer: Publications

Key Documentation:

Key Personnel: TD Brewer, 509-375-4552, TD\_BREWER@PNL.GOV

Lab Capabilities Applied: Separations and hydrothermal processing



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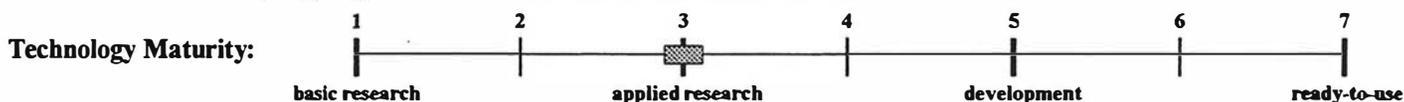
Category: Environmental & Regulatory (5)

Laboratory: Pacific Northwest Laboratory      Contact: Brian Shaw, 509-372-6157,  
BR\_SHAW@PNL.GOV

Title: U. S. Coast Guard Human Factors Engineering

Description: Task order contract to investigate human factors issues in commercial shipping. Tasks to date have included studies of vessel manning patterns and crew fatigue, research to support the development of an automated training simulator to examine deck watch officers on their knowledge of Rules of the Road, and the effects of watch keeping schedules on crew safety and performance.

91-95 Funding (\$K): 3943      Dates: 1994 - 1999



Technology Transfer: Reports to the client, publications in open literature, staffing model prototype (software)

Key Documentation: Task Reports

Key Personnel: TF Sanquist, 206-528-3240; JD Lee, 206-528-3227; A Bittner, 206-528-3263; J Morgan, 206-528-3225

Lab Capabilities Applied: Staff expertise in human factors and software development



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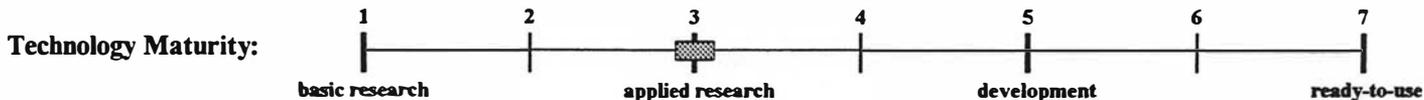
Category: Environmental & Regulatory (4, 6, 7, 12); Oil Processing & Refining

Laboratory: Pacific Northwest Laboratory      Contact: Brian Shaw, 509-372-6157, BR\_SHAW@PNL.GOV

Title: Petroleum Sludge Treatment; Spent Catalyst Processing

**Description:** Petroleum refineries in the United States must dispose of over 850,000 tons of petroleum oil-in-water emulsions each year. Battelle, Pacific Northwest Laboratory's new treatment process could reduce the original amount of waste requiring disposal by as much as 95% at a cost that is 10% of the cost of incineration. The Petroleum Sludge Treatment (PST) Process separates highly stable emulsified petroleum wastes into oil, water, and solids. The oil is recovered and returned to the refinery for processing, and the water is suitable for discharge to the refinery wastewater treating plant or to a publicly owned treatment plant, leaving a greatly reduced volume of solids for disposal. The process has been successfully demonstrated in a bench scale, batch separator. The CRADA with SunPro calls for a continuous flow, small-pilot separator to be built and demonstrated over the next two years. The purpose of this project is to demonstrate PNL's Petroleum Sludge Treatment Process (PST) in a continuous prototype unit. Upon successful demonstration, the CRADA partner, Sunpro, Inc., seeks to commercialize PST through a licensing arrangement. A modest PST unit serving one average oil refinery would benefit the user by recovering an additional 20,000 barrels of oil per year and avoiding more expensive waste treatment options for about 25,000 tons per year of sludge. The economic benefit to the end user could easily be in excess of \$1 million/yr per unit. The purpose of this project at Phillips Petroleum and Pacific Northwest Laboratory (PNL) is to develop a novel approach for separating metals from spent catalyst. Deposition of metals on petroleum resid upgrading catalysts limits the economic life of these catalysts. Also, increasing concern for pollution prevention and waste disposal creates a need for clean alternatives for spent catalyst recovery or disposal. The Battelle technology developed at PNL uses electrochemistry to remove carbon, hydrocarbons, metal sulfides and/or metal oxides adhered to spent catalyst. The metal sulfides are converted to aqueous metal ions and sulfate. The metal constituents are then separated and recovered. Major advantages of the technology include operation at low temperature (less than 200F) operation, no emissions of hydrocarbons, SOx, or NOx, and favorable kinetics. The extraction and electrochemical steps are clean and contain catalyst contaminants in manageable product streams.

91-95 Funding (\$K): 1100      Dates: 1995 - Present



Technology Transfer: Publications

Key Documentation: U. S. Patents 4,971,703 and 5,100,559. A CRADA with Sunpro is currently being negotiated. PNL CRADA No. 38 with Phillips Petroleum. A U.S. Patent is pending.

Key Personnel: EG Baker, 509-376-1494, EG\_BAKER@PNL.GOV; LJ Silva, 509-372-4590, LJ\_SILVA@PNL.GOV; DC Elliott, 509-375-2248, DC\_ELLIOTT@PNL.GOV

Lab Capabilities Applied: Separations and hydrothermal processing; Hydrothermal processes, PST; Experience in catalysis and heavy oil processing, electrochemistry, and advanced separations



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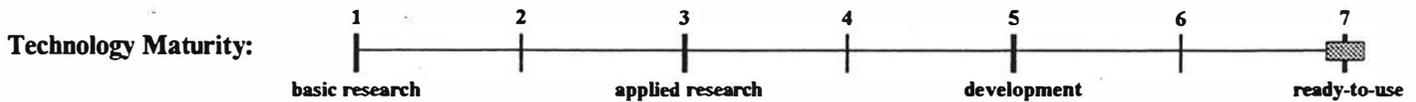
Category: Environmental & Regulatory (5, 6)

Laboratory: Pacific Northwest Laboratory      Contact: Brian Shaw, 509-372-6157, BR\_SHAW@PNL.GOV

Title: Toxicological Monitoring of Ballast-Water Effluent Discharge

Description: A program for toxicity testing with Alyeska's effluent was expanded beyond permit requirements to provide data during periods when specified test organisms were not available. A suite of alternative test species were selected from laboratory-cultured organisms for which standard protocols have been published. Native and commercially-important species were tested simultaneously with laboratory-cultured species to assess if alternate species would be comparable indicators of effluent toxicity. If so, a toxicity testing program could be designed with scheduling flexibility and no restrictions based on seasonal availability of test organisms. Correlations were made in the sensitivity of native, commercially-important and alternative test species to Alyeska's effluent. When test results in 1990 and 1991 were compiled, a substantial data base was available for assessment of numerous issues, including sensitivity of 8 test species to Alyeska's effluent, seasonal availability of native species for toxicity testing, and temporal and seasonal variability in effluent toxicity. This data is being used to design a site-specific testing program for effluent toxicity monitoring.

91-95 Funding (\$K): 300      Dates: 1991 - 1992



Technology Transfer:

Key Documentation: Antrim, LD, JQ Word. 1991. Toxicity Testing in Support of Acute and Chronic "Water Quality Criteria" for Balast-Water Effluent. Prepared for Alyeska Pipeline Service company, Anchorage, Alaska, by Battelle/marine Sciences Laboratory, Sequim, Washington.

Key Personnel: RM Ecker, 360-683-4151, RM\_ECKER@PNL.GOV; WH Pearson, 360-681-3610, WH\_PEARSON@PNL.GOV; JQ Word, Jr., 360-681-3668, JQ\_WORD@PNL.GOV; EA Crecelius, 360-681-3604, EA\_CRECELIUS@PNL.GOV

Lab Capabilities Applied:



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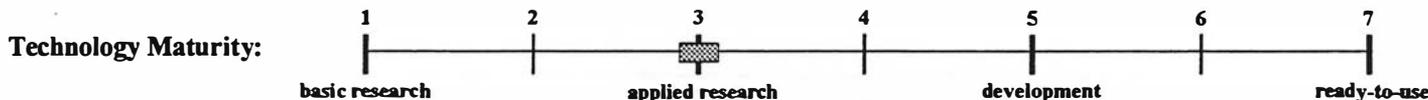
Category: Environmental & Regulatory (4, 5)

Laboratory: Pacific Northwest Laboratory Contact: Brian Shaw, 509-372-6157, BR\_SHAW@PNL.GOV

Title: Perform Field Assess of Possible Damage to Eelgrass in Fidalgo Bay, WA During Oil Spill Cleanup, Investigate Effects of Oil on Kelp Nereocystis Luetkeana, Conduct Analyses Using SPMD to Estimate Bioconcentration Potential of Oil Additives in Aquatic Life

Description: Three study sites were selected within Fidalgo Bay. One site received oil, one site was not oiled (reference site), and one site was not oil, but may have been affected by skimmer activity. All three sites contained eelgrass. Transects were set up within each area, and density measurements made at 10 meter intervals using a 0.25 m2 quadrat. The transect lines were surveyed at low tide, which was from 7 p.m. - 1 a.m. in December, 1991. Impacts to the eelgrass were inferred following a statistical analysis of the density and percent cover data taken along the transects. The key issue in the kelp investigation was the effect of various product type and level of weathering on the survival and productivity of kelp. There was no industry involvement, other than ARCO supplied crude oil used in the experiments. The results showed that weathered diesel was most toxic. There was a final report. These results changed the way the state assessed damages from spills. The purpose of the analyses to estimate the bioconcentration potential of oil additives in aquatic life was to provide Chevron with a scientifically sound, yet fast and inexpensive testing, to estimate the potential for bioaccumulation of oil additives in aquatic life. Semipermeable membrane devices (SPMDs) similar to those that have been developed by the United States Fish and Wildlife Service will be used for this work because they function as "model fish" with selective membranes and lipid reservoirs that can concentrate organic compounds from water.

91-95 Funding (\$K): 152 Dates: 1991 - Present



Technology Transfer: NRDA analysis pursuant to CERCLA; report submitted to Texaco, Inc., Anacortes, WA. (Proprietary). The results of the kelp study were published in the "Marine Biology" journal and presented at 2 professional meetings.

Key Documentation: Report to Texaco, Inc., Anacortes, WA.

Key Personnel: RC Phillips, 509-372-2691, RC\_PHILLIPS@PNL.GOV; RM Thom, 360-681-3657, RM\_THOM@PNL.GOV; EA Crecelius, 360-681-3604, EA\_CRECELIUS@PNL.GOV

Lab Capabilities Applied: Paper Study, Report, Computer Model (designed by CA Brandt); large flaming seawater systems with state of the art treatment system was essential to the kelp project; trace contaminant analysis, semipermeable membrane devices.



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Category: Environmental & Regulatory (5, 6)

Laboratory: Pacific Northwest Laboratory

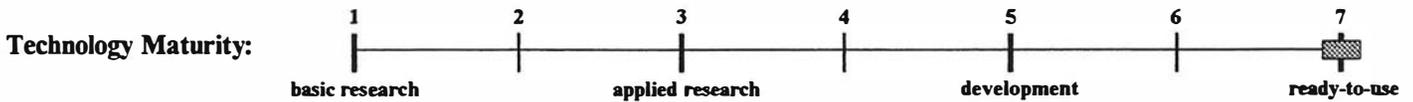
Contact: Brian Shaw, 509-372-6157, BR\_SHAW@PNL.GOV

Title: Conduct Histopathological Evaluation and Body Burden Analysis of Alaska Salmon Potentially Affected by the Exxon Valdez Oil Spill

Description: Evaluate tissues of marine fish (herring and salmon) for evidence of damage resulting from oil exposure. Measure and evaluate numerical indices of salmon and herring condition and health from oil exposed and non-exposed fish.

91-95 Funding (\$K): 100

Dates: 1991



Technology Transfer: Publications in open literature

Key Documentation:

Key Personnel: RA Elston, 360-683-4151, RA\_ELSTON@PNL.GOV

Lab Capabilities Applied: Histopathology laboratory, pathology, necropsy laboratory



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Category: Environmental & Regulatory (5, 6)

Laboratory: Pacific Northwest Laboratory

Contact: Brian Shaw, 509-372-6157,  
BR\_SHAW@PNL.GOV

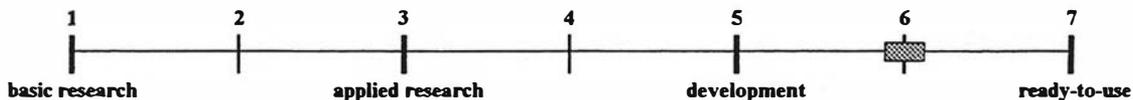
Title: Alyeska Sediment Studies

**Description:** The first phase of the Alyeska Sediment Program involved choosing candidate organisms for use in toxicity testing and evaluating their response to the fine-grained sediments which predominate in Port Valdez. Species showing promise as monitoring organisms were then evaluated for sensitivity to Alaska North Slope crude oil through a series of spiked sediment tests during Phase 2 of the study. ANS crude oil was chosen as it was the most likely contaminant that would influence sediment quality in Port Valdez. Organisms showing sensitivity to the crude oil were then incorporated into a long-term monitoring study of Port Valdez sediment quality.

91-95 Funding (\$K): 250

Dates: 1991 - Present

Technology Maturity:



Technology Transfer: Private contract

**Key Documentation:** Ward, JA, JQ Word, and LD Antrim. 1990. Toxicological Evaluation of Sediment Samples from Port Valdez, Alaska, Using Three Species of Marine Amphipods. Prepared for Alyeska Pipeline Service Company, Anchorage, Alaska, under contract TAPS 4875, by Battelle/Marine Sciences Laboratory, Sequim, Washington.

**Key Personnel:** RM Ecker, 360-683-4151, RM\_ECKER@PNL.GOV; WH Pearson, 360-681-3610, WH\_PEARSON@PNL.GOV; JQ Word, Jr., 360-681-3668, JQ\_WORD@PNL.GOV; EA Crecelius, 360-681-3604, EA\_CRECELIUS@PNL.GOV

Lab Capabilities Applied:



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Category: Environmental & Regulatory

Laboratory: Pacific Northwest Laboratory

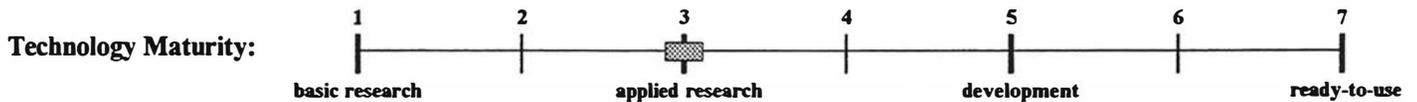
Contact: Brian Shaw, 509-372-6157,  
BR\_SHAW@PNL.GOV

Title: Soil Washing for Removal of Heavy Metals and Radionuclides

**Description:** The objective of this program is to evaluate the use of soil washing techniques to remove contaminants from soils on the Hanford site. Primary contaminants of concern are uranium, chromium, cesium-137, Strontium-90, Cobalt-60, and Europium-152. The program includes the comprehensive characterization of soils to determine the association of contaminants as a function of particle size and mineralogy. This data is used to design bench scale tests used to assess various soil washing unit operations. Bench scale tests include, physical separation, attrition scrubbing, autogenous grinding, chemical extraction, and waste water treatment. Once bench scale tests identify the most effective unit operations and operating conditions, batch recycle tests are conducted to determine effects of buildup of competing ions on the removal of contaminants. Tests completed to date have shown that uranium can be successfully removed from 300 area pond soils with physical separation and attrition scrubbing with water. Tests on 100 area soils showed that Europium-152 and Cobalt-60 can easily be removed but cesium-137 requires additional unit operations to meet performance objectives. Full scale tests with commercial equipment has been successfully completed on 300 area soils and tests on 100 area soils are currently underway. Analysis of data from the 100 area full scale tests will continue in FY95.

91-95 Funding (\$K): 1214

Dates: 1994 - Present



Technology Transfer: Publications

Key Documentation:

Key Personnel: HD Freeman, 509-376-8561, HD\_FREEMAN@PNL.GOV; RJ Serne, 509-376-8429, RJ\_SERNE@PNL.GOV

Lab Capabilities Applied: Separations and hydrothermal processing



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Category: Oil Processing &amp; Refining (4, 20, 24, 25, 27)

Laboratory: Sandia National Laboratories

Contact: Jean-loup Faulon (505) 844-3345

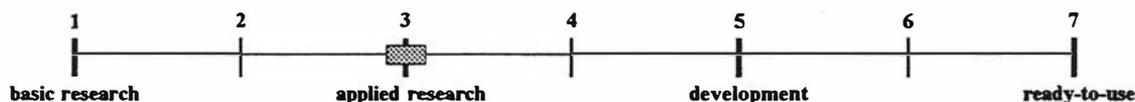
Title: Molecular Modeling of Macromolecular Structure of Complex Hydrocarbons and Fuels

**Description:** The goal of this program is to use computer-aided molecular design (CAMD) techniques to increase our understanding of the macromolecular structures of complex hydrocarbons and fuels. For this purpose, we have developed a computer program (the SIGNATURE program) that produces models based solely on qualitative and quantitative experimental data. The SIGNATURE program has been used with lignin, humic acids, kerogen, asphaltenes, and coal. We also have developed a computer technique based on finite element theory that calculates physical characteristics (density, micropore volume, surface area, and fractal dimension) of three-dimensional molecular models. This technique has been applied with coal models generated by the SIGNATURE program, and it was shown that the physical characteristics computed matched the corresponding experimental data. Recently, we have coupled our CAMD effort with kinetics modeling. We have modified the SIGNATURE program in order to apply chemical reactions to three-dimensional molecular models. The input of our kinetics program is a molecular model, a reaction mechanism with associated rates. The output of the program is the distribution of the products of the reactions. We believe this new technique is more accurate than classical Monte Carlo kinetics programs, because our simulations are carried out in three-dimensional space. We have applied our kinetics program to investigate wood coalification and the pyrolysis of coal.

91-95 Funding (\$K): 750

Dates: 1990-present

Technology Maturity:



Technology Transfer: Informal collaborations with universities and oil companies; staff visits; open literature publications.

**Key Documentation:** Faulon, J., G. A. Carlson et al., "Statistical Models for Bituminous Coal: A Three-Dimensional Evaluation of Structural and Physical Properties Based on Computer-Generated Structures," *Energy and Fuels* 1993, 7, 1062.  
 Faulon, J., "Stochastic Generator of Chemical Structure: Application to the Structure Elucidation of Large Molecules," *J. Chem. Inf. Comput. Sci.* 1994, 34, 1204.

**Key Personnel:** Jean-loup Faulon, 505-844-3345  
 David Hobbs, 505-844-5571  
 Gary Carlson, 505-844-8116  
 Howard Stephens, 505-844-9178

**Lab Capabilities Applied:** Unique molecular builder methodology providing capabilities for physical properties prediction and petroleum process modeling capabilities; world's fastest massively parallel computer; computer-aided molecular design



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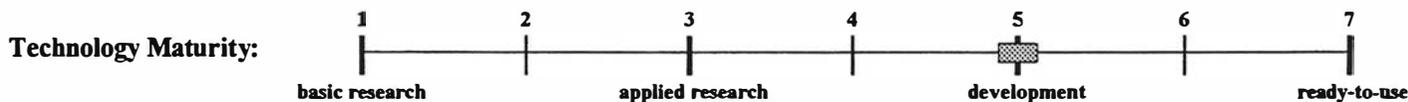
Category: Environmental & Regulatory (10, 11, 12)

Laboratory: Sandia National Laboratories Contact: Michael R. Prairie (505) 844-7823

Title: Photocatalytic Detoxification of Organic Contaminants

**Description:** The goal of this program is to investigate the feasibility of photocatalytic processes for treating water contaminated with organics and heavy metals. Specific tasks include treatability studies on industrial waste (Microelectronics water contaminated with organics, photographic waste contaminated with silver, water contaminated with high explosives, textile waste, etc.), and fundamental studies (w/the University of New Mexico) to elucidate and model redox kinetics of photocatalytic processes. Sandia performs laboratory research and feasibility studies for Strategic Environmental Research and Development Program (SERDP of DoD) and Intel Corporation. SERDP is interested in new ways to treat explosives contaminated water and Intel is interested in photocatalysis as a pretreatment for recycling water at microelectronics fabrication plants. With the National Renewable Energy Laboratory, Sandia is helping to develop solar photocatalytic technology for a variety of applications. This work is funded by DOE/EE-222. Specific applications of current interest are found in the microelectronics, groundwater treatment, fuel spill remediation, and photoprocessing industries. Sandia's work with DuPont is via a CRADA with DOE funds. This project will result in the development of a phenomenological model that describes photocatalytic oxidation and reduction kinetics in terms of external variables. Sandia will use the model to optimize photocatalyst performance. DuPont will use it to characterize and improve the performance of systems for deactivating pigment grade titanium dioxide.

91-95 Funding (\$K): 3200 Dates: 1991 - present.



Technology Transfer: Publications, presentations, brochures, patent applications, CRADAs.

Key Documentation: Pacheco, J.E. and Yellowhorse, L. Summary of Engineering-Scale Experiments for the Solar Detoxification of Water Project. Sandia National Laboratories Report SAND92-0385, 1992. Prairie, M.R., Evans, L.R., Stange, B.M., and Martinez, S.L. An investigation of TiO<sub>2</sub> photocatalysis for the treatment of water contaminated with metals and organics. Envir. Sci. Tech. 27, 1776-1782 (1993).

Key Personnel: M.R. Prairie, 505-844-7823  
 S.K. Showalter, 505-844-6412  
 P.Rodacy, 505-844-1665  
 J.M. Chavez, 505-844-4485

Lab Capabilities Applied: Quantitative analysis of low levels of metals and organics, by-product identification, catalyst preparation and characterization, explosives handling and trace analysis, electrochemistry, kinetic modeling, photochemistry.





**Index:** 333

**Category:** Drilling & Completion (6, 1, 3, 5, 10), Production (11, 13, 25)

**Laboratory:** Sandia National Laboratories

**Contact:** Dale S. Preece, 505-844-6259, dspreec@sandia.gov

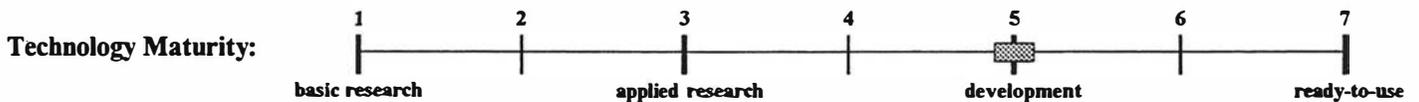
**Title:** Near Wellbore Mechanics (ACTI)

**Description:** The objective of this project is to integrate, apply and transfer computational mechanics tools available at SNL to better model near wellbore mechanics. We intend to move the assessment of sand production and wellbore stability to a new level by: 1) better assessment of wellbore stress state and stability for all well orientations, 2) prediction of perforation induced formation damage with its effect on well performance, and 3) more accurate prediction of sand production onset and rates to facilitate successful well operation with higher production rates than other conservative approaches currently in use. This sand production predictive capability will be applicable to all wells that produce from zones of weakly consolidated sandstones.

Major and minor oil companies as well as service companies and universities are involved in this project. The oil companies are contributing the time and expertise of their staff, core and sand production data. The service companies are contributing rock testing and computer codes as well as the time and expertise of their staff. This ACTI project builds upon a sand control project begun with industry in 1994.

The deliverable of this project is a set of Sandia structural mechanics computer codes customized for solving Near Wellbore Mechanics problems. The development of this code system will be guided through interaction with industry partners.

**91-95 Funding (\$K):** 1700      **Dates:** 1994-present



**Technology Transfer:** The system of computer codes developed by this project will be commercialized in some manner during the third year. It is perceived that this would best be accomplished through a private company working closely with Sandia and the industry partners.

**Key Documentation:** "CTH Reference Manual: Johnson Holmquist Ceramic Model," SAND92-0576.  
"JAC3D - A Three-Dimensional Finite Element Computer Program for Nonlinear Quasi-Static Response of Solids with the conjugate Gradient Method," SAND87-1305.

**Key Personnel:** Dale S. Preece, 505-844-6259, dspreec@sandia.gov  
Paul Yarrington, 844-7504, pyarrin@sandia.gov  
Robert K. Thomas, 844-7450, rkthoma@sandia.gov  
Harold S. Morgan, 844-7045, hsmorga@sandia.gov  
Wolfgang R. Wawersik, 844-4342, wrwawer@sandia.gov

**Lab Capabilities Applied:** Computational Physics, Computational Structural Mechanics, Discrete Element Modeling, Shock Physics Laboratory, Rock Mechanics Laboratory.



Index: 334

Category: Environmental & Regulatory (9, 5), Drilling & Completion (11), Development (4)

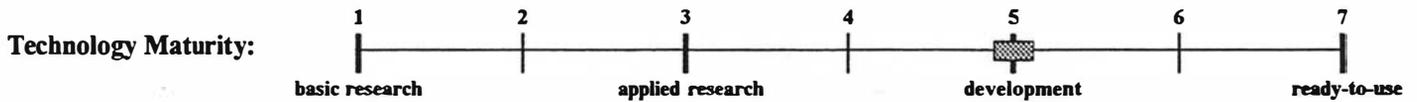
Laboratory: Sandia National Laboratories Contact: David Betsill, 505-844-9578

Title: Monitoring of Contaminants, In-Situ Remediation, Subsurface Barriers, and Landfill Covers Using Tracers

**Description:** Recent studies on contaminant transport in the vadose indicate that the use of tracers to emulate and/or monitor contaminant transport, remediation, and post-closure activities offer non-hazardous and cost-effective methods for modeling and verifying these processes. Areas of capabilities and research include: (1) Gas and liquid conservative tracers to evaluate natural properties that affect contaminant transport, remediation, and containment. (2) Sorptive gas tracers to assess the amount of contaminant that may exist in the unsaturated zone. (3) Conservative, reactive, and sorptive and reversible tracers to emulate contaminants of concern in natural flushing, sorption, reduction, and remediation processes. (4) Conservative and sorptive tracers to estimate the degree of contaminant removal and effectiveness of in-situ remediation processes. (5) Microsphere tracers to emulate microbial movement and transport in support of in-situ bioremediation processes. (6) Gas and liquid tracers to evaluate and verify the effectiveness of landfill covers and subsurface barriers to contain and isolate wastes.

An associated capability is measurement-while-drilling for real time field screening of contaminants, where downhole sensors are located behind the drill bit and linked by a high-rate data transmission system to the surface. The current measurement system is compatible with dry compaction boring, a directional drilling technique that uses minimal drilling fluids and generates little to no secondary waste. The data transmission techniques and data reduction hardware are based on proven military technology.

91-95 Funding (\$K): 970 Dates: 1993-present



Technology Transfer: Technical publications

Key Documentation: Betsill, J. D. and R. D. Gruebel, 1995 (in preparation), "Verification and Monitoring Options Study," Sandia National Laboratories Document No. SAND95-XXXX.  
G.J. Lockwood, et al., "Environmental Measurement-While-Drilling System for Real-Time Field Screening of Contaminants," North American No-Dig Conference, Toronto, May 1995.

Key Personnel: David Betsill, 505-844-9578  
Cecilia V. Williams 505-844-5722  
Dianne C. Marozas, 505-844-5504  
Grant J. Lockwood, 505-845-7007  
Randy A. Norman, 505-845-9675

Lab Capabilities Applied: Hydrogeology, Tracers, Geochemistry, Modeling, Environmental Monitoring, Geology, Tracers, Telemetry, Radiation Physics, Geophysics, Drilling Technologies.



Index: 335

**Category:** Development (8), Environmental & Regulatory (9, 12), Exploration (9), Drilling & Completion (2, 6)

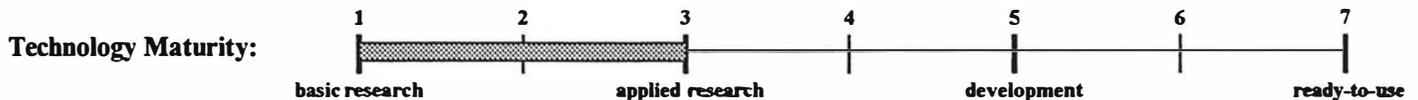
**Laboratory:** Sandia National Laboratories

**Contact:** Henry R. Westrich, 505-844-9092,  
hrwestr@sandia.gov

**Title:** Fluid/Rock Interactions - Mineral Dissolution and Precipitation Kinetics, Sorption, and Surface Charge Speciation

**Description:** Ongoing projects focus on experiments, molecular and conceptual modeling, and high resolution surface analysis of fluid/rock interactions pertinent to sedimentary basin diagenesis, scale formation, environmental remediation, and oil recovery. Dissolution and precipitation kinetic data and sorption isotherms are included in geochemical models (e.g. The Geochemist's Workbench, C. M. Bethke) and coupled reaction/transport models (e.g. CIRF, P. Ortoleva; REACT, C. Moore) used in industry. Data can be used to predict porosity and permeability and to model paleothermometric mineral reactions. Potential applications include migration pathway modeling and fault/seal analysis. Comprehensive mechanistic rate laws have been developed for feldspar and orthosilicate dissolution. Current work includes quantifying effects of organic acid anions on mineral diagenesis, e.g. kaolinite dissolution and growth. Possible applications include prediction of mineral reactions during enhanced oil recovery. Molecular modeling of clay and oxides surfaces, and crystal morphologies can be applied to formulating scale inhibitors and potentially to interpretation of NMR and resistivity logs. Mechanistic models of radionuclide sorption onto kaolinite and montmorillonite and of organic molecule adsorption onto calcite are underway. Sorption isotherm data and conceptual modeling result in bulk distribution coefficients for predicting retention of radionuclides (e.g. cesium) and toxic contaminants (e.g. cadmium) in groundwater hydrologic systems. Models for predicting sorption as a function of oxide components of mineral surfaces are being developed. Other potential areas for applying work results and methodologies include treatment of NORM, drilling fluid design and disposal, and wettability models.

**91-95 Funding (\$K):** 1800

**Dates:** 1987-present

**Technology Transfer:** Peer-reviewed journal articles, scientific conference presentations, staff exchange, government reports

**Key Documentation:** H. R. Westrich, R. T. Cygan, P. V. Brady, K. L. Nagy, H. L. Anderson, Y. Kim, and R. J. Kirkpatrick, 1995, The Sorption Behavior of Cs and Cd onto Oxide and Clay Surfaces, Waste Management '95, Conference Proceedings.  
W. H. Casey, C. Eggleston, P. A. Johnsson, H. R. Westrich, and M. F. Hochella, Jr., 1992, Aqueous Surface Chemistry and Corrosion of Minerals, Materials Research Society Bulletin 17, 23-29.

**Key Personnel:** Patrick V. Brady, 505-844-7146, pvbrady@sandia.gov  
Randall T. Cygan, 505-844-7216, rtcygan@sandia.gov  
Kathryn L. Nagy, 505-844-5337, klnagy@sandia.gov  
Henry R. Westrich, 505-844-9092, hrwestr@sandia.gov

**Lab Capabilities Applied:** Ion beam (RBS & ERD), direct current plasma, NMR, and X-ray photoelectron spectroscopies; TEM, SEM, scanning probe microscopy, XRD, ion chromatography, surface titrations, batch & stirred-flow reactors, molecular modeling, cold-seal & Dickson P vessels.



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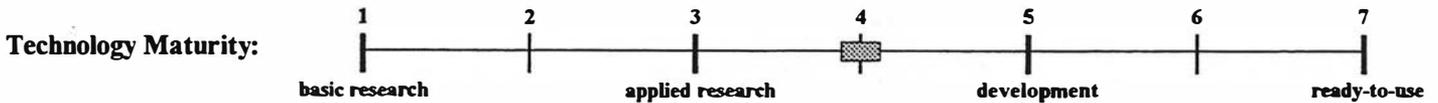
Category: Oil Processing & Refining (11,4), Environmental & Regulatory (10)

Laboratory: Sandia National Laboratories Contact: W. T.(Ted) Wheelis (505) 845-9298

Title: Organic Destruction/Re-Use and Recycling Methodologies

**Description:** Sandia National Laboratories has many years experience evaluating, developing and demonstrating technologies and systems for recycle (both liquids and solids). This includes systems for separation prior to recycle, evaluation and modification of equipment components, and development and demonstration of automated recycle/treatment systems. For solids, This includes an abrasive water-jet with real-time X-ray system for removal of hazardous components; a remotely operated, cryogenically cooled forge hammer system for size reduction prior to recycle; and evaluation of various physical separation systems (e.g. eddy current and electrostatic separators, shaker tables, etc.). Sandia has worked extensively with industrial companies on new technologies for the recycle (for instance into hydrogen or syn-gas fuels)/destruction of organic materials & metals recycling. Sandia's contributions in this area have included developing test plans, defining monitoring parameters (e.g. particularly with respect to evaluating environmental impact), refractory & fluxing agent issues and risk/reliability improvement, e.g. through work in risk analysis, metal processing, high temperature sensors, instrumentation, feed systems, and modelling. In addition, Sandia has performed cost-benefit analyses to quantify the economics of disposal, treatment, or recycle of organic and metal bearing components. Current activities also include investigation of methods for producing high-value products from low value (or waste) sludges at petroleum refineries and benchmarking of best-in-class waste minimization practices.

91-95 Funding (\$K): 2300 Dates: 1993-Present



Technology Transfer: Publications in Open Literature, Conference Presentations, Trade Shows, Technology Development with Industry

Key Documentation: 1.) Report: Waste Component Recycle, Treatment, & Disposal Integrated Demonstration (WeDID) Program, Activities summary report, FY92 & FY93  
 2.) Demilitarization & Disposal Technologies for Conventional Munitions & Energetic Materials, SAND94-2223C

Key Personnel: Al Lemieux 505-844-7251  
 Stuart Purvis 505-845-8392  
 Jim Lutz 505-844-9082  
 Victoria Levin 505-844-8956

Lab Capabilities Applied: Systems Engineering, Environmental Assessments, Chemistry/Materials Science, Benchmarking Methodologies



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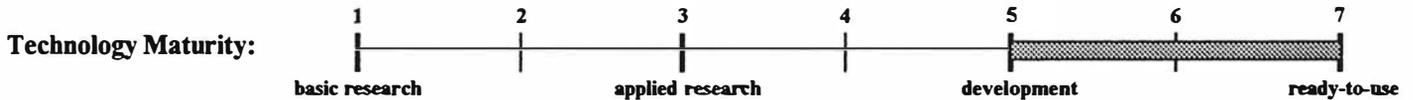
Category: Environmental & Regulatory (5), Gas Gathering (2)

Laboratory: Sandia National Laboratories      Contact: Robert G. Knowlton, 505-848-0425

Title: Leak Detection Using Horizontal Logging and Electromagnetic Sensor Techniques

Description: Sandia has already demonstrated capabilities in horizontal logging with neutron/density probes for leak detection, as well as developed unique electromagnetic sensor capabilities for moisture determinations in multiplexed arrays and automated logging. Cone penetrometer push technologies have also been developed by Sandia for leak detection and hydrologic characterization. Additional work is being considered to promote the concept of pushing dedicated sensors into the subsurface for routine monitoring. A method for monitoring design and leak detection has also been developed and is in the process of being published.

91-95 Funding (\$K): 500      Dates: 1992-present



Technology Transfer: Neutron logging commercialized, electromagnetic techniques are under consideration for patenting/copyrighting.

Key Documentation: Documentation in development. Several conference papers presented already.

Key Personnel: Robert G. Knowlton, 505-848-0425

Lab Capabilities Applied: Applied engineering; monitoring/characterization technologies; electronics.



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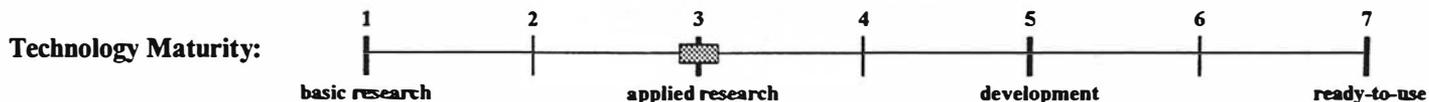
Category: Oil Processing & Refining (11), Environmental & Regulatory (10)

Laboratory: Sandia National Laboratories Contact: Chris F. Edwards 510/294-2008

Title: The Origin and Fate of Toxic Combustion By-Products in Process Heaters

**Description:** Toxic combustion by-products, or air toxics, are regulated under the Clean Air Act Amendments of 1990. A source of air toxics at oil refineries is the air emissions from petrochemical process heaters. These heaters use refinery fuel gas (RFG), a mixture of varying composition of hydrogen, methane, propane, and other hydrocarbons that is an off-product of the refinery process. RFG provides most of the fuel at refineries. The goals of the program are: 1) to assess the state of air toxics emission in existing burners used in process heaters, 2) to evaluate candidate burners and combustion control strategies that would lessen air toxics generation, 3) to provide a fundamental understanding of the contributory fluid mechanics, the combustion and high temperature chemistry, and the process thermal environments that lead to the production and release of air toxic emissions, and 4) to develop computer models that enable site evaluations and predictions. Work to achieve these goals is progressing at three laboratories with guidance, industrial information, and direct and in-kind financial support provided by the industrial partners. At SNL, fundamental experiments are being conducted in the flame research laboratory and applied experiments with industrial burners in the Burner Engineering Research Laboratory-BERL (jointly sponsored by OE/EE and GRI). A key piece of the experiments in the BERL will be an experimental representation of the convective cool-down sections used in process refineries. In cooperation with LNL, SNL is building models of the pertinent chemical submechanisms. SNL will incorporate the chemistry as defined by LLNL and the fluid mechanics as defined by SNL to model the burner and the cool down sections. At LLNL, chemical kinetics models are being built that describe the formation of the air toxics in the combustion zone and their fate as they pass out of the combustion one and through the convective cool-down section. UCLA is performing fundamental experiments in specially designed and instrumented burners to provide the experimental basis for the LLNL chemical kinetics models.

91-95 Funding (\$K): 2140 Dates: 1994-present



**Technology Transfer:** data base to be extended to refinery evaluation, code for predicting refinery performance, participation in analysis of refinery measurements, joint publications as appropriate

**Key Documentation:** CRADA No: SC93/01203 The Origin and Fate of Toxic Combustion By-Products in Petrochemical Process Heaters: Research to Enable Efficient Compliance with the Clean Air Act

**Key Personnel:** Chris F. Edwards 510-294-2008  
Neal R. Fornaciari 510-294-2472  
Charles M. Hartwig 510-294-3047

**Lab Capabilities Applied:** advanced optical diagnostics, burner combustion research laboratory, BERL, combustion engineering, fluid mechanics modeling, combustion science modeling, quantum chemistry model development



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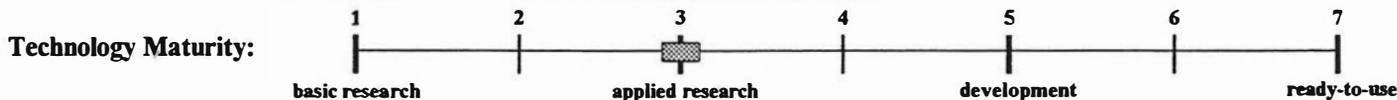
**Category:** Oil Processing & Refining (1, 4, 19), Gas Processing (4, 5, 6)

**Laboratory:** Sandia National Laboratories **Contact:** Mark Phillips, (505) 844-8969

**Title:** Design and Development of Smart Membranes for Small Molecule Separations

**Description:** We are developing molecular sieve films for use as light gas separation membranes and catalyst supports. Polymer membranes, on which current gas membrane technology is based, cannot separate gases based on molecular size or shape and do not perform well at elevated temperatures. We are synthesizing membranes that consist of microporous crystalline (zeolitic) films supported on porous substrates. Our goal is to develop a family of zeolitic films that offer permeability and selectivity exceeding those of polymer membranes, allowing gas membranes to compete with cryogenic and adsorption technologies for large-scale gas separation applications. Films must be made thin and leak-free in order to be both permeable and selective. This may be accomplished by nucleating and crystallizing zeolitic phases from nutrients previously deposited on porous ceramic supports. These nutrients consist of sol-gel, metal, and clay films. The resulting film is ideally a composite of zeolitic crystallites within a matrix of uncrystallized nutrient film. The nutrient matrix improves film durability and can prevent gas leakage through gaps between crystals. Ultimately, such films could be used in a catalytic membrane reactor in which catalytic and separation processes (e.g., dehydrogenation) are performed by a single membrane element. We are working with Golden Technologies, Inc. on this project. Thin film zeolites have been synthesized and gas permeability measurements made. Processes are currently being optimized. Very significant energy savings will result if these membranes can be economically applied to gasification products and other refining applications. Energy-intensive processes in petrochemicals manufacture (catalytic oxidation and dehydrogenation, Haber process, distillation) will also benefit from this technology.

**91-95 Funding (SK):** 2100 **Dates:** 1989-present



**Technology Transfer:** Informal collaboration, staff visits, annual reports.

**Key Documentation:** Frye, G. C. et al., "Sol-Gel Coatings on Acoustic Wave Devices: Thin Film Characterization and Chemical Sensor Development," Mat. Res. Soc. Symp. Proc. 1993, 180, 583.  
 Brinker, C. J. et al., "Review of Sol-Gel Film Formation," J. Non-cryst. Solids 1992, 147/148, 424.

**Key Personnel:** Mark Phillips, 505-844-8969  
 Carol Ashley, 505-845-8931  
 Jeff Brinker, 505-845-8930

**Lab Capabilities Applied:** Advanced materials synthesis; sol-gel techniques; advanced gas adsorption and permeation characterization techniques



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Category:

Laboratory:  Contact:

Title:

Description:

91-95 Funding (\$K):  Dates:

Technology Maturity:   
 1                      2                      3                      4                      5                      6                      7   
 basic research                      applied research                      development                      ready-to-use

Technology Transfer:

Key Documentation:

Key Personnel:

Lab Capabilities Applied:



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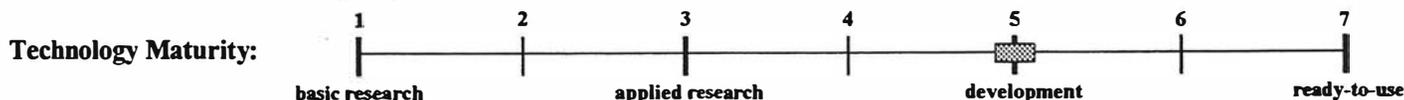
Category: Development (10, 3), Exploration (3, 10, 14, 16)

Laboratory: Sandia National Laboratories Contact: Bob Cutler, (505) 844-5576, rputc@sandia.gov

Title: Three Component Borehole Seismic Source

**Description:** Project Goal: Develop and make commercially available a high force, wide bandwidth, three axis, easily deployable, clamped borehole seismic source for crosswell, reverse VSP, and single-well seismic surveys.  
 Project Team: The tool is being jointly developed and funded by DOE and Industry. Development team members include Chevron, Conoco, Amoco, Exxon, Sandia National Laboratories/DOE, Gas Research Institute, E-Systems, Pelton.  
 Results and Deliverables: The source will be deployed on a special heavy-duty wireline and will consist of a downhole Electronics Module, a downhole Hydraulic Power Supply Module, and one of three interchangeable vibrator modules. The first of these is a clamped Vertical Vibrator Module containing a high bandwidth hydraulic actuator and a reaction mass. The vertical vibrator module was completed and tested in 1994. A complete single axis version of the tool, including all downhole and uphole support equipment, the electronics module and hydraulic power supply module, and surface control electronics, will be ready for initial field tests in August, 1995. Work on the the other two vibrator modules will follow successful field testing of the single axis version. The tool is intended for use over wide well spacings (~2000'), in deep wells (>15,000') and at high temperatures (>150 C). Tool characteristics include: 6000 lb. peak force, present useful bandwidth ~30-500 Hz (with plans to extend to ~800 Hz), fiber optic telemetry from tool to surface, capability to attach seismic receiver string below tool, 4.4" tool O.D., clamped for good coupling to formation, easy deployment.  
 Applications and Impacts: This tool should significantly advance the state of the art in borehole seismic applications including crosswell, reverse VSP, and single well imaging, by making these tests viable over typical existing well separation distances.

91-95 Funding (\$K): 3160 Dates: 1991- 1995



Technology Transfer: E-Systems and Pelton will sell tools to any interested party. A small commercial service company is being established to operate the existing hardware in field surveys. The results of initial field tests will be published in the open literature.

Key Documentation: CRADA 1074 Seismic Source Development, Dec 1992

Key Personnel: Bob Cutler, (505) 844-5576, rputc@sandia.gov; Chad Harding, (505) 844-0780, rshardi@sandia.gov

Lab Capabilities Applied: Dynamic modeling, borehole tool design, thermal modeling, high temperature electronics, fiber optic telemetry, corrosion, materials, program management



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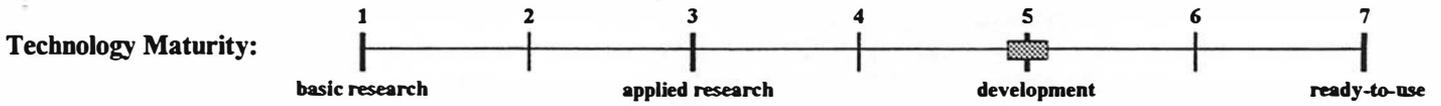
Category: Environmental & Regulatory (10), Gas Processing (6)

Laboratory: Sandia National Laboratories Contact: Nina Bergan French 510/294-3185

Title: Laser-Spark Spectroscopy for Continuous Metal Emissions Monitoring

Description: The objective of this task is to develop and demonstrate an instrument using Laser-Spark-emission Spectroscopy (LASS) as a continuous monitor to measure metal emissions from offgas of thermal treatment units. The project will address several important issues for the instrument, including sensitivity (at least ppm concentration for metals governed under the clean air act), calibration, durability, and reliability, and accuracy. The purpose of this development is to design, build, and test a field instrument at a DOE facility by March 1995. This instrument would have wide applicability to many different industries.

91-95 Funding (\$K): 1800 Dates: 1993-present



Technology Transfer: reports and publications, field test demonstrations, concept and design transfer, fieldable instrument

Key Documentation:

Key Personnel: Nina Bergan French 510-294-3185  
William Flower 510-294-2046

Lab Capabilities Applied: optical diagnostics, laser applications, uv and optical spectroscopy, system design



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Category: Drilling & Completion (9,11)

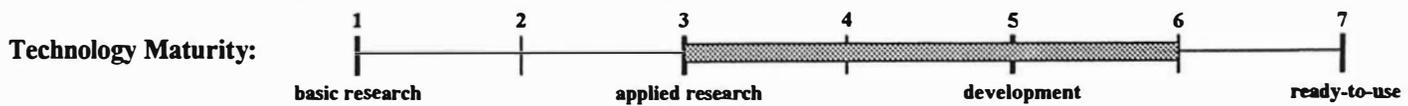
Laboratory: Sandia National Laboratories      Contact: P.C. Lysne, 505-844-8885, pclysne@sandia.gov

Title: Downhole Instruments for Slim, High-Temperature Wells

**Description:** Slim (4 inch diameter) holes are used in geothermal exploration since diamond coring operations are economically competitive over conventional rotary drilling. However, small diameter logging instruments capable of working at high temperatures (700 degrees Fahrenheit) are not commonly available. A suite of electronic memory tools is being developed to make appropriate measurements and promulgate the use of logs in geothermal holes.

Three tools are in the advanced prototype stage. A pressure/temperature tool features an on-board computer that may be programmed, thereby making the tool "smart". A fluid/gas sampler tool may be joined with the P/T tool to sample formation materials or injectates used in tracer tests. A spectral gamma tool returns conventional KUT data. All tools are Dewared, and they are short and light weight so they may be transported by passenger air service. A "slick line" of the sort found at most drilling sites is necessary for deployment. Operation is through a menu routine located on a personal computer. Measurements are traceable to DOE standards.

91-95 Funding (\$K): 2000      Dates: 1991- Present



Technology Transfer: Geothermal Operators and Service Companies

Key Documentation: "Design of a Pressure/Temperature Logging System for Geothermal Applications", Peter Lysne and Joseph Henfling, Proc. DOE Geothermal Review Number XII, San Francisco, March, 1994.

Key Personnel: Peter Lysne, 505-844-8885, pclysne@sandia.gov, Joseph Henfling, 505-844-6720, jahenfli@sandia.gov

Lab Capabilities Applied: Electronics, calibration, downhole testing



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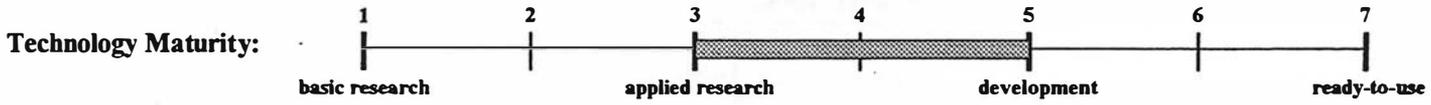
**Category:** Environmental & Regulatory

**Laboratory:** Sandia National Laboratories **Contact:** Charles Hickox, 505-844-5882, cehicko@sandia.gov

**Title:** Transport and Fate of Oil Spilled in a Marine Environment

**Description:** The purpose of the project is to improve the response to and remediation of marine oil spills and to provide a basis from which to assess important physical processes and the role of field measurements. An advanced simulation tool has been created and compared to OILMAP, the current state of the art simulation tool used in the industry for field response. The advanced simulation capability uses a three-dimensional hydrodynamic model for modeling circulation in upper region of the ocean and assumes turbulent transport of oil. The project will provide significant simulations of oil spills using historical data, make comparisons with OILMAP and develop requirements for remote data acquisition and real-time oil spill fate simulations. This simulation capability can be coupled with oil transport and ocean current simulations. These are based upon high-resolution, high-performance (massively parallel) simulations using a unique overset grid approach. The ocean circulation modeling has been done in conjunction with the Eddy Joint Industry Project (EJYP).

**91-95 Funding (\$K):** 600 **Dates:** 1994-present



**Technology Transfer:** Publications in the open literature, joint industry project.

**Key Documentation:** D. Barnette et al., "Progress Report on High-Performance, High-Resolution Simulation of Coastal and Basin-Scale Ocean Circulation," 2nd Overset Composite Grid & Solution Technology Symposium, 10/25-28, 1994.

**Key Personnel:** Charles Hickox, 505-844-5882, cehicko@sandia.gov  
Daniel Barnette, 505-845-7874, dwbarne@cs.sandia.gov

**Lab Capabilities Applied:** Advanced computational fluid dynamics modeling, high performance computing.



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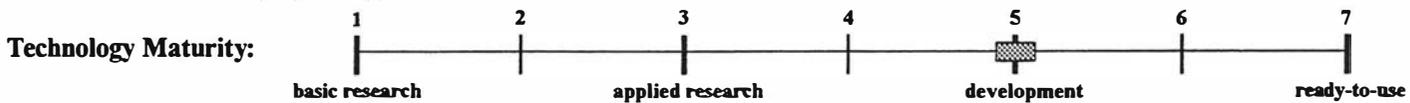
Category: Gas Gathering (2), Environmental & Regulatory (5,10)

Laboratory: Sandia National Laboratories Contact: Thomas J. Kulp 510/294-3676

Title: The Development of a Real-Time Video Imaging System for Natural Gas Leaks

**Description:** The detection of gas leaks represents a critical operation performed regularly by the gas industry to maintain the integrity and safety of its vast network of piping, both above and below the ground. These operations are mandated to occur at regular time intervals by regulatory agencies, and represent a major cost for gas utility companies. Other motivations for gas leak detection include: (1) energy conservation, (2) reduction of greenhouse gas emissions, and (3) safety and emergency response applications. This project is directed at the development of a new technology to vastly accelerate the rate at which gas leak detection is carried out. The end product of the research will be an instrument that will allow real-time television images of gas plumes to be generated. The use of an imaging technology to identify and locate gas leaks will be superior to presently used point sensor ("sniffer") technologies for several reasons, all stemming from its inherent two-dimensional operation. The primary attributes are the ability to search wide areas at a given instant in time (thereby greatly accelerating search procedures) and the ease with which an operator can locate a gas leak by viewing it in a television picture. The specific focus of our project is to demonstrate a new means of generating natural gas imagery using a pulsed infrared laser and an infrared focal-plane array sensor. The work builds on past work in which the ability to image natural gas plumes was demonstrated using a scanned imaging camera. The scanned work was successfully demonstrated at a number of gas industry facilities. It was, however, limited in its range of operation. The new technology will allow ranges that are of interest to the gas industry and will allow many more hydrocarbon vapors to be imaged as well. If the technology demonstration is successful, the project is expected to proceed to a prototype development stage.

91-95 Funding (\$K): 800 Dates: 1995-present



Technology Transfer: reports, site testing, fieldable instrument

**Key Documentation:**  
 1. T.G. McRae and T.J. Kulp, "Backscatter Absorption Gas Imaging - A New Technique for Gas Visualization," Appl. Opt. 32 4037-4050 (1993).  
 2. T.J. Kulp, R. Kennedy, M. Delong, D. Garvis, and J. Stahovec, "The Development and Testing of a Backscatter Absorption Gas Imaging System Capable of Imaging at a Range of 300 m", in Proceedings of SPIE, Applied Laser Radar Technology, (Society of Photo-Optical Instrumentation Engineers, Bellingham, WA, 1993) Vol. 1936, pp 204-212.

**Key Personnel:** Thomas J. Kulp 510-2943676  
 Charles M. Hartwig 510-294-3047

**Lab Capabilities Applied:** laser applications, infrared spectroscopy, optical remote diagnostics



Index: 346

Category: Development (14, 2, 9, 25, 33)

Laboratory: Sandia National Laboratories

Contact: W. R. Wawersik, 505-844-4342,  
wrwawer@sandia.gov

Title: Geomechanics of Petroleum Reservoirs

**Description:** Geomechanics, in regard to petroleum reservoirs, concerns the understanding of the initial mechanical conditions within the reservoir and the response of the reservoir to drilling, completions, production, or any other induced processes. Understanding the development of a reservoir, the changes in stress state and permeability, and the effects of and on wellbores is critical to efficient reservoir management and development. Geomechanics addresses problems such as subsidence of reservoirs, permeability degradation with drawdown, and difficulties with production from fractured reservoirs.

Sandia involvement in geomechanics began with studies of the Ekofisk reservoir for Phillips and has continued with studies of the Austin Chalk for Oryx, Lisbourne field for Arco, and others. In these studies, industry core, log, drilling, completion, and production results are used, together with Sandia measurements on core or within the reservoir, to obtain information critical to effective reservoir management.

This project has produced many important results, ranging from the determination of the stress state throughout the Ekofisk reservoir, the characterization of the mechanics responsible for subsidence in the Ekofisk field, poroelastic measurements of rock deformation and permeability behavior, the development of several methods for core-based stress measurements, the analysis of coring induced fractures and their relation to the stress state in the reservoir, and other aspects of reservoir mechanical behavior.

This technology has application in all aspects of production and injection of fluids and solids from and into reservoirs, has crucial importance in subsiding reservoirs, naturally fractured reservoirs and many other marginal reservoir types, and is necessary for developing mechanical basin analyses.

91-95 Funding (\$K): 1400

Dates: 1986-present

1 2 3 4 5 6 7

Technology Maturity:

basic research applied research development ready-to-use

**Technology Transfer:** Technology transfer occurs through journal articles (SPE), reports, joint projects, help and consultation on industry projects, industry and professional forums and reviews, and university contacts.

**Key Documentation:** Warpinski, N. R. and L. W. Teufel, "Determination of the Effective Stress Law for Permeability and Deformation in Low Permeability Rocks," SPE Formation Evaluation, Vol. 7, pp. 123-131, June 1992.

**Key Personnel:** L. W. Teufel, 505-844-8680  
N. R. Warpinski, 505-844-3640  
W. R. Wawersik, 505-844-4342, wrwawer@sandia.gov  
D. J. Holcomb, 505-844-2157, djholco@sandia.gov

**Lab Capabilities Applied:** Rock mechanics, Geotechnical modeling, Natural fracture expertise, Rock mechanics testing facility.



Index: 347

Category: Oil Processing &amp; Refining (1, 6, 7, 12, 16, 22)

Laboratory: Sandia National Laboratories

Contact: N. B. Jackson, (505)-844-0940

Title: Catalyst Assessment and Reactor Hydrodynamics for Indirect Liquefaction

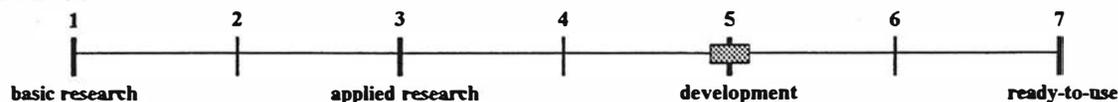
**Description:** The objectives of this project are to understand and prevent the causes of attrition of Fischer-Tropsch (FT) catalysts used in slurry-phase bubble column reactors (SPBR), and to develop diagnostic instrumentation to understand better the hydrodynamics of SPBR's in order to assist in the scale up of these reactors. Catalyst attrition studies are correlated with FT catalyst synthesis, pretreatment, and reactor conditions. Catalyst characterization techniques, including XPS, TEM, FTIR, Mossbauer, and temperature programmed desorption and oxidation, are used to design an attrition resistant catalyst. Two diagnostic techniques are being developed to study the hydrodynamics of SPBRs, gamma-densitometry tomography (GDT) and electrical impedance tomography (EIT). GDT will be set up for measurements at the LaPorte Alternative Fuel Development Unit (AFDU), operated by Air Products and Chemicals, for measurement of gas holdup. EIT validation experiments will be conducted with a hot model bubble column. Both GDT and EIT can also be used to characterize the hydrodynamic behavior of other types of reactors, such as ebullated-bed reactors used for hydroprocessing petroleum resids. Collaboration with industrial and academic partners is an integral part of the characterization activity.

91-95 Funding (\$K):

2500

Dates: 1989-present

Technology Maturity:



Technology Transfer:

Project Meetings, quarterly reports, publications.

Key Documentation:

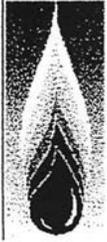
S. D. Kohler, M. S. Harrington, and N. B. Jackson, "Attrition and Carbon Formation on Iron Catalysts" Preprints of Papers, 39 (4), 1122, (1994), Fuel Division, American Chemical Society.  
M. D. Shroff, D.S. Kalakkad, K. E. Coulter, S. E. Kohler, M. S. Harrington, N. B. Jackson, A. G. Sault, and A. K. Datye, "Activation of Precipitated Iron Fischer-Tropsch Synthesis Catalysts," Journal of Catalysis, submitted.

Key Personnel:

N. B. Jackson, 505-844-0940  
A. G. Sault, 505-844-8723  
J. R. Torczynski, 505-845-8991  
T. J. O'Hern, 505-844-9061  
K. A. Shollenberger, 505-844-9132

Lab Capabilities Applied:

Catalyst evaluation, advanced instrumentation, fluid dynamics and thermal sciences engineering analysis.



**Index:** 348

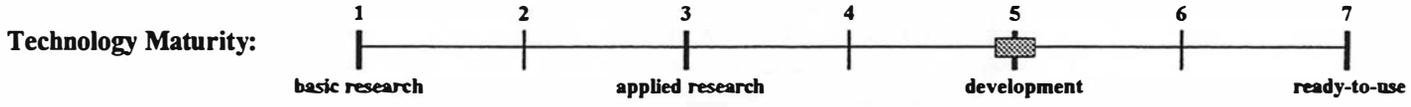
**Category:** Drilling & Completion (3), Production (11, 25)

**Laboratory:** Sandia National Laboratories **Contact:** N. R. Warpinski, 505-844-3640

**Title:** Hydraulic Fracturing Diagnostics

**Description:** The Sandia hydraulic fracturing diagnostics project is concerned with the development of existing or new technology for imaging hydraulic fracture growth at depth. The key technology being developed is seismic based, but seismic results are being confirmed with downhole strain measurements and direct coring of fractures so that seismic methods can be validated for the first time. Industry is involved through the Gas Research Institute (GRI) Project Advisory Group (PAG) which consist of oil company advisors, and also through a cooperative effort with an industrial partner (BOLT Technologies, Inc.) to market the technology developed here. Sandia also conducts experiments with interested oil companies to assure that the technology meets their needs. The ultimate deliverable of this project is to develop a real-time fracture diagnostic service industry that can be contracted to image a fracture in many different environments. The development of this industry requires new software algorithms, advanced multi-level receiver technology, and fast transmission and data-acquisition capabilities, all based on PC systems familiar to the oil industry. Previous results include detailed images of fracture experiments and their development with time, evaluation of multi-level technology, and optimization analyses of required receiver capabilities for accurate imaging. The applications of this technology are foremost for hydraulic-fracture stimulation, including tight gas sands and oil-well fracturing, but also including drill-cutting re-injection, waste disposal, EOR processes and other production activities. A successful hydraulic fracture is the single most important element in economic gas wells and observing the fracture's behavior is the key missing element for process optimization. Monitoring of cutting and waste injection may become mandatory, so imaging capabilities will be essential for this technology.

**91-95 Funding (\$K):** 3500 **Dates:** 1976-present



**Technology Transfer:** Journal articles (SPE), reports, joint projects, help and consultation on industry projects, licensing of advanced receiver technology, work with an industrial partner, and participation in GRI sponsored forums and reviews.

**Key Documentation:** U. S. Patent 5,189,262 Advanced Motor Driven Clamped Borehole Seismic Receiver, February 23, 1993. The use of Broadband Microseisms for Hydraulic Fracture Mapping, SPE 26485, Proc. 68th Annual SPE Conf., Houston, TX, pp. 707-717, October 1993 (To be published in one of the SPE Journals).

**Key Personnel:** N. R. Warpinski, 505-844-3640  
C. J. Young, 505-844-8329  
R. S. Harding, Jr., 505-844-0780

**Lab Capabilities Applied:** Instrumentation Expertise, Digital Signal Processing, Seismic Modeling, Geomechanics.



Index: 349

Category: Environmental & Regulatory (6), Development (31)

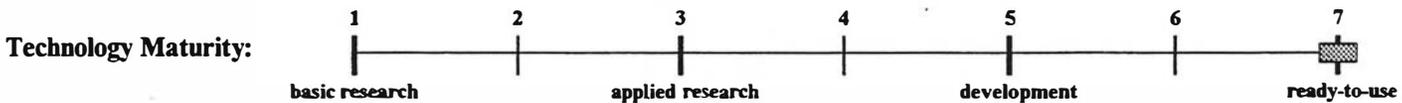
Laboratory: Sandia National Laboratories Contact: Sanford Ballard, 505-844-6293, sballar@sandia.gov

Title: In Situ Permeable Flow Sensor

**Description:** The In Situ Permeable Flow Sensor uses a thermal perturbation technique to directly measure the full three-dimensional groundwater flow velocity vector in saturated, unconsolidated sediments. The basic operating principle of the technology is to bury a thin, cylindrical heater in the ground at the point where the groundwater flow velocity is to be measured. When the heater is activated, a spatially uniform heat flux out of the cylinder is established. After thermal equilibrium is achieved, which generally takes 24 to 48 hours, the temperature distribution on the surface of the cylinder will vary as a function of the direction and magnitude of the groundwater flow velocity past the cylinder. In essence, relatively warm temperatures are observed on the downstream side of the probe and relatively cool temperatures on the upstream side as some of the heat introduced into the formation by the heater is advected around the instrument by fluid flow past the tool. The technology can measure groundwater flow velocities in the range of about .000005 to .001 cm/s.

Flow sensors are simple and inexpensive foam cylinder surrounded by a thin film flex circuit heater with an array of 30 thermistors and a waterproof jacket. The sensor is permanently buried in the soil using a hollow-stem auger, allowing the soil to collapse in around the probe after insertion. The probe data are collected via a remote data acquisition system that can be monitored remotely. Crucial to the application of the hardware is a computer program that uses an inversion technique to determine the groundwater flow given the thermistor temperature distribution.

91-95 Funding (\$K): 1520 Dates: 1990-1994



Technology Transfer: Publications, staff exchange, licensed product, presentations

Key Documentation: Ballard, S. The In Situ Permeable Flow Sensor: a groundwater flow velocity meter, accepted, Journal of Groundwater, 1995.  
Ballard, S. A test of the In Situ Permeable Flow Sensor at Savannah River, SC, accepted, Journal of Groundwater, 1995.

Key Personnel: Sanford Ballard, 505-844-6293, sballar@sandia.gov  
Glenn Barker, 505-844-7481, gtbarke@sandia.gov

Lab Capabilities Applied: Fluid Dynamics, Thermal Geophysics, Electrical Engineering, Data Acquisition, Instrumentation, materials science, numerical modeling



**Index:** 350

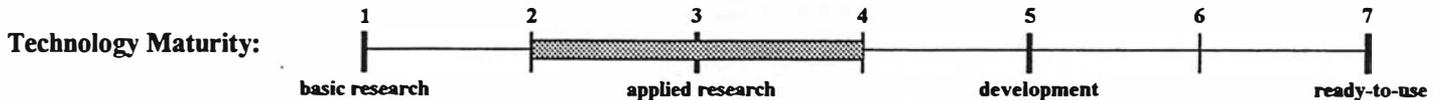
**Category:** Development (9, 2, 5, 14, 18), Exploration (1, 9)

**Laboratory:** Sandia National Laboratories      **Contact:** W. R. Wawersik, 505-844-4342, wrwawer@sandia.gov

**Title:** Rock Mechanics Investigations

**Description:** Knowledge of rock properties and the deformation and failure of rocks are vitally important to the gas and oil industry in exploration, development, and production. We have continuing efforts in experimental and analytical applied rock mechanics which are centered around four themes: (1) Shear strain localization and fracture/fault evolution. A phenomenological material model captures the major characteristics of rock behavior and describes faulting as a constitutive instability. The experimental part is based on advanced true-triaxial testing to measure the onset of localization as a function of the stress state. (2) Micromechanics of failure. The objective is a basic understanding of the effects of grain boundary structure and cementation, damage state, and load path (via triaxial tests) on the deformation and failure mode of brittle porous geologic materials by measurement of the mechanical behavior under high pressure and deviatoric stress, quantitative microstructural characterization of pristine and deformed samples, and theoretical analysis. The micromechanical processes are described quantitatively using light microscopy, laser scanning confocal microscopy, and scanning electron microscopy. (3) Characterization of creep. Creep in such rocks as salt and diatomite is measured in triaxial laboratory test machines at constant applied stress and in variable stress-path tests with and without pore fluids. The results are used to develop constitutive models for use in computer codes and engineering design, and have been extensively applied in geotechnical studies supporting the Strategic Petroleum Reserve. (Creep studies in salt began in 1972.) (4) Transport paths in single natural fractures. This study uses quantitative visual observations of flow and two-phase flow in discrete fractures. Quantitative measurements of fracture aperture are obtained by combining optical imaging and nuclear magnetic resonance imaging. Parallel work is directed at using graph, effective-medium, and percolation theories to analyze the topology of the conducting networks of void space.

**91-95 Funding (\$K):** 2070      **Dates:** 1993-present



**Technology Transfer:** Open literature, industry working groups, staff exchange.

**Key Documentation:** Holcomb, D. J., Localization studies under triaxial conditions, in Proc. 33rd U. S. Symp. Rock Mech., pp. 661-670, 1992.  
Brown, S.R., Simple mathematical model of a rough fracture, J. Geophys. Res., in press.

**Key Personnel:** D. J. Holcomb, 505-844-2157, djholco@sandia.gov  
S.R. Brown, 505-844-0774, srbrown@sandia.gov  
W. A. Olsson, 505-844-7344, waolssso@sandia.gov  
J.T. Fredrich, 505-844-2096, fredric@sandia.gov  
D.H. Zeuch, 505-844-6829, dhzeuch@sandia.gov

**Lab Capabilities Applied:** Rock mechanics testing facility, high pressure and true triaxial loading and creep test machines, permeability laboratory, microscopy (optical, SEM, laser scanning confocal), non-contacting laser profiler.



Index: 351

Category: Deepwater Offshore (9, 16)

Laboratory: Sandia National Laboratories

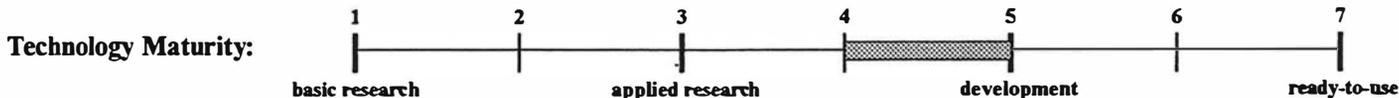
Contact: R. K. Thomas, 505-844-7450, rkthoma@sandia.gov

Title: Advanced Computational Models for Deep Water Oil and Gas Production (ACTI)

**Description:** This project is a collaboration between Sandia and the DeepStar Consortium, a cooperative oil and gas industry endeavor to develop leading edge technologies that will open new oil and gas fields in deep water (>6000 ft.). Over the past five years, in excess of 3.2 billion barrels of oil have been discovered in the deep water Gulf of Mexico. By comparison, the Alaskan North Slope contains an estimated 3.5 billion barrels. Today the US imports 50% of its total daily oil consumption of 16 million barrels. With deep water production, imports will be reduced through the early part of the next century, and approximately 40,000 jobs could be created.

Deep water oil production in the Gulf of Mexico is not commercially feasible with present technology. One component requiring major technical advances in the design of deep water risers and umbilicals used to transport oil to surface facilities. The goal of this project is to develop computational methods for structural analysis and material selection of deep water risers using Sandia's expertise in large-scale computations and DeepStar Consortium's expertise in design and operation. We will specifically address (1) stresses on flexible deep water risers resulting from ocean currents and platform motions, and (2) the strength of composite material risers and adhesive joints.

91-95 Funding (\$K): 650      Dates: 1995-present



Technology Transfer: DeepStar Consortium Working Group, staff exchange, Sandia short courses, ASME and SPE papers and symposia, News Releases, Trade Journal Articles, INTERNET Home pages.

Key Documentation: Proc. of the Forum on Vortex Methods for Engineering Applications, Sponsored by Sandia National Laboratories, February 22-24, 1995, Albuquerque, NM.  
 E. D. Reedy, Jr., and T. R. Guess, Composite-to-Metal Tubular Lap Joints: Strength and Fatigue Resistance, Int. Jour. of Fracture, 63, p. 351-367, 1993.

Key Personnel: James H. Strickland, 505-844-8421, jhstric@sandia.gov  
 Frank J. Mello, 505-844-5357, fjmello@sandia.gov  
 Don W. Lobitz, 505-844-9398, dwlobit@sandia.gov  
 E. Dave Reedy, 505-844-3297, edreedy@sandia.gov

Lab Capabilities Applied: Offshore Dilling Technology, Engineering Sciences, Structural Mechanics, Fluid Mechanics, Fluid/Structure Interaction, Finite Element Methods, Material Science, Bonding, Fatigue Analysis, High Performance Computing, Diagnostics, Instrumentation.



Index: 352

Category: Oil Processing &amp; Refining (1, 4, 11, 25)

Laboratory: Sandia National laboratories

Contact: John Shelnett, (505) 844-8856

Title: Conversion of Carbon Dioxide Using Biomimetic Catalysts

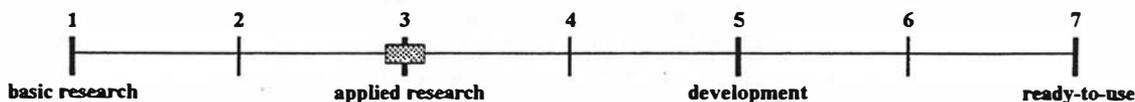
**Description:** The goal of this project is to use computer-aided molecular design to develop catalysts that electrochemically reduce carbon dioxide to chemicals that are commercially useful such as methanol and formaldehyde. This process would simultaneously destroy a greenhouse gas and develop an underutilized carbon source. Initial catalyst choices are based on molecules found in the enzymes that activate many small molecules, including carbon dioxide, oxygen and nitrogen. The effects of geometry, binding pockets, hydrogen bonding and ionic interactions are studied theoretically, and then molecules found to be optimal for binding carbon dioxide are synthesized and tested for electrocatalytic activity in the laboratory. Our unique laboratory capabilities include a state-of-the-art computing facility utilizing massively parallel processing and graphics workstations that allow us to model these large and complicated molecules. Experimental testing includes Raman and NMR spectroscopy which yield conformational data needed to verify modeling parameters and chemical and electrochemical instrumentation for measuring catalytic activity and product yields. Biosym, the world's largest producer of computational software for chemical catalysis, has provided much of the molecular and quantum mechanics computer code as well as the programming and development assistance necessary to measure accurately both the structure and reactivity of catalysts which will reduce CO<sub>2</sub>. A CRADA under development with Dupont proposes that Dupont will provide synthesis capabilities to make the computer-designed molecules for testing in Sandia Laboratories and will do pilot plant testing on promising catalysts. Computer-aided catalyst design will greatly reduce costs associated with developing catalysts by rapidly identifying key molecular features necessary to drive the desired reaction. In the particular case of carbon dioxide conversion, an understanding of which elements in natural systems are required for activating this extremely stable molecule will be gained and applied to catalyst development.

91-95 Funding (\$K):

1500

Dates: 1990-Present

Technology Maturity:



Technology Transfer:

Informal collaborations, staff visits, open literature publications, annual reports, graduate students.

Key Documentation:

Medforth, C.J., J. A. Shelnett et al., "Control of Axial Ligand Orientations in Highly Nonplanar Metalloporphyrins and Implications for the Design of Porphyrins and Regio- and Stereo-Specific Oxidation Catalysts," *J. Chem. Soc., Chem. Commun.* 1994 (in press).  
 Hobbs, J. D., J. A. Shelnett et al., "Structural Heterogeneity and Coordination Chemistry of Nickel(II) Octaethyl-meso-nitroporphyrins," *J. Am. Chem. Soc.* 1994, 116, 3261.

Key Personnel:

John Shelnett, 505-844-8856  
 David Hobbs, 505-844-5571  
 Gail Ryba, 505-844-1802

Lab Capabilities Applied:

Computer-aided molecular design; Raman spectroscopy; advanced materials synthesis techniques; electrocatalytic testing



Index: 353

Category: Drilling & Completion (9)

Laboratory: Sandia National Laboratories      Contact: John Finger, 505-844-8089

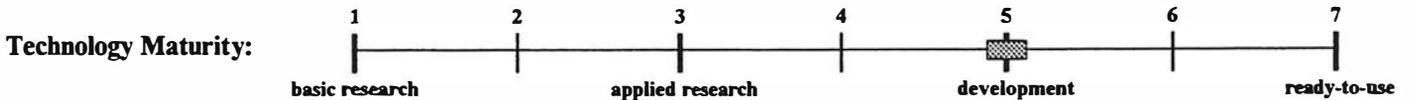
Title: Slimhole Drilling for Geothermal Exploration and Reservoir Assessment

**Description:** The slimhole drilling program accrues benefits for the geothermal industry in three major areas: increased exploration, reduced environmental impact, and deferred costs in power plant construction. Smaller rigs, crews, drill sites, and less consumable goods are some of the reasons that slimhole drilling is cheaper than production-size wells at many locations; these same reasons mean reduced environmental impact. Because cost savings are so site-specific, it is difficult to generalize, but a reasonable estimate is that slimhole exploration wells will cost approximately half as much as production-size wells. This leads to twice as many exploration wells, and in environmentally sensitive areas, may make exploration wells possible at all.

In traditional power plant development, production wells are used for exploration as well as to prove the reservoir in order to secure financing and permits for power plant construction. These large wells are thus drilled long before the plant is built and starts returning revenue that can pay off development costs. If the reservoir can be proven with slimhole exploration, this long term debt service can be reduced by drilling the production wells later in the course of development.

There are presently three major activities in this program: (1) Acquisition of data from slimholes and nearby production wells; (2) Analysis of these data to determine whether the slimhole measurements adequately predict performance of production wells; (3) Transfer of this information to industry through meetings, professional papers, industry contacts, and, eventually, a handbook on drilling, completing, testing, and analyzing exploratory slimholes.

91-95 Funding (\$K): 5000      Dates: 1991 - Present



**Technology Transfer:** DOE Geothermal Program Review, Geothermal Industry Advisory Panel, Sandia SAND Report, article in Geothermal Resources Council "Bulletin", paper at World Geothermal Congress

**Key Documentation:** Finger, J. T., Jacobson, R. D., Hickox, C. E., Eaton, R. R., "Steamboat Hills Exploratory Slimhole: Drilling and Testing"; Sandia Report SAND94-0551; Oct. 94  
 Finger, J. T., Jacobson, R. D., Hickox, C. E., Eaton, R. R., "Slimhole Drilling for Geothermal Exploration", Proceedings of World Geothermal Congress; Florence, Italy; May 95

**Key Personnel:** John Finger, 505-844-8089  
 Ron Jacobson, 505-844-0938  
 Charles Hickox, 505-844-5882  
 Roger Eaton, 505-844-4063

**Lab Capabilities Applied:** Drilling Engineering, Mechanical Engineering, Fluid Flow, Heat Transfer, Wellbore Modeling, Finite-Element Modeling, Reservoir Modeling, Instrumentation



Index: 354

Category: Drilling & Completion (3), Production (11, 13, 25)

Laboratory: Sandia National Laboratories

Contact: N. R. Warpinski, 505-844-3640

Title: Hydraulic Fracturing

**Description:** Many of the basic mechanisms controlling hydraulic fracture behavior are still poorly understood, cannot be duplicated in the lab, and are questionably represented by fracture models. Starting with mineback experiments in the early 1970's and continuing through Multiwell field experiments and more recently the coring of a hydraulic fracture, this project has endeavored to provide real field evidence of operating mechanisms in the fracturing process and an unbiased comparison with available models.

Sandia has continually been involved with industry through technical advisory panels, joint modeling forums, service company involvement in fracturing tests, and testing of new technology and concepts. Results of this project have led to new technologies being applied by industry (e.g., extreme overbalanced perforating) and new mechanisms have been incorporated in models (e.g., multiple fractures).

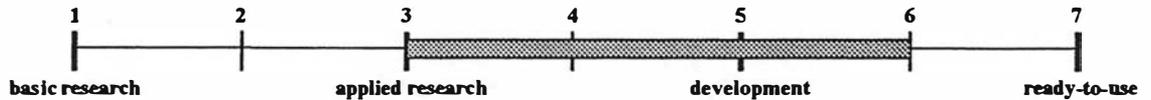
Results of this project have included a recovery of core through a hydraulic fracture in a deep gas well (at the Multiwell site) and a documentation of the implications of the complicated fracturing seen in that core, the assembly of calculations from most available fracturing simulators in a comparison study based upon the GRI Staged-Field Experiment results, and detailed evaluations of stress measurement techniques for fracture model input.

Application of this technology has resulted in improvement in fracture models and design calculations which has helped to optimize fracture performance. The in situ stress techniques developed during this project have now become the standard for industry stress measurements. Extreme overbalanced perforating, first used in this project, has become an important industry tool.

91-95 Funding (\$K): 600

Dates: 1976-present

Technology Maturity:



**Technology Transfer:** Technology transfer occurs through journal articles (SPE), reports, help and consultation on industry projects, participation in forums and reviews, and joint projects with oil companies in GRI sponsored projects.

**Key Documentation:** Warpinski, N. R., J. C. Lorenz, P. T. Branagan, F. R. Myal and B. L. Gall, "Examination of a Cored Hydraulic Fracture in a Deep Gas Well," SPE Production & Facilities, Vol. 8, pp. 150-158, August 1993.  
Warpinski, N. R., Z. A. Moschovidis, C. D. Parker and I. S. Abou-Sayed, "Comparison Study of Hydraulic Fracturing Models - Test Case: GRI Staged Field Experiment No. 3," SPE Production & Facilities, Vol. 9, pp. 7-16, February 1994.

**Key Personnel:** N. R. Warpinski, 505-844-3640  
L. W. Teufel, 505-844-8680  
A. R. Sattler, 505-844-1019

**Lab Capabilities Applied:** In Situ Stress expertise, Fracture modeling, Geomechanics, High energy gas fracturing.



Index: 355

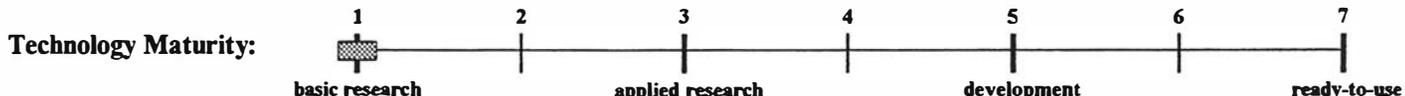
Category: Oil Processing & Refining (1, 25)

Laboratory: Sandia National laboratories Contact: Gary Carlson, (505) 844-8116

Title: Study of Catalysts Using ab initio Codes on Massively Parallel Computers.

**Description:** To model or theoretically study advanced catalytic materials requires a combination of high-performance computing resources and a variety of computational and theoretical techniques and methods. The objective of this project is to develop these techniques and methods and then apply them to the study of real or potential catalytic systems using Sandia National Laboratories' (SNL) high-performance massively parallel computers. Our approach is: 1) To develop, implement, and test numerical libraries for use with massively parallel computers, 2) To integrate these libraries into Biosym Technologies' molecular modeling codes, as well as into SNL's in-house codes, and 3) To apply these codes to the study of catalytic systems. To study the subtle electronic and structural interactions that take place in catalysts requires a quantum mechanical level of study. For this reason we employ the Density Functional Theory (DFT) approach in this work. Using SNL's unique massively parallel computing resources and expertise in designing algorithms and codes that make use of these resources, we have developed parallel numerical libraries which have been integrated into two separate DFT codes - DMOL (from Biosym Technologies, Inc.) and QUEST (an in-house SNL code). Biosym Technologies has participated in this project by integrating these libraries into their DMOL code as well as participating in the use of this code to study catalytic systems. Systems of catalytic interest that have been studied include bulk metal surfaces, transition metal nanoclusters, biomimetic molecules, and membrane materials including the interaction of reactant molecules with these systems. This approach allows researchers to study systems of unprecedented size with quantum mechanical accuracy, elucidating the processes that occur in real catalytic systems and allowing the design of new catalysts for applications of industrial interest.

91-95 Funding (\$K): 1050 Dates: 1992-Present



Technology Transfer: CRADA with BIOSYM Technologies, Inc.; staff visits, open literature publications.

Key Documentation: Li, Y. S., T. Klitsner, et al., "Density Functional Methods as Computational Tools in Materials Design," J. Computer-aided Materials Design 1993, 1, 199.  
Li, Y.S., T. Klitsner et al., "Mesh-based LDA Electronic Structure Calculations on a Parallel Computer," presented at the High Performance Computing '94 Meeting, La Jolla, CA, April, 1994 (to be published).

Key Personnel: Tom Klitsner, 505-844-1901  
Mark Sears, 505-845-7194  
Peter Schultz, 505-845-7771  
Tony Martino, 505-844-4332

Lab Capabilities Applied: Massively parallel computer (Paragon), quantum codes, computer-aided molecular design; nanocluster materials synthesis



**Index:** 356

**Category:** Development (7, 17, 18)

**Laboratory:** Sandia National Laboratories      **Contact:** J. C. Lorenz, 505-844-3695

**Title:** Natural Fractures

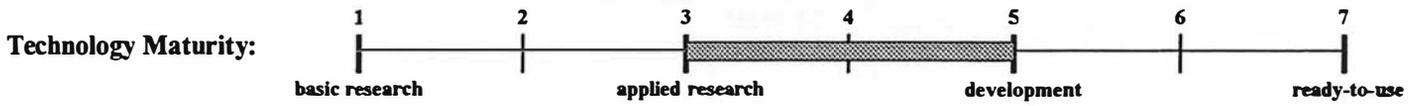
**Description:** Natural fractures are the key production mechanism in an ever-increasing number of U. S. and international reservoirs. They provide the pathways by which oil and gas migrate to the wellbore and are produced. Natural fractures, however, have strong preferential orientations, stress sensitivity, relations to bedding, and other features that make them difficult to exploit. This project determines fracture characteristics and the important geomechanical relationships that exist at depth in the reservoir so that exploitation of the reservoir can be optimized.

Studies and analyses of natural fracture systems have been carried out in producing reservoirs in conjunction with many oil companies (e.g., UPRC, Amoco, Oryx, Arco, Phillips). In other reservoirs, results of detailed studies have been requested and used by producers (e.g., Barrett, Mobil, Shell).

This project has used actual field studies to show the characteristics of regional fractures (e.g., Mesaverde, Austin Chalk and Frontier formations) and structurally related fractures (e.g., Ekofisk). Stress sensitivity of the fracture systems, production characteristics, relationships between outcrop and downhole fracture data, methodology for evaluating natural fractures from core and logs, relationships between fractures and bedding, and many other important aspects of natural fracture systems have been documented, employed in reservoir studies, and requested by oil companies.

Applications of these natural fracture studies include use in horizontal drilling, optimization of well spacing and layout, evaluation of stimulation and enhanced recovery technology, evaluation of secondary recovery and infill drilling potential, development of new fracture identification technology, and improvement of reservoir simulators.

**91-95 Funding (\$K):** 1800      **Dates:** 1981-present



**Technology Transfer:** Technology transfer occurs through journal articles (SPE and AAPG), reports, help and consultation on industry projects, field trips, and GRI and industry sponsored forums.

**Key Documentation:** Lorenz, J. C., L. W. Teufel and N. R. Warpinski, "Regional Fractures I: A Mechanism for the Formation of Regional Fractures at Depth in Flat-Lying Reservoirs," AAPG Bulletin, Vol. 75, No. 11, pp. 1714-1737, November 1991.  
Lorenz, J. C., N. R. Warpinski and L. W. Teufel, "Rational for Finding and Exploiting Fractured Reservoirs, Based on the MWX/SHCT-Piceance Basin Experience," SAND93-1342, Sandia Natl. Labs Report, 150 pp., July 1993.

**Key Personnel:** J. C. Lorenz, 505-844-3695  
N. R. Warpinski, 505-844-3640  
L. W. Teufel, 505-844-8680

**Lab Capabilities Applied:** Natural Fracture Expertise, Geomechanics, Rock Mechanics Testing Facility.



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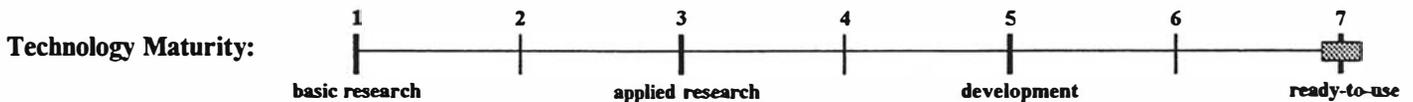
Category: Development (10, 3), Exploration (3, 10, 14, 16)

Laboratory: Sandia National Laboratories      Contact: R. S. Chad Harding, (505) 844-0780, rshardi@sandia.gov

Title: Advanced Borehole Seismic Receiver

**Description:** Project Goal: Develop and make commercially available an advanced three-component multi-station borehole seismic receiver.  
 Project Team: The receiver was jointly developed and funded by DOE and Industry. The engineering design and testing was performed by Sandia National Laboratories. The hardware fabrication and tool commercialization was performed by OYO -Geospace. The high temperature fiber optic wireline was fabricated and commercialized by Rochester.  
 Results and Deliverables: The goal of this project was to develop a three component multi-station borehole seismic receiver with improved bandwidth, faster data acquisition and transfer, and higher signal-to-noise than presently available receivers. An advanced receiver sonde was developed which has the following features. It is much shorter and lighter (16" L x 4" O.D., 30 lbs) than most receivers which increases its mechanical resonance from the 150-400 Hz. of presently available receivers to ~2000 Hz. The receivers are modular, and a number of them can be strung together in a receiver string, reducing data collection time. Each receiver contains its own digitizing circuitry, so that only digital data is transferred between sondes. The output of all of the sondes is sent to a data formatter/telemetry module where the data is converted to optical signals which are sent to the surface over a special fiber optic wireline. This dramatically increases the data transfer rate and allows a number of sondes to be operated in a string with no time penalty. Up to 30 sondes can be interconnected and collect 1/8 msec sample data in real time. The sondes use an advanced three axis accelerometer, with improved noise characteristics at high frequency. The sondes incorporate a new wall locking piston type clamp for improved bandwidth. The sondes are designed for 10,000 psi external pressure and >125 C well temperature. The sondes have been field tested in a number of surveys, and are now commercially available through OYO-Geospace, or as a field service thru Bolt International. As part of this project, a high temperature fiber optic wireline was fabricated and commercialized by Rochester. It contains 7 conductors and 1 multi-mode fiber and is designed with armor similar to conventional 7 conductor wirelines. It is operational to 200 C.

91-95 Funding (\$K): 3100      Dates: 1989-1994



Technology Transfer: OYO has a non-exclusive license to produce and market the receiver. Rochester will offer the fiber optic wireline as a commercial item. A complete development report is being published in a SAND document and will be widely available.

Key Documentation: Report SAND 94-2162, Development of a Multi-Level Seismic Receiver, February 1995, 228 pp. U.S. Patent # 5189262 Advanced Motor Driven Clamped Borehole Seismic Receiver Feb 23, 1993.

Key Personnel: Ron Franco, (505) 845-8654, Gerry Sleaf, (505) 844-2195, Bruce Engler, (505) 844-7419, Bob Cutler, (505) 844-5576

Lab Capabilities Applied: Dynamic modeling, borehole tool design, seismic testing, vibration testing, high temperature electronics, mechanical design, fiber optic telemetry, materials, program management



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**Category:** Oil Processing & Refining (9, 1, 7, 16), Environmental & Regulatory (10)

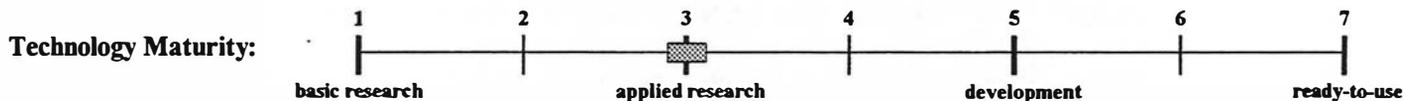
**Laboratory:** Sandia National Laboratories

**Contact:** Nancy Jackson, (505) 844-0940

**Title:** Replacement of Liquid H<sub>2</sub>SO<sub>4</sub> and HF Acids with Solid Acid Catalysts in the Paraffin Alkylation Process

**Description:** This effort investigates using hydrous titanium oxides (HMOs) and crystalline silicotitanates (CSTs) as paraffin alkylation catalysts. Paraffin alkylation (PA) is a petrochemical process that is used to produce high-octane, yet clean burning, low-emission gasoline additives. The products of PA are highly branched alkanes, which do not have the toxicity or emission problems found with other high-octane blending components such as benzene or xylene. The problem with PA is that at present the only technologies available require either liquid sulfuric acid (H<sub>2</sub>SO<sub>4</sub>) or liquid hydrofluoric acid (HF) as a catalyst. These mineral acids represent serious safety and environmental hazards. Despite the environmental drawbacks to the process, demand for these compounds will increase not only domestically but worldwide as fuel standards become more stringent, since the PA process produces clean-burning low emission compounds for gasoline blending. We propose to replace H<sub>2</sub>SO<sub>4</sub> and HF with solid acid catalysts developed from HMO and/or CST materials. Results from experimental work with HMOs and CSTs as catalysts for other petrochemical reactions indicate that these materials may be very good solid acid catalysts.

**91-95 Funding (\$K):** 765

**Dates:** 1995-present

**Technology Transfer:** Informal collaboration, staff visits, annual reports.

**Key Documentation:** N. B. Jackson, "Replacement of Liquid H<sub>2</sub>SO<sub>4</sub> and HF Acids with Solid Acid Catalysts in the Paraffin Alkylation Process," Sandia National Laboratories LDRD Proposal 95-t-00138, June 15, 1994.  
J. E. Miller, R. G. Dosch, & L. I. McLaughlin, "Hydrous Metal Oxide Catalysts for Oxidation of Hydrocarbons," Sandia National Laboratories Report SAND93-1039, 1993.

**Key Personnel:** N. B. Jackson, 505-844-0940  
C. Ashley, 505-845-8931  
J. A. Voight, 505-845-9044  
T. Nenoff, 505-844-0340  
T. Gardner, 505-845-7502

**Lab Capabilities Applied:** Advanced materials synthesis; materials characterization; catalyst evaluation; and laboratory-scale process simulation.



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Category:

Laboratory:  Contact:

Title:

Description: The Geothermal Drilling Organization is a non-profit organization of geothermal operating and service companies. These companies join with DOE to jointly fund near-term projects that result in a product or service. Development contracts are placed by Sandia, and Sandia personnel follow progress of all contracted work and serve as technical consultants. Typically, new projects are started each year. Currently, the following three projects are active: (1) improved positive displacement motors for operation at high temperature with air, (2) adaptation of a retrievable whipstock to geothermal well conditions, and (3) development and testing of new cementitious lost circulation materials.

91-95 Funding (\$K):  Dates:



Technology Transfer: GEO projects include participants that are all commercial suppliers of drilling technology. Successful projects can, therefore, be rapidly commercialized by the supplier.

Key Documentation:

Key Personnel:

Lab Capabilities Applied:



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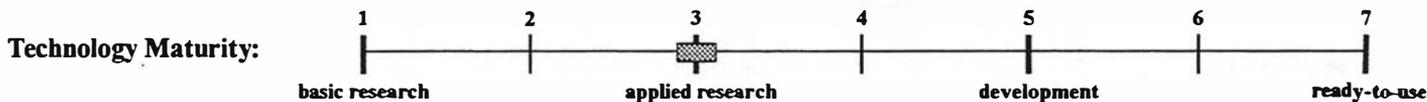
**Category:** Environmental & Regulatory (12, 9)

**Laboratory:** Sandia National Laboratories **Contact:** James M. Phelan, 505-845-9892

**Title:** Numerical Modeling of Thermal Enhanced Vapor Extraction Remediation Technology

**Description:** The past three years experience working with the Thermal Enhanced Vapor Extraction System (TEVES), and Sandia's development of new numerical codes using massively parallel computing for the TEVES system design and evaluation, has contributed to our capability of expansion in these areas. Our TEVES experience includes engineering design, numerical modeling, permitting of field demonstrations, and actual field demonstration of the TEVES technology.

**91-95 Funding (\$K):** 2500 **Dates:** 1993-present



**Technology Transfer:** Transfer of numerical codes, publications.

**Key Documentation:** Phelan, J. M. and S. W. Webb, Thermal Enhanced Vapor Extraction Systems - Design, Application, Performance Prediction, including Contaminant Behavior. In proceedings of: Thirty-Third Hanford Symposium on Health and the Environment, Insitu Remediation: Scientific Basis for Current and Future Technologies, November, 1994.  
 Webb, S. W. TOUGH2 Simulations of the TEVES Project Including the Behavior of a Single-Component NAPL. Sandia National Laboratories, Albuquerque, NM. SAND94-1639. January, 1995.

**Key Personnel:** James M. Phelan, 505-845-9892  
 Stephen W. Webb, 505-848-0623  
 Mario J. Martinez, 505-844-8729

**Lab Capabilities Applied:** Massively parallel computing, environmental remediation technology, site demonstrations of thermal enhanced vapor extraction remediation technology.



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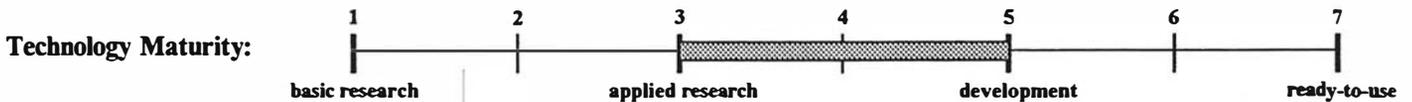
Category: Development (3, 10), Exploration (4, 14)

Laboratory: Sandia National Laboratories Contact: Richard S. Harding, Jr. - (505) 844-0780

Title: Single-well Imaging of Salt Dome Flanks (ACTI)

**Description:** Surface seismic and salt proximity surveys sometimes fail to provide the high resolution images of salt flank and subsalt geology required for efficient development of petroleum reserves. By placing seismic sources and receivers in the same well, the recording datum is both close and subparallel to the target, and higher resolution data can potentially be obtained. As borehole instrumentation required to perform single-well imaging nears implementation, seismic modeling and imaging tools tailored to the single-well geometry and recording environment are required to assist instrumentation development, design surveys, and process collected data. In this project, seismic modeling and imaging codes will be developed to bring single-well seismic imaging of salt dome flanks to maturity. In the first year code development will include 3D viscoelastic finite difference forward modeling with adaptive grids, and 3D Kirchhoff migration using operator aperture limits based on arrival angle of incident reflection energy. Tube wave modeling will be performed to assist field survey design, and development of a tube wave suppression algorithm. Field data will be acquired in the project. In the first year field data will be acquired in dual-well configuration. In the second and third years, single-well data will be acquired. Field data from the salt dome site will be analyzed using codes developed in the project. Computationally demanding codes will be implemented on Sandia's parallel distributed workstation array. Industry participation is organized by the new Salt Imaging Consortium. Commercialization of developed codes will be provided by Advance Geophysical/Landmark.

91-95 Funding (\$K): 1550 Dates: 1995 - present



Technology Transfer: CRADA/licensing agreements.

Key Documentation: Proposal is available from Sandia contact. Detailed Work Plan is in preparation.

Key Personnel: R. C. Armstrong, (510) 294-2470  
R. S. Harding, (505) 844-0780

Lab Capabilities Applied: Borehole Seismic Data Processing, Distributed Systems Computing, Borehole Source and Receiver Technology



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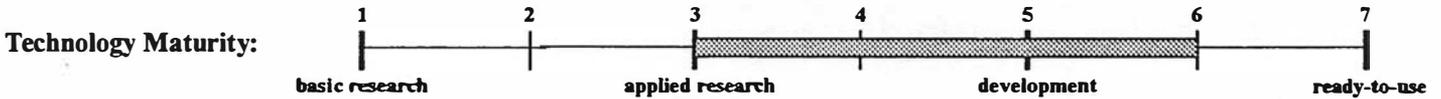
Category: Development (10, 6, 14), Environmental & Regulatory (10), Exploration

Laboratory: Sandia National Laboratories      Contact: R.S. Chad Harding, 505-844-0780, rshardi@sandia.gov

Title: Electromagnetic Reservoir Characterization

**Description:** The Electromagnetic (EM) Reservoir Characterization program at Sandia has focused on developing and proving new EM methods for characterizing reservoirs or environmental sites. The work has covered the spectrum from reservoir engineering (to understand the properties to be measured and interpret the results of field tests), through instrumentation development, to EM modeling (to investigate how to invert or interpret field data).  
 Specific techniques developed include: surface electrical potential (SEP), controlled source audio magnetotellurics (CSAMT), cross-well EM imaging, borehole radar, and borehole-to-surface imaging. Some of these techniques are now being used commercially. Modeling has included reservoir simulation of electromagnetic properties during EOR processes, expected responses from different source-receiver configurations, and expected responses for algorithm development. Significant development of algorithms have been direct inversion methods and integral wave field migration imaging. Significant instrumentation development include establishing the borehole-to-surface method to image oil reservoirs and for environmental characterization. A patent application, "Radar System for geologic Analysis" #966,917 Oct. 27, 1992, has been submitted for the borehole radar. Key to the program has been joint field testing of techniques with industry in producing fields.

91-95 Funding (\$K): 3700      Dates: 1987-present



Technology Transfer: SEG Papers, Forums, SPE Papers, Joint Field Tests with Industry, Patents

Key Documentation: 1) Bartel, L.C.: "Application of EM Holographic Methods to Borehole Vertical Electric Source Data to Map a Fuel Oil Spill," Technical Program Expanded Abstracts, Society of Exploration Geophysicists, 63 Annual Meeting and International Exposition, Washington DC, September 1993. 2) Newman, G A.: "Cross well EM inversion using integral and differential equations," Geophysics, May/June 1995.

Key Personnel: Lew Bartel, 505-844-6902, lcbarte@sandia.gov  
 Gregory Newman, 505-844-8158, ganewma@sandia.gov  
 John Waggoner, 505-844-2100, jrwaggo@sandia.gov  
 Thurlow Caffey, 505-844-4217, twcaffey@sandia.gov  
 A.J. (Chip) Mansure, 505-844-9315, ajmansu@sandia.gov

Lab Capabilities Applied: Geophysics, EM Modeling, Reservoir Engineering, Electrical Engineering, Instrumentation, Inversion Techniques, Simulation, Field Testing, Diagnostics



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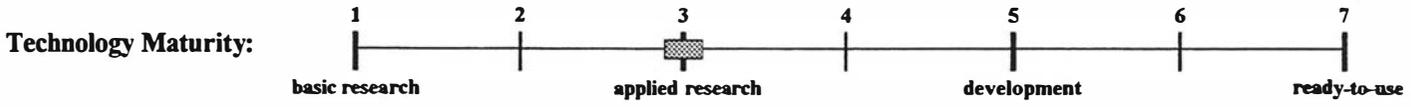
Category: Development (2), Exploration (5, 9, 11)

Laboratory: Sandia National Laboratories      Contact: Harold S. Morgan, 505-844-7045, hsmorga@sandia.gov

Title: Computational Geomechanics for Geologic Structure and Reservoir Mechanics (ACTI)

**Description:** Large-strain, quasistatic, structural mechanics finite element codes, developed at Sandia for nuclear weapon and energy and environment programs, will be adapted and enhanced to simulate, in three-dimensions, the mechanical response of rocks over spatial and temporal scales of interest to the oil and gas industry. On the field scale, applications driving the code development are predictions of subseismic faulting, fracturing, and folding associated with geologic scale deformations to allow better interpretation of seismic data, understanding of stress fields resulting from tectonic plate motion, etc. On the reservoir scale, applications are predictions of the structural response of weak porous rock as reservoirs are produced to understand changes in transport properties due to production induced compaction and fracturing. Coupling to multi-phase flow response will also be addressed. The computational tools already in existence at Sandia can currently be used to address some of the simpler of these applications. This technology will be transferred to the oil and gas industry at the beginning of the project and periodically thereafter as new developments are completed. The participants, which include Amoco, Chevron, Conoco, Exxon, and Mobil, will provide manpower to become familiar with the codes, to provide feedback on performance, and to identify new features that need to be added. They will also provide data for constitutive model development and code validation. The bulk of the project is devoted to research in the areas of progressive fracture with iterative finite element codes, constitutive modeling, and adaptive meshing that is needed to provide the features needed for more complex applications.

91-95 Funding (\$K): 1250      Dates: 1995-present



Technology Transfer: Transfer of licensed codes to industry, consultation and training on use, publications.

Key Documentation: ACTI Proposal: Computational Geomechanics for Geologic Structure and Reservoir Mechanics.

Key Personnel: H. S. Morgan, 505-844-7045, hsmorga@sandia.gov  
 C. M. Stone, 505-844-5113, cmstone@sandia.gov  
 J. G. Arguello, 505-844-1482, jgargue@sandia.gov  
 W. R. Wawersik, 505-844-4342, wrwawer@sandia.gov

Lab Capabilities Applied: Computational structural mechanics, computational and experimental geomechanics, rock mechanics test facility.



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Category: Environmental & Regulatory (9, 5)

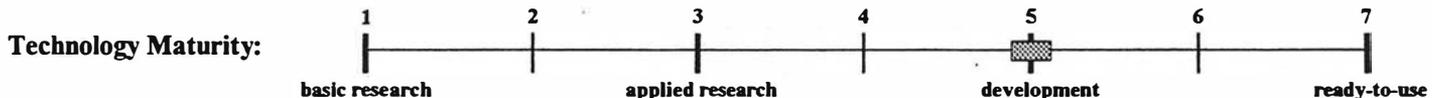
Laboratory: Sandia National Laboratories      Contact: Dianne C. Marozas, 505-844-5504

Title: Natural Geochemical Attenuation and Chemical Manipulation to Stabilize Groundwater Contaminants

**Description:** Sandia is investigating the role of natural attenuation reactions and the use of permeable reaction walls to chemically manipulate groundwater in order to immobilize contaminants in the subsurface. Natural subsurface reactions can be a significant part of a remediation program to meet closure requirements for sites affected by contaminated groundwater. Regulators are beginning to accept results from research that shows that natural fluid/rock interactions have a significant capacity to partition solutes from the fluid to the solid phase, thereby inhibiting their subsurface migration (Marozas, 1992). Sandia is currently conducting research to develop accepted protocols for quantifying the effect of natural attenuation at DOE's uranium mill tailings sites. Sandia's research approach includes the use of computer modeling to analyze subsurface contaminant behavior and transport for extended periods of time.

Natural attenuation mechanisms can also be enhanced by manipulating groundwater chemistry with permeable reaction walls that combine subsurface fluid flow management systems with designed treatment zones. Sandia is currently emplacing a permeable treatment wall at a DOE uranium mill tailing site to test different reactive treatments and to test different subsurface flow management designs. Sandia is uniquely qualified to develop reaction wall engineering designs based on its history of field demonstrations of subsurface barrier emplacement and remediation (Dwyer, 1994).

91-95 Funding (\$K): 580      Dates: 1995-present



Technology Transfer: Results of the field demonstrations will be described in Technical papers and presentations; groundwater remediation programs used by DOE's commercial remediation contractors.

Key Documentation: Dwyer, B. P., 1994, Feasibility of Permeation Grouting For Constructing Subsurface Barriers, in: In-Situ Remediation: Scientific Basis for Current and Future Technologies, edited by Gee, G. W. and Wind, N. R., pp. 3-26.  
 Marozas, D. C., 1992, Results of Attenuation Capacity Testing, Chapter 15, in Aquifer Protection Permit Application for In Situ Mining Test: Santa Cruz In Situ Copper Mining Research Project, Pinal County, Arizona, pp. 127-146.

Key Personnel: Patrick V. Brady, 505-844-7146  
 Brian Dwyer, 505-844-9894  
 Dianne C. Marozas, 505-844-5504  
 Malcolm Siegel, 505-844-5426

Lab Capabilities Applied: Subsurface Remediation, Impermeable Barrier Emplacement, Geochemistry, Hydrology, Computer Modeling, Massively Parallel Computing.



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Category: Production (10, 3, 5, 7, 8)

Laboratory: Sandia National Laboratories      Contact: David A. Northrop, 505-844-2302, danorth@sandia.gov

Title: Applied Production Technology

**Description:** Oil and gas production in the US has reached a point where significant effort is required to forestall declining production and stop the abandonment of significant unproduced resources. New technology is needed, however, because lifting costs are high relative to oil prices, the petroleum industry is downsizing and spending less developing new technology. The goal of Sandia's Applied Production Technology (APT) project is to extend the life of marginally economic wells by reducing the negative impacts of persistent production problems. The approach is to use "Sandia Technology" to rapidly diagnose industry-defined production problems and then propose or develop improved technology utilizing the needs and capabilities of industry.

Currently the APT project includes four tasks: a) Sucker Rod Failures, b) Automatic Casing Swab, c) Paraffin Control, and d) Field Measurement of Oil Properties. In addition, the project helps small businesses in the oil patch obtain technical assistance through Sandia's Tech Transfer Organization. Many small companies are faced with significant technical challenges requiring expertise beyond their capabilities. There are a number of DOE initiatives to provide such technical assistance to small business. The APT project helps small businesses in the oil patch obtain technical assistance at Sandia.

The Sucker Rod Failures and Paraffin Control tasks are industry lead through Working or Pilot Groups. These groups provide guidance to Sandia and play a significant technology transfer role. Through the groups, Sandia has catalyzed work within industry, thus broadening the project beyond what Sandia could do alone by promoting technology transfer within the industry.

91-95 Funding (\$K): 1700      Dates: 1991-present

1	2	3	4	5	6	7
basic research	applied research		development		ready-to-use	

**Technology Transfer:** Paraffin Control Working Group, Sucker Rod Working Group, Southwest Petroleum Shortcourse, Seminars, SPE Papers, Hot Oiling Spreadsheet, News Releases, Trade Journal Articles, INTERNET home pages

**Key Documentation:**

- 1) Waggoner, J.R., and Buchheit, R.G.: "Analysis of Sucker Rod and Sinkerbar Failures," Proc. of the 40th Annual Southwestern Petroleum Short Course, Lubbock, TX (1993).
- 2) Mansure A.J., and Barker, K.M.: "Practical Hot Oiling and Hot Watering for Paraffin Control," Proc. of the 41th Annual Southwestern Petroleum Short Course, Lubbock TX, April 94.

**Key Personnel:** A.J. (Chip) Mansure, 505-844-9315, ajmansu@sandia.gov  
 John R. Waggoner, 505-844-2100, jrwaggo@sandia.gov  
 Katherine N. Gaither, 505-844-5019, kngaith@sandia.gov

**Lab Capabilities Applied:** petroleum engineering, reservoir engineering, engineering analysis, fluid dynamics, mechanical engineering, corrosion, metallurgy, fatigue analysis, diagnostics, instrumentation, simulation, field testing, material science, quartz crystal microbalance.



**Index:** 366

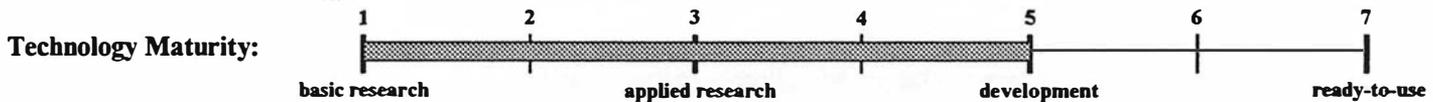
**Category:** Development (8), Environmental & Regulatory (6)

**Laboratory:** Sandia National Laboratories **Contact:** Peter B. Davies, 505-848-0709, pbdavie@nwer.sandia.gov

**Title:** Flow Visualization Laboratory for Multiphase Flow Processes

**Description:** Experimental capabilities of this laboratory are focused on visualization of multiphase flow processes in fractured and porous media through integration of physical experimentation, conceptual model formulation, and mathematical modeling of detailed processes. Specific capabilities include: 1) medium and high resolution transmitted light image capture for detailed flow/transport process characterization in fracture casts and translucent porous media; 2) high resolution X-ray image capture for characterization of multiphase flow process in 2-dimensional rock systems; 3) automated experimental systems for saturated, unsaturated, multiphase, and/or non-isothermal experiments; 4) rotating test stands for analysis of gravitational effects; 5) image analysis for quantitative evaluation of spatial and temporal changes in multiphase flow parameters and solute dispersion; 6) numerical and analytical modeling of flow and transport processes.

**91-95 Funding (\$K):** 5000 **Dates:** 1987-present



**Technology Transfer:** Publications in open literature, staff exchange, post docs, graduate and undergraduate student programs

**Key Documentation:** Glass, R.J. and Tidwell, V.C., 1991, Research Program to Develop and Validate Conceptual Models for Flow and Transport Through Unsaturated, Fracture Rock, SAND90-2261, Sandia National Laboratories  
Tidwell, V.C. and Glass, R.J., 1994, X-ray and Visible Light Transmission for Laboratory Measurement of 2-Dimensional Saturation Fields in Thin Slab Systems, Water Resources Research, Vol. 30, no. 11, p. 2873-2882

**Key Personnel:** Bob Glass, 505-848-0556, rjglass@nwer.sandia.gov Vince Tidwell, 505-848-0574, vctidwe@nwer.sandia.gov, Cliff Ho, 505-848-0712, ckho@nwer.sandia.gov Mike Nicholl, M.J., 505-848-0554, mjnichol@nwer.sandia.gov

**Lab Capabilities Applied:** non-destructive testing, numerical code development



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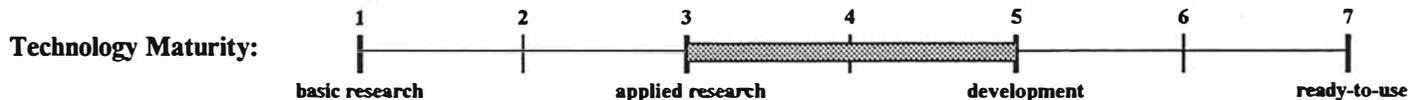
**Category:** Drilling & Completion ( 6, 1, 3), Development (9, 26), Production (11, 25), Environmental & Regulatory (1, 2)

**Laboratory:** Sandia National Laboratories      **Contact:** John R. Waggoner, 505-844-2100, jrwapgo@sandia.gov

**Title:** Increased Effectiveness Of Hydraulic Fracturing Through Advanced Computational Technology (ACTI)

**Description:** Hydraulic fracturing is the primary well stimulation technology for the recovery of gas and oil from low permeability reservoirs. Because such reservoirs are of great importance in the U.S., and because the costs of hydraulic fracturing represent the major part of the well completion costs, significant improvements in the design of hydraulic fracturing treatments have great potential for increasing production and reducing costs. The goal of this project is to increase the effectiveness of hydraulic fracturing by enhancing the industry's leading 3D simulator, TerraFrac™, to make it more versatile, easy-to-use, cost effective, and reliable, and to provide the advanced computational capability required for simulating hydraulic fracturing in such new technologies as horizontal drilling and waste injection. These significant improvements in the design of hydraulic fracturing treatments will substantially increase oil and gas production and will reduce costs. These objectives will be achieved by combining the complementary modeling and verification capabilities of TerraTek and SNL, with strong guidance from the industry group of TerraFrac™ users. To meet these objectives, TerraFrac™ will be extended to cover horizontal drilling applications, develop better physical descriptions for the modeling of slurry flows, and provide fast, interactive input, convenient flexible meshing, and modern visualization of results. TerraTek will assume responsibility for the commercialization of results, and updated TerraFrac™ code will be released as various milestones are reached. Quarterly reports will ensure that the industry is informed of the availability of the newly developed capability for increasing oil and gas production and for reducing costs.

**91-95 Funding (\$K):** 825      **Dates:** 1995 - present



**Technology Transfer:** TerraFrac™Group, technical publications, commercially available software.

**Key Documentation:** ACTI project proposal.

**Key Personnel:** John R. Waggoner, 505-844-2100, jrwapgo@sandia.gov  
 Lisa A. Mondy, 505-844-1755, lamondy@sandia.gov  
 Larry A. Schoof, 505-844-5156, laschoo@sandia.gov  
 Greg D. Sjaardema, 505-844-2701, gdsjaar@sandia.gov  
 Norm R. Warpinski, 505-844-3640, nrwarpi@sandia.gov

**Lab Capabilities Applied:** Suspended-Particle Flow Experiments, Suspended-Particle Flow Numerical Simulation, Finite Element Analysis, Microseismicity, Mesh Generation, Computer Graphics, Petroleum Engineering, Graphical User Interface Design.



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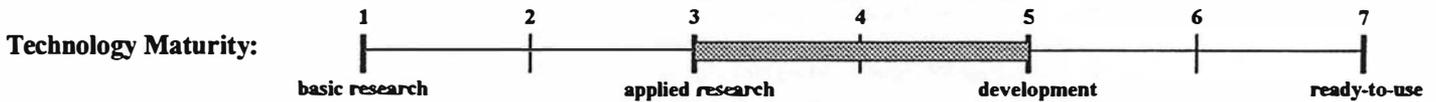
Category: Exploration (4, 3, 10, 13)

Laboratory: Sandia National Laboratories      Contact: Elaine Gorham 505-844-1401  
edgorha@sandia.gov

Title: 3-D Seismic Imaging of Complex Geologies: Remote and Rapid Processing of Terabyte Data Sets (ACTI)

Description: Sandia National Laboratories and its partners propose to greatly reduce the time and cost required to perform 3-D, finite difference, prestack depth migrations and to enable remote iterative processing and interpretation of terabyte data sets. Major products will be advanced, scaleable, finite difference, prestack depth migration algorithms that execute efficiently on all classes of high performance computers, techniques for management of large scale I/O and data sets on massively parallel computers, algorithms validated on synthetic and real world data sets, and a remote seismic processing environment. Software created in this project will provide a template for continued scaleable algorithm and software development. As a result of the development of these technologies, both service companies and oil companies will be able to provide exploration teams with more accurate and timely recommendations.

91-95 Funding (\$K): 1650      Dates: 1995-present



Technology Transfer: High performance depth imaging seismic research working group, industry collaboration, technical presentations, graduate student support.

Key Documentation: ACTI Proposal: 3-D Seismic Imaging of Complex Geologies: Remote and Rapid Processing of Terabyte Data Sets

Key Personnel: Elaine Gorham, 505-844-1401, edgorha@sandia.gov; David Womble, 505-845-7471, dewombl@cs.sandia.gov; Sudip Dosanjh, 505-845-7018, ssdosan@cs.sandia.gov; David Greenberg, 505-845-7601, dsgreen@cs.sandia.gov; John VanDyke, 505-845-7248, jpvandy@cs.sandia.g

Lab Capabilities Applied: Software and algorithm development for massively parallel architectures, large scale I/O optimization and data management for massively parallel architectures, infrastructure development for remote processing, object oriented processing, scaleable soft



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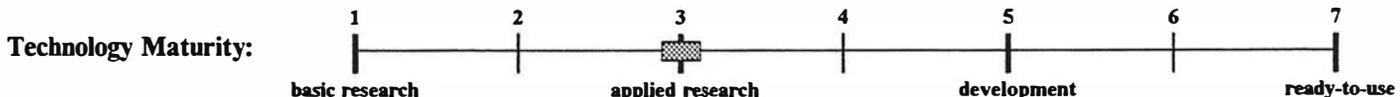
Category: Oil Processing & Refining (1, 21, 22)

Laboratory: Sandia National Laboratories Contact: Tony Martino (505) 844-4332

Title: Highly Dispersed Catalysts

**Description:** The objective of this research is to synthesize colloidal sized dispersed metal, metal oxide, and metal sulfide clusters for applications in catalysis. Applicable catalytic reactions include hydrogenation, synthesis gas conversion, and hydrogen generation. Highly dispersed clusters 1- 3 nm in diameter are potentially good catalysts, because they exhibit ultra-high surface areas and unique material properties. We are studying the formation of clusters using two different synthesis procedures: (1) clusters formed in microemulsions and (2) clusters formed from organometallic precursors. These procedures have in common the ability to control particle size and shape and to stabilize the colloids in organic solutions. We are capable of forming noble metals, base metals, mixed metals, sulfides, and oxides. Thus, we form catalysts widely applicable to many reaction processes. Particle size and composition are determined with transmission electron microscopy, electron diffraction, x-ray photoelectron spectroscopy, and Mossbauer spectroscopy. Current research includes the development of procedures to isolate the particles in a variety of forms. Emphasis is on the isolation of the particles as powders, the re-dispersion of the powders into a variety of solvents, and the mating of the particles with amorphous solid support materials.

91-95 Funding (\$K): 1200 Dates: 1989-present



Technology Transfer: Subcontracts with universities; staff visits; open literature publications.

Key Documentation: Martino, A. et al., "Synthesis and Characterization of Coal Liquefaction Catalysts in Inverse Micelles," Energy and Fuels (in press). Martino, A. et al., "Synthesis of Transition Metal Clusters and Their Catalytic and Optical Properties," Mater. Res. Soc. Symp. Proc. 1993, 286, 131.

Key Personnel: Tony Martino, 505-844-4332  
 Doug Loy, 505-844-4445

Lab Capabilities Applied: Nanocluster materials - metals, bimetallics, oxides, sulfides; catalytic testing; quantum mechanical calculations



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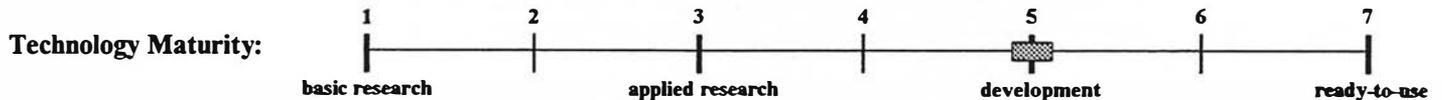
Category: Development (9, 3), Deepwater Offshore (1, 16)

Laboratory: Sandia National Laboratories Contact: R. S. Harding, (505) 844-0780

Title: Seafloor Earthquake Measurement System (SEMS)

**Description:** This seafloor seismic instrumentation system was developed to characterize the response of seafloor sediments to earthquake-related ground motion. Measured in-situ ground motion were used to guide the engineering design of offshore petroleum production platforms, primarily in State and Federal waters off the California coast. Project funding was provided by DOE, the Minerals Management Service (MMS), and a group of oil companies. The system functions as a stand-alone digital event-detection and recording system using three component accelerometer sensors. The SEMS unit is deployed in a seafloor penetration probe from a small barge or boat. Command and interrogation of the unit from the ocean surface using acoustic telemetry allows data gathering without retrieval of the installed unit. Real-time digital filtering enhances event detection and reduces false triggers. Three component accelerometer orientation is determined from onboard magnetometers. The system employs a low power electronics package, battery operated for long stand-alone life (up to 7 years). System dynamic range permits recording of 0.1 to 2.0 G signals, over a bandwidth from .05 to 20 Hz. Installed SEMS systems successfully recorded earthquake events off Long Beach, in the Santa Barbara Channel, the Santa Maria basin, and in the Bering Sea. The SEMS system offers the capability of recording seismic shear waves in a marine environment. Potential new applications of the SEMS technology include monitoring the seismicity of petroleum reservoirs for study of production-related subsidence and compaction effects, e.g., at Ekofisk, and using three component reverse-VSP monitoring for characterization of offshore reservoirs.

91-95 Funding (\$K): 700 Dates: 1977 - present



Technology Transfer: Collaboration with industry, technical reports

Key Documentation: SAND89-0107, "Measurements of Earthquake-Induced Seafloor Motions Offshore California," G.E. Sleaf

Key Personnel: D. E. Ryerson, (505) 845-9627  
B. P. Engler, (505) 844-7419

Lab Capabilities Applied: Seismic Instrumentation, Acoustic Telemetry, Seismic Data Processing



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**Category:** Drilling & Completion (13), Environmental & Regulatory (12)

**Laboratory:** Sandia National Laboratories **Contact:** Robert Wemple, 505-844-2230

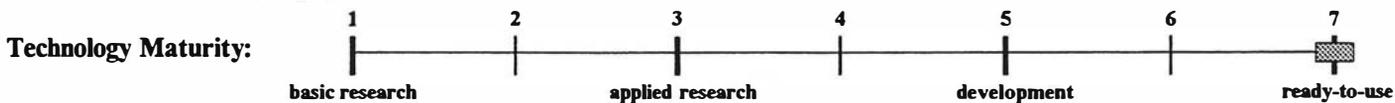
**Title:** Shallow Directional Drilling Development for Environmental Use

**Description:** Shallow directional drilling for environmental applications has been adapted from the underground utilities installation industry. SNL and its industrial partner, The Charles Machine Works, better known by the trademark of DITCH WITCH, have developed a new class of cost effective machinery. This partnership, now in the fifth year, has tested prototype machinery with improved onboard tracking, increased depth, and extended lateral range capabilities at the DOE-Savannah River Site (coastal plain sediments), SNL in New Mexico (aluvial fill), and the DOE-Hanford (glacial till) site. Successful boreholes were emplaced at SRS (600' in length, 40' deep) and at SNL (420' in length, 30' deep). The Hanford test was used to evaluate the limits of the technology and did not produce a usable borehole.

The SNL test drilling cost was approximately \$60/ft. This compares to a project goal of \$25 to \$75/ft., not including the casing/screen cost. This technology is not applicable to all geologies, but where usable in mainly compactable soils, is more cost effective, with less site disturbance, less fluid used, and minimal secondary waste generated as compared to other directional drilling methods such as river crossing or oil/gas technologies.

Charles Machine Works has commercialized and is successfully marketing this technology to world wide markets. The SNL/CMW partnership continues with ongoing technology transfer to the environmental industry.

**91-95 Funding (\$K):** 1600 **Dates:** 1991 - Present



**Technology Transfer:** DOE Model Conferences, DOE TIE Workshops, DoD Environmental Workshop, SAND Reports, Project Brochures, Marketing Brochures.

**Key Documentation:** (1) R. P. Wemple, R. D. Meyer, G. E. Staller, R. R. Layne, "Final Report for SNL/NM Environmental Drilling Project", SAND94-2388, Nov., 94.  
 (2) R. P. Wemple, R. D. Meyer, R. D. Jacobson, R. R. Layne, "Continued Development of Directional Boring Technology", Proceedings of 7th DOE Model Conference, Oct. 91.

**Key Personnel:** R. P. Wemple, 505-844-2230;  
 R. R. Layne, 405-336-3591;  
 R. D. Meyer, 505-844-4181;  
 G. E. Staller 505-844-9328

**Lab Capabilities Applied:** Environmental and Geothermal Drilling Development with Engineering, Applications, Instrumentation and Testing Capabilities



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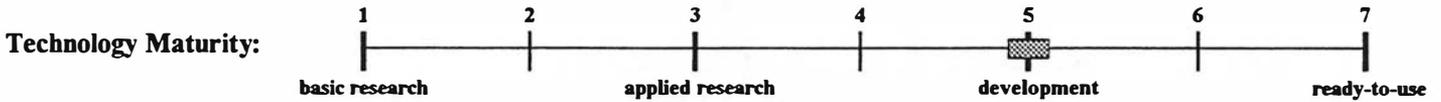
Category: Oil Processing & Refining (12, 3, 6), Production (5)

Laboratory: Sandia National Laboratories Contact: James Miller, (505)-844-2565

Title: Advanced Thermally Stable Jet Fuels and Field Measurement of Oil Properties

Description: This project has focused on the development and application of two sensor techniques, photon correlation spectroscopy (PCS) and the quartz crystal microbalance (QCM), for in situ monitoring of the processes involved in thermal degradation and solids deposition when aviation fuels are thermally stressed. The PCS system has been used to determine the kinetics of formation of particle formation and growth during the thermal degradation of jet fuels as a function of temperature and ambient conditions. The QCM system can determine surface deposition rates of fuel degradation products to a resolution of better than 0.3 micrograms/cm<sup>2</sup> hr. The system has been operated to pressures of 1000 psig and temperatures to 300 C. Additionally the QCM system can be used to obtain viscosity-density data for fuels as a function of temperature. The QCM system is currently being considered for use in qualifying the thermal stability properties of jet fuels. Both the QCM and PCS systems can be applied to monitoring feed and product streams in fuel refining and storage operations and to detecting fouling conditions in refinery operations. QCM technology is also being applied to measure such liquid hydrocarbon properties as viscosity, density, cloud-point, and freeze-point. The sensor technology offers substantial advantages and it is robust and suitable for field environments. We are teaming with Petrolite to develop a field cloud-point system to measure the paraffin solubility characteristics of crude oil in the field. This technique has the potential of transforming a lab measurement normally taking days to weeks into a field measurement requiring tens of minutes.

91-95 Funding (\$K): 2660 Dates: 1989-present



Technology Transfer: Licensing agreements, quarterly and annual reports, project meetings, publications.

Key Documentation: T. J. O'Hern, W. M. Trott, S. J. Martin, and E. A. Klavetter, "Advanced Diagnostics for In Situ Measurement of Particle Formation and Deposition in Thermally Stressed Jet Fuels," AIAA Paper, AIAA-93-0363, 1993. S. J. Martin, V. E. Granstaff and G. C. Frye, "Characterization of a Quartz Crystal Microbalance with Simultaneous Mass and Liquid Loading," Anal. Chem. 63, 2272-2281, 1991.

Key Personnel: J. E. Miller 505-844-2565  
E. A. Klavetter, 505-844-9119  
S. J. Martin, 505-844-9723  
T. J. O'Hern, 505-844-9061  
A.J. Mansure, 505-844-9315

Lab Capabilities Applied: Advanced sensors; petroleum product properties, microelectronics engineering.



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Category: Oil Processing &amp; Refining (1,7,16,22)

Laboratory: Sandia National Laboratories

Contact: T. Gardner, (505) 845-7502

Title: Catalyst Development for Direct Liquefaction and Dehydrogenation Processes

**Description:** Energy efficiency improvements in coal liquefaction can be obtained by developing catalysts with better activity, selectivity, and life. We have developed catalysts synthesized via hydrous metal oxide (HMO) ion exchangers that were found to have potential for application to a number of reactions associated with the conversion of coal to liquid fuels. In addition, these catalysts can also be used for processing other hydrocarbon fuels sources, such as petroleum. The development effort has proceeded to the point where HMO catalysts can be made which have hydrocracking, hydrodenitrogenation, and hydrodesulfurization activities better than the best commercial catalysts. A number of areas of development are being pursued that may lead to catalysts with even higher activities and lower costs than the present HMO catalysts. The HMO catalysts will continued to be valuated under conditions that are representative of commercial processes. The goal of this effort is to develop catalysts that will result in further improvements in yields and product quality for coal liquefaction through better understanding of the catalyst synthesis reactions, and long-term evaluation in laboratory and bench-scale coal liquefaction processes.

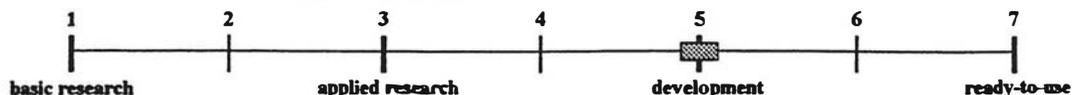
Anticipated environmental regulations are expected to increase the demand for oxygenated fuel additives such as methyl-tert-butyl ether (MTBE), which is synthesized from methanol and isobutene. New demand for isobutene will result in an increase in the importance of catalytic dehydrogenation of isobutane. Another goal of this project is to synthesize and test bulk forms of hydrous titanium oxide (HTO) supported iron and chromia catalysts for the selective dehydrogenation of isobutane to isobutene. In addition, thin films of the most promising HTO catalysts on various substrates will also be evaluated. Such thin film catalysts have unique potential in membrane reactor applications, as they can be coated directly onto the membrane, thereby increasing conversions obtainable with only a bulk catalyst inside a membrane tube. The successful development of these catalysts is expected to improve the economic viability of the isobutane dehydrogenation process by allowing better utilization of feedstocks, thereby resulting in savings in energy and raw materials.

91-95 Funding (\$K):

4350

Dates: 1988-present

Technology Maturity:



Technology Transfer:

Patents, reports, journal articles.

Key Documentation:

R. G. Dosch, H. P. Stephens and F. V. Stohl, "Catalysis Using Hydrous Metal Oxide Ion Exchangers," U.S. Patent 4,511,455, April 16, 1985.

R. G. Dosch, L. I. McLaughlin, H. P. Stephens, and T. J. Headley, "Development of Thin Film Hydrous Metal Oxide Supported Catalysts for Direct Coal Liquefaction," Preprints of Papers, Amer. Chem. Soc., Div. Fuel Chem. 37 (1), 141 (1992).

Key Personnel:

T. Gardner, 505-845-7502

Allen Sault, 505-844-8723

S. E. Lott, 505-844-1889

L. I. McLaughlin, 505-844-7294

E.P.Boespflug, 505-844-0983

Lab Capabilities Applied:

Advanced materials synthesis and characterization; catalyst evaluation and characterization; lab-scale process simulation; continuous bench-scale hydroprocessing; hydrocarbon feed &amp; product characterization; statistical experiment design; surface analysis



Index: 374

Category: Environmental & Regulatory (4, 6, 9, 14)

Laboratory: Sandia National Laboratories Contact: Robert G. Knowlton, 505-848-0425

Title: Risk-Based Decision Analysis Tools for Remedial Alternatives Selection Based on Probabilistic Flow and Transport Simulators

Description: Sandia has developed a suite of decision analysis tools for risk assessment, sampling/monitor well network design, and remediation costing. These tools, along with some new applications for remedial design options, are being packaged as a decision analysis tool for selecting treatment and disposal methods. Factors such as human health risk, ecological risk, worker risk, transportation risk, and cost will influence the decision making process and are an integral part of these tools. The risk tools would also be used to provide a scientific basis for risk-based regulation. The risk tool provides a method to calculate the statistical distribution of risk, and therefore one can estimate the probability of a given risk occurrence, and quantifying the uncertainty in risk. The costing tool is probabilistic and gives the mean and variance of a cost scenario, based on uncertainty in the site knowledge and resource allocations. This gives the user a more defensible handle on budget contingencies. The sampling/monitor well network design software uses probabilistic flow and transport simulators to define network adequacy. The code is unique in its application of the probabilistic approach combined with a post-conditioning alternative. In other words, the output of the probabilistic simulations is conditioned, or has to match within prescribed tolerances, any observed concentrations of constituents of interest. This feature causes the code to function in sort of an auto-calibration mode. The code is quite user-friendly, and runs on the Macintosh, PC Windows, and Windows NT platforms. The code is already in use for monitor well network design using state-of-art optimization methods.

91-95 Funding (\$K): 2200 Dates: 1993-present



Technology Transfer: Copyrighting and licensing software.

Key Documentation: Conference presentations, technical publications (in preparation).

Key Personnel: Robert G. Knowlton, 505-848-0425  
Brian M. Rutherford, 505-844-3120

Lab Capabilities Applied: Advanced computational methods, Hydrogeology, Remediation, Costing, Optimization.



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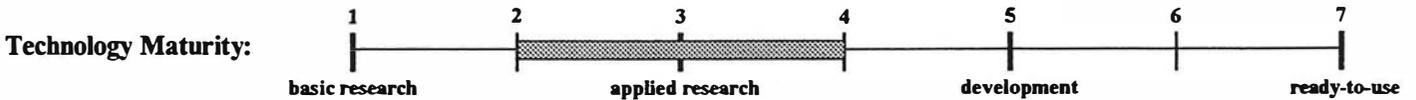
Category: Production (17), Environmental & Regulatory (9)

Laboratory: Sandia National Laboratories      Contact: Henry R. Westrich, 505-844-9092, hrwestr@sandia.gov

Title: Macroscopic Transport in Geologic Media: A Lattice Gas Automata Study

**Description:** Development of Lattice Gas Automata (LGA) computer codes model complex fluid and solute phenomena in porous geologic media using collections of discrete particles that are constrained to move on geometric grids, undergo simple collisions, and conserve momentum. Averages over time or space obey Navier-Stokes and advection-diffusion relations. The LGA codes will accurately model microscopic (fracture- and pore-scale) diffusion, flow, immiscibility, adsorption/desorption of solutes and particles, and density-driven convection for complex geometries. There are several advantages of LGA calculations over the finite-element (analytical solutions) codes which are currently being used for the petroleum industry, usually on massively parallel computers. First, complex boundary conditions can be addressed in LGA simulations; these codes are numerically stable, and, for 2-D simulations, they can be run on a personal computer. More complex 3-D LGA simulations would require use of a multiprocessor workstation. LGA results would be tested against analytic solutions to assess the accuracy of approximations, estimate scaling effects, and suggest experimental strategies for obtaining greater accuracy. Work is continuing to develop more efficient, PC-based LGA codes. Potential applications include simulation of Rayleigh-Taylor instability for immiscible fluids, dispersion or fingering in a porous medium due to flow, density or viscosity, and interpretation of NMR resistivity and mercury porosity logs. These results have implications for NMR well logging, advanced recovery processes, hydrologic modeling, and remediation schemes for drilling waste products.

91-95 Funding (\$K): 500      Dates: 1992-present



Technology Transfer: Peer-reviewed journal articles, scientific conference presentations, staff exchange

Key Documentation: Stockman, H. W. (1994) Estimation of scaling errors via Lattice Gas Automata: Application to diffusion and adsorption, American Geophysical Union Chapman Conference, June 6-9, Lincoln, NH.  
Stockman, H.W.; C.T. Stockman and C.R. Carrigan (1990) Modelling viscous segregation in immiscible fluids using lattice-gas automata. Nature 348, pp 523-525.

Key Personnel: Harlan W. Stockman, 505-844-0975, hwstock@sandia.gov  
Kathryn L. Nagy, 505-844-5337, klnagy@sandia.gov

Lab Capabilities Applied: Pentium personal computer- and multiprocessor RISC workstation-based code development



Index: 376

Category: Oil Processing &amp; Refining (22, 23, 25)

Laboratory: Sandia National laboratories

Contact: Margaret Showalter (505) 844-7014

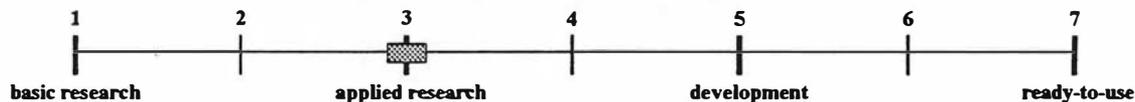
Title: Catalysts for the Conversion of Light Hydrocarbons to Alcohols

**Description:** The objective of this project is to develop biomimetic catalysts for the direct conversion of light hydrocarbon gases to alcohols and/or other valuable oxygenates. A fundamental goal of this research is to develop a better understanding of the structure-activity relationships of biomimetic catalysts, and to apply that understanding to rational catalyst design. The current focus is on development of novel porphyrin metal complexes for use as homogeneous alkane oxidation catalysts. Our stepwise approach to catalyst development involves first using Computer Aided Molecular Design to design and model potential metalloporphyrin catalysts with desired structural features, followed by synthesis and characterization of promising catalysts, and finally testing the porphyrins in bench scale oxidation reactions. Catalyst design and modeling, structural characterization, and activity testing are performed at Sandia National Laboratories. Researchers at Florida International University and University of California at Davis synthesize and characterize the new porphyrins.

91-95 Funding (\$K): 1125

Dates: 1991-present

Technology Maturity:



Technology Transfer: Subcontracts with universities; staff visits; open literature publications.

**Key Documentation:** Showalter, M. et al., "Light Hydrocarbon Gas Conversion Using Halogenated Iron Dodecaphenylporphyrin Catalysts,": in Coal Liquefaction and Gas Conversion, Proc., Vol. I, U.S. DOE, PETC, Pittsburgh, PA., 1993, 249.  
 Medforth, C. J. et al., "Novel Ligand Orientations in Pridine and Imidazole Complexes of a Highly Substituted Nonplanar Porphyrin, and Implications for the Design of Porphyrins as Regio- and Stereo-Specific Oxidation Catalystse," J. Chem. Soc., Chem. Commun. 1994, 1994, 1843.

**Key Personnel:** Margaret Showalter 505-844-7014  
 John Shelnett 505-844-8856

**Lab Capabilities Applied:** Computer-aided molecular design; Raman spectroscopy; advanced materials synthesis techniques; catalyst testing.



Index: 377

Category: Oil Processing &amp; Refining (22, 4, 21, 16)

Laboratory: Sandia National Laboratories

Contact: F. V. Stohl, (505) 844-7991

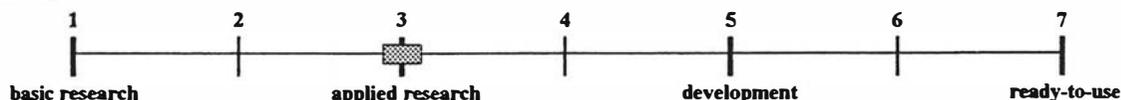
Title: Advanced Direct Liquefaction Concepts for Improved Efficiency and Economics in the Refining of Coal-Derived Liquids

**Description:** Coal Liquefaction research in the United States has led to strategic reductions in process costs with advances in oil yield and quality. Previous work has shown that coal liquefaction reactions proceed rapidly to form soluble, yet nondistillable products. The nondistillable products or residual (resids) are recycled as a major portion (about 40%) of the liquefaction feed to the first stage reactor of a two-stage process. This project explores hydrolysis as a means of converting residuum to distillable liquids while selectively avoiding costly hydrocarbon gas formation. Analysis has shown that hydrolysis processing could simplify the reactor design for liquid fuels production from coal. The objectives of this project are: 1) to apply catalytic hydrolysis to coal liquefaction resid (ashy and deashed) at various temperatures and hydrogen pressures, 2) to hydrotreat a light coal-derived resid to increase its hydrogen donor content and 3) to test solvent quality by using heavy residuum-like materials for direct coal liquefaction. The effort also examines the effects of hydrotreating conditions on hydroaromatic compound formation with the aim of improving distillate production in coal liquefaction. Another objective of this project is to experimentally evaluate options for hydrotreating coal liquids and various distillate cuts of coal liquids, and to develop a database relating hydrotreating parameters to feed and product quality. The hydrotreating effort is being conducted with a bench-scale continuous flow trickle-bed reactor that enables us to evaluate many hydrotreating options in a rapid and cost effective manner. Data gathered is used by program participants to develop algorithms that are used in refinery linear programming models to identify the most cost effective options for introducing and processing coal liquids in a refinery. This project is integrated with the efforts of other DOE project participants, including Bechtel, Southwest Research Inc., Amoco, M. W. Kellogg, and the MITRE Corporation.

91-95 Funding (\$K): 715

Dates: 1993-1995

Technology Maturity:



Technology Transfer:

Project Meetings, quarterly &amp; annual reports, publications.

Key Documentation:

R. Anderson, et. al., "Advanced Process Concepts for Coal Liquefaction: Process Simulation Testing," Proceedings of the Eleventh AIST-NEDO/DOE-PETC Joint Technical Meeting on Coal Liquefaction, Albuquerque, NM, September 27-28, 1994.

R. J. Kottenstette and H. P. Stephens, Progress in Donor Assisted Coal Liquefaction: Hydroaromatic Compound Formation, Preprints of Papers, Amer. Chem. Soc., Div. Fuel Chem. 39 (1), 98 (1994).

Key Personnel:

F. V. Stohl, 505-844-7991

H. P. Stephens, 505-844-9178

S. E. Lott, 505-844-1889

Lab Capabilities

Applied:

Continuous bench-scale hydroprocessing, catalyst characterization, hydrocarbon feed &amp; product characterization, and statistical experimental design.



Index: 378

Category: Drilling & Completion (4, 3, 13)

Laboratory: Sandia National Laboratories      Contact: D. A. Glowka, 505-844-3601  
daglowk@sandia.gov

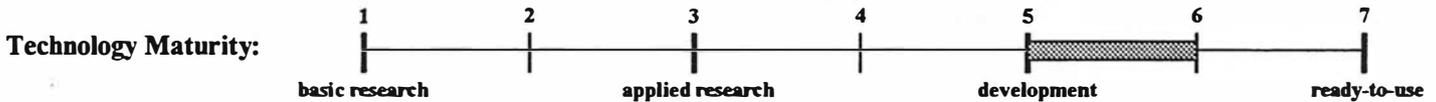
Title: Lost Circulation Technology

**Description:** The most common and costly problem routinely encountered in drilling geothermal wells is lost circulation. Approximately 10-20% of the cost of a typical geothermal well is attributable to lost circulation. Because well costs represent about 50% of the total cost of a geothermal power plant, the incentives for reducing lost circulation costs are apparent. The goal of this project is to reduce lost circulation costs in geothermal drilling by 30-50%.

This project is developing technology in two areas: lost circulation diagnostic techniques and lost circulation control. Under the first topic, hardware and software are being developed to provide information related to the onset of lost circulation and the location, size, and severity of the loss zone. Work is concentrating on: developing and testing flow meters for measuring inflow and outflow rates for the well while drilling; and data acquisition hardware and software for using this information to provide guidance to the driller for treating any loss zones encountered. Under the second topic, downhole tools and fluids are being developed for treating loss zones. These tools include: a drillable straddle packer for isolating the loss zone and improving the efficiency of cement jobs; and a wireline-deployable porous packer for delivering a two-component polyurethane foam to the loss zone.

Industry involvement includes laboratory and field testing of hardware and software developed under this project. In addition, Sandia is participating in field testing of fluids developed by industry for lost circulation control.

91-95 Funding (\$K): 3000      Dates: 1988- Present



Technology Transfer: Publications in open literature, loan of equipment to industry for testing, joint field testing

Key Documentation: Glowka, D. A.: "Lost Circulation Technology Development Projects," presented at DOE Geothermal Program Review VIII, San Francisco, CA, April 18-20, 1990.  
Schafer, D. M., Loeppke, G. E., Glowka, D. A., Scott, D. D., and Wright, E. K.: "An Evaluation of Flowmeters for the Detection of Kicks and Lost Circulation During Drilling," paper IADC/SPE 23935, presented at 1992 IADC/SPE Drilling Conference, New Orleans, LA, February 18-21, 1992.

Key Personnel: David A. Glowka, 505-844-3601, daglowk@sandia.gov, and George E. Staller, 505-844-9328

Lab Capabilities Applied: Data analysis, model development, hardware and software design, material science, laboratory testing, field testing



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Category: Gas Processing (4, 8)

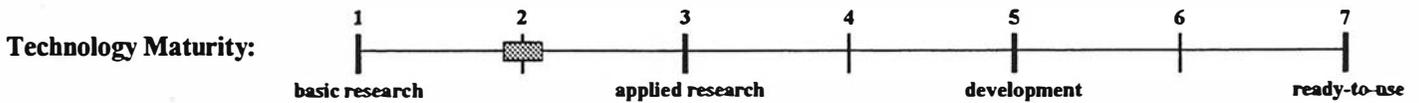
Laboratory: Sandia National Laboratories

Contact: Robert R. Lagasse, 505-845-8333, rrlagas@sandia.gov

Title: Microengineered Polymer-Derived Adsorbents for Natural Gas

**Description:** The goal of this project was to a) evaluate a porous polymer as a precursor for producing high capacity, monolithic carbon adsorbents for methane and b) correlate the methane capacity of these materials with their pore structure. The motivation was that filling a storage tank with a porous adsorbent for natural gas can reduce the pressure needed to store a given amount of gas. Reducing storage pressure for natural gas may open large new markets, such as natural gas powered vehicles. Although carbon adsorbents are common in many areas of industrial technology, their capacity is normally evaluated on a weight basis instead of the volume basis important for natural gas storage. In order to achieve the highest possible capacity on a volume basis, the adsorbent must be produced in a monolithic form, instead of the more common particulate form, and the pores should be smaller than 2 nm. Processes were developed for a) converting an example polymer, poly(acrylonitrile), into monolithic porous precursors and b) pyrolyzing the precursors to produce carbon monoliths. The highest methane storage capacity achieved in these carbon materials was 45 cc@STP/cc at 500 psi and 58 cc@STP/cc in the carbons that had been activated. Finally, an improved correlation of the methane capacity of the monolithic carbons with their pore structure was developed. Compared to existing empirical correlations, the new one may be more reliable for a broad range of materials, since it has no adjustable parameters. This correlation was successful in predicting the methane capacity of not only the polymer derived monoliths, but also conventional particulate carbons.

91-95 Funding (\$K): 300      Dates: 1993-1994



Technology Transfer: Contractor reports, publications, GRI review board, graduate student

Key Documentation: R.R. Legasse, "Microengineered Polymer-Derived Adsorbents for Natural Gas," Final Report to Gas Research Institute, Contract 5091-260-2228, August 1994

Key Personnel: Robert R. Lagasse, 505-845-8333

Lab Capabilities Applied: Polymer synthesis and characterization, pore-structure characterization,



Index: 380

Category: Exploration (4), Development (33)

Laboratory: Sandia National Laboratories

Contact: Raymond E. Cline, Jr., 510-294-1395, rec@sandia.gov

Title: Gas and Oil National Information Infrastructure (GONII)

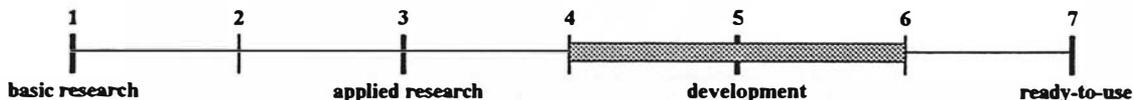
**Description:** This broad information-based program consists of five overall activities: (1) Synthetic Seismic Dataset: The labs are working with the Society of Exploration Geophysicists to generate a synthetic seismic dataset for the development, verification, and validation of seismic processing tools used in the gas and oil industry. At the completion of the project, the developed tools will be made available to the industry for commercialization. (2) GONII Testbed Emulation: This activity provides a testbed which the industry can use to evaluate, benchmark, and access new technologies of interest to them. It will simulate long-haul high performance networks with access to supercomputers, clusters, and mass storage in a transparent distributed computing environment. (3) ARIES Testbed Partnership: The Aries Testbed is a partnership between Amoco and 15 industrial communications and computing vendors to explore the use of ATM in the gas and oil business sector. The labs are offering their network and distributed computing technology in order to obtain interoperability information and further knowledge of a prospective customer - the gas and oil industry. (4) Information Access for Independent Oil Producers: The labs are providing enabling capabilities of information technology to the Petroleum Technology Transfer Council (PTTC), which is tasked with establishing 10 regional resource centers to provide a mechanism of tech transfer to the nation's independent oil and gas producers. The aim is to use telephone modems coupled with Mosiac/World Wide Web systems to bring an information system to the independent community. (5) Satellite Communications for the Gas and Oil Industry: Several institutions are negotiating for a joint demonstration of satellite communications capabilities as applied to the gas and oil industry as a means of retrieving seismic and reservoir data from remote sites. The scope could include the development of stabilized ship-board T3 ground terminals in seismic data collection. (Sandia collaborates with three other National Laboratories (Lawrence Livermore, Los Alamos, and Oak Ridge) on this overall GONII program.)

91-95 Funding (\$K):

4500

Dates: 1993-present

Technology Maturity:



Technology Transfer: Publications in the open literature, presentations and demonstrations at technical symposia, collaborative projects with industry

Key Documentation:

Key Personnel: Raymond E. Cline, Jr., 510-294-1395, rec@sandia.gov

Lab Capabilities Applied: Massively parallel computers, systems for remote data access and browsing, systems interactions, large-scale data storage, transparent distributed computing environments, satellite communications



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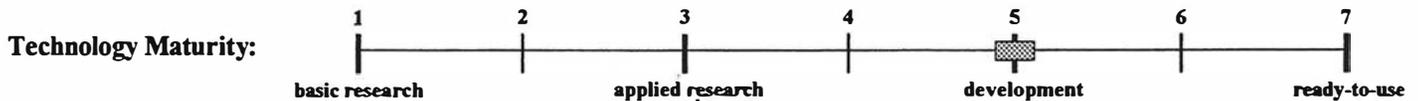
**Category:** Oil Processing & Refining (1, 16), Environmental & Regulatory (10)

**Laboratory:** Sandia National Laboratories      **Contact:** S. E. Lott, (505) 845-1889

**Title:** Reduction of Nitrogen Oxide Emissions for Lean Burn Engine Technology

**Description:** The goal of this project is to develop advanced catalysts and catalytic converter system concepts to meet current and near future mandated Clean Air Act standards for motor vehicle emissions, with the emphasis on reduction of nitrogen oxides emissions. The development and implementation of catalysts and converter systems will aid the commercialization effort of lean burn engines that represent the next technical step in fuel efficiency and automobile performance. This project is focused on (1) quantitative understanding of catalytic processes in current catalysts; (2) design, development and testing of novel catalytic materials; (3) predictive simulation of catalytic systems; and (4) evaluation of catalyst systems under engine conditions. Sandia is focusing its efforts on the application of the hydrous metal oxide (HMO) ion exchanger system to use for nitrogen oxide reduction catalysts. HMOs can be used to tailor catalytic systems by forming a thin-film of the catalytically active phase on virtually any surface. Catalysts and small-scale converter systems are evaluated with an atmospheric pressure, gas-phase flow reactor system. This technology can be applied to the development of many other catalysts systems for the treatment of emissions.

**91-95 Funding (SK):** 2000      **Dates:** 1993-present



**Technology Transfer:** CRADAs, quarterly reports, project meetings.

**Key Documentation:** R. G. Dosch, H. P. Stephens and F. V. Stohl, "Catalysis Using Hydrous Metal Oxide Ion Exchangers," U.S. Patent 4,511,455, April 16, 1985.

**Key Personnel:** S. E. Lott, 505-844-1889  
 T. Gardner, 505-845-7502  
 S. Lockwood, 505-844-1186  
 L. I. McLaughlin, 505-8447294

**Lab Capabilities Applied:** Advanced materials synthesis; materials characterization; catalyst evaluation; laboratory-scale process simulation, catalyst characterization, continuously operated gas-phase reactor evaluation, and statistical experimental design.



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Category: Oil Processing & Refining (21, 25)

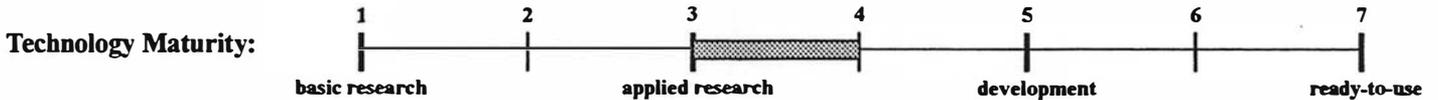
Laboratory: Sandia National Laboratories      Contact: James L. Tomkins, 505-845-7249

Title: Simulation of Residual Oil Hydroprocessing Units on Massively Parallel Supercomputers

**Description:** Sandia and Los Alamos National Laboratories are cooperating through separate CRADAs in a joint research project with Amoco Oil Company to investigate the process used by Amoco to transform heavy crude oil into light synthetic crude oils. Amoco processes heavy crude oils in a fluidized-bed catalytic reactor called a Residual oil Hydroprocessing Unit (RHU). Heavy crude oil and hydrogen are pumped into the bottom of the RHU where they are combined, in the presence of a catalyst, at high temperature and pressure. The goal of this research is to improve the overall efficiency of the process by increasing the efficiency of the conversion and by increasing the percentage of time that the RHU is operational.

To achieve this goal a three-dimensional multi-phase reactive flow code is being developed to accurately simulate the complex physical processes that occur in an operating RHU. Los Alamos has primary responsibility for the physics model development while Sandia's primary responsibility is for development of the massively parallel vision of the code. Amoco is responsible for building a cold flow experimental model and for providing RHU operational data that will be used to benchmark the computer code.

91-95 Funding (\$K): 800      Dates: 1992-present



Technology Transfer: Technology transfer will occur through publications in the open literature and through licensing of the computer code developed through the project.

Key Documentation: CRADA Number 01110 (DOE TTI Number 92-Mult-057-B1).

Key Personnel: James L. Tomkins, 505-845-7249

Lab Capabilities Applied: Massively Parallel Computing, Domain Decomposition, and Sparse Matrix Solvers.



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Category: Gas Storage (7)

Laboratory: Sandia National Laboratories      Contact: James K. Linn, 505-844-6813  
 jklinn@sandia.gov

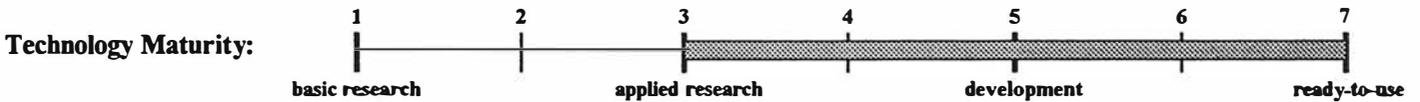
Title: U.S. Strategic Petroleum Reserve Geotechnical Support

**Description:** Sandia provides geotechnical engineering for the U.S. Strategic Petroleum Reserve Program. Sixty three (63) caverns in salt with a total underground volume of nearly 750 million barrels of space have been converted or developed for underground crude oil storage (equally applicable for gas or other hydrocarbon storage). Key technical developments include:

- ( 1) a salt solution mining code (interactive, flexible leach/fill schedules),
- ( 2) cavern testing techniques,
- ( 3) salt mechanics modeling of salt creep and surface subsidence,
- ( 4) salt dilatancy modeling,
- ( 5) site planning and characterization,
- ( 6) downhole sonar, temperature, and pressure tool development,
- ( 7) brine disposal,
- ( 8) corrosion resistant materials,
- ( 9) geophysical diagnostics,
- (10) natural radioactive materials monitoring, and in situ permeable flow sensors.

Since 1989, Sandia have applied many of the above capabilities in direct support of the commercial gas storage industry. Key technologies that have been developed and applied are horizontal, controlled cavern leaching (patent pending), leaching under a gas blanket, gas storage cavern shape optimization, and geomechanics analyses of arrays of gas storage caverns.

91-95 Funding (\$K): 16500      Dates: 1979 to present



Technology Transfer: Publications in Open Literature, Solution Mining Research Institute technical papers and presentations

Key Documentation: SANSMIC code, SAND83-1150, A. J. Russo, "A User's Manual for the Salt Solution Mining Code, SANSMIC," September 1983.  
 "A User's Manual for the Computer Code HORSMIC," A.J. Russo, SAND93-3841, Jan. 1994.

Key Personnel: James K. Linn, 505-844-6813 jklinn@sandia.gov  
 James T. Neal, 505-844-7715  
 Thomas E. Hinkebein, 505-844-6985  
 Anthony Russo

Lab Capabilities Applied: Instrumentation development, 2-D and 3-D modeling, Materials development, Engineering analyses, Geodiagnosics, Process chemistry, Geomechanics modeling



**PART II**  

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**ENABLING CAPABILITIES**



Capability	Key Word(s)	Applicable Technology Need
<b>Argonne National Laboratory</b>		
1. Site Characterization		Environmental & Regulatory (3)
2. Site Remediation	Remed(ial), Remediation	Environmental & Regulatory (12)
3. Environmental Control Technology	Environment(al)	Environmental & Regulatory (10)
4. Chemical and Physical Analysis	Chemi(cal), Chemistry	Oil Processing & Refining (24)
5. Corrosion		Production (3)
6. Geotechnical Modeling	Geo(logy), Geophysics	Development (25)
7. Gas Production	Production	Production (2)
8. Fluid Dynamics	Fluid	Oil Processing & Refining (25)
9. Chemistry and Catalysis	Cataly(st), Catalysis	Oil Processing & Refining (1)
10. Computer Applications	Comput(er), Computing, Computation	Development (25)

## Brookhaven National Laboratory

1. The National Synchrotron Light Source	Light Source	Exploration, Development, Production, Oil Processing & Refining
2. High Flux Beam Reactor		Oil Processing & Refining (1, 9, 24), Development (5, 9)
3. Applied Physical Sciences Division		Oil Processing & Refining (1, 22, 23), Gas Storage, Exploration, Development
4. Materials Science Division	Material(s)	Production (3), Oil Processing & Refining (5)
5. Biosystems and Process Sciences Division	Process(es)	Production (18, 21)
6. Energy Efficiency and Conservation Division		Oil Processing & Refining (16, 17, 18, 27)
7. Chemical Sciences Division	Chemi(cal), Chemistry	Production (24), Gas Storage
8. Analytical Sciences Division		Exploration (12), Development (2, 28, 33), Environmental & Regulatory (8)
9. Environmental Chemistry Division	Environment(al)	Development (4, 21), Gas Gathering (2), Gas Storage (2), Environmental & Regulatory (5, 10)
10. Environmental and Waste Technology Center	Waste	Environmental & Regulatory (4, 9, 10, 14)
11. Seismic and Structural Engineering Evaluation Programs	Seism(ology)	Exploration (6), Development (3, 14, 28)

Capability	Key Word(s)	Applicable Technology Need
12. New Infrastructure Technologies for the 21st Century		Oil Processing & Refining (3, 5, 6, 11, 13), Gas Gathering, Gas Storage (2, 4, 7)
13. High Temperature Combustion Facility	Combustion	Production (24)

## Idaho National Engineering Laboratory

1. Engineering Mechanics, Fracture Mechanics, and NDE	Mechanic(s)	Oil Processing & Refining (12, 13, 3)
2. Advanced Materials and Processing	Material(s)	Oil Processing & Refining (5), Deepwater Offshore (16)
3. Advanced Manufacturing	Manufacturing	Oil Processing & Refining (5, 14)
4. Sensors and Controls	Control	Oil Processing & Refining (26), Deepwater Offshore (3)
5. Robotics and Smart Systems	Robotic(s)	Oil Processing & Refining (14), Deepwater Offshore (3)
6. Reservoir Modeling	Reservoir	Development (25)
7. Computational Fluid Dynamics	Comput(er), Computing, Computation	Oil Processing & Refining (25), Production (22)
8. AI/Expert Systems	System(s)	Oil Processing & Refining (26)
9. Integrated Visualization	Visual(ization)	Exploration (13)
10. Simulation Based Design	Simulation	Deepwater Offshore (7, 16), Arctic Region Activities (6)
11. Chemical Processing	Chemi(cal), Chemistry	Environmental & Regulatory (11), Oil Processing & Refining (4, 1, 7, 11, 19)
12. Biotechnology	Bio(logy), Biological	Oil Processing & Refining (11), Environmental & Regulatory (12), Production (21)
13. Risk and Reliability Analysis	Risk	Environmental & Regulatory (14), Oil Processing & Refining (8)
14. Human Factors		Oil Processing & Refining (3, 15)
15. Environmental Technologies	Environment(al)	Environmental & Regulatory (4, 10, 11, 12, 14)
16. Earth Sciences	Earth	Exploration (7, 9, 15, 16), Development (2, 4, 8, 14)

## Lawrence Berkeley Laboratory

1. Advanced Light Source	Light Source	Oil Processing & Refining (1, 5, 7, 9)
2. Barrier Fluid Technology for Production Enhancement and Waste Isolation	Waste	Production (16), Drilling & Completion (6), Environmental & Regulatory (12)

Capability	Key Word(s)	Applicable Technology Need
3. Center for Atmospheric and Biospheric Effects of Technology (CABET)	Bio(logy), Biological	Environmental & Regulatory (7, 8, 10, 12)
4. Center for Computational Seismology	Comput(er), Computing, Computation	Exploration (4, 6, 14, 16), Development (3, 10, 11, 12)
5. Chemical Energy Research	Chemi(cal), Chemistry	Oil Refining & Processing, Gas Processing
6. Chemical Physics	Chemi(cal), Chemistry	Oil Refining & Processing, Gas Processing
7. Combustion Science	Combustion	Environmental & Regulatory (10), Oil Refining & Processing (16, 24, 28)
8. Database Management		Exploration, Development, Drilling & Completion, Production, Environment & Regulatory
9. Distributed Computer Systems and Networking	System(s)	Exploration, Development, Drilling & Completion, Production, Environment & Regulatory
10. Drilling	Drilling	Drilling & Completion (13)
11. Ecological Systems	System(s)	Environmental & Regulatory (14)
12. Flue-Gas Chemical Research	Chemi(cal), Chemistry	Environmental & Regulatory (10)
13. Isotope Geochemistry	Geo(logy), Geophysics	Exploration (1), Development (1, 4, 8)
14. Materials Energy Research	Material(s)	Oil Processing & Refining (1, 5, 7, 9), Exploration (16), Development (10, 12)
15. National Center for Electron Microscopy (NCEM)	Electro(nics), Micro-, Opto-	Oil Processing & Refining (1, 3, 5, 6, 7)
16. Neutron Source Development		Development (17)
17. Reservoir Characterization	Reservoir	Development (1, 4, 6, 14, 21)
18. Reservoir Simulation	Simulation	Development (25, 26, 28, 30, 33)
19. Scientific Visualization	Visual(ization)	Development (25, 30, 33)
20. Subsurface Imaging	Surface, Subsurface	Development (10, 12, 14, 15, 16, 17)
21. Surface Reactivity	Surface, Subsurface	Oil Processing & Refining (3, 5, 7, 8, 9, 11)

## Lawrence Livermore National Laboratory

1. Materials Testing and Advanced Materials	Test(ing), Testbed	Drilling & Completion (8, 12), Production (3), Deepwater Offshore (7, 8, 9, 16), Oil Processing & Refining (5)
2. Mass Spectroscopy		Exploration (7), Development (4, 21), Oil Processing & Refining (24), Environmental & Regulatory (10, 15)
3. System and Decision Sciences Capability	System(s)	Exploration (2), Development (28, 33), Oil Processing & Refining (8, 11, 15), Environmental & Regulatory (14)

Capability	Key Word(s)	Applicable Technology Need
4. Scientific Basis for Risk-Based Regulation	Risk	Environmental & Regulatory (4, 7, 14)
5. Nondestructive Evaluation (NDT)	Nondestructive	Development (5, 12, 15, 22), Drilling & Completion (11), Production (10), Deepwater Offshore (7, 16), Oil Processing & Refining (12, 13)
6. Parallel Linear System Solvers and Adaptive Numerical Methods	System(s)	Exploration (1), Development (15, 16, 17, 25), Production (8, 11), Oil Processing & Refining (6, 25), Environmental & Regulatory (6)
7. Atmospheric Modeling	Model(s), Modeling	Environmental & Regulatory (7, 8)
8. Systems Engineering for Complex Industrial Systems	System(s)	Production (14), Oil Processing & Refining (2, 3, 6, 8, 11, 14), Environmental & Regulatory (7, 10, 11)
9. Computer Simulation of Mechanical and Thermal Processes	Comput(er), Computing, Computation	Exploration (1), Development (2, 25), Production (8, 11), Deepwater Offshore (6, 9, 16), Oil Processing & Refining (3, 13)
10. Electromagnetics	Electro(nics), Micro-, Opto-	Development (10, 15, 16, 17, 18, 30), Drilling & Completion (11), Oil Processing & Refining (12), Environmental & Regulatory (5)
11. Micro Technology Capability	Micro(scop)y	Development (34), Oil Processing & Refining (12), Gas Processing (5, 8), Environmental & Regulatory (10)
12. High-Powered Lasers		Exploration (8), Gas Storage (2), Environmental & Regulatory (5, 10)
13. Neural Networks		Exploration (1, 3, 4, 12), Development (11, 14, 28, 33)
14. Rock Mechanics	Mechanic(s)	Exploration (1, 9, 16), Development (3, 5, 9, 12, 18)
15. Large Scale Plant Process Control System	Control	Oil Processing & Refining
16. Computational Earthquake Initiative	Earth	Environmental & Regulatory
17. Robotics for Hazardous Materials Handling	Robotic(s)	Environmental & Regulatory

## Los Alamos National Laboratory

1. Computational Testbed for Industry	Comput(er), Computing, Computation	Development (25, 2, 27), Exploration (3, 4, 6, 13), Environmental & Regulatory (8, 9)
2. The Advanced Computing Laboratory	Comput(er), Computing, Computation	Exploration (4, 3, 6, 13), Development (2, 25, 27), Environmental & Regulatory (8, 9)
3. The High Performance Parallel Processor Program	Process(es)	Development (25, 14), Oil Processing & Refining (6, 11, 21, 24, 25), Environmental & Regulatory (9)
4. Multiphase Flow Computer Code Library	Comput(er), Computing, Computation	Oil Processing & Refining (25, 6, 21, 24), Production (22)

<b>Capability</b>	<b>Key Word(s)</b>	<b>Applicable Technology Need</b>
5. Applications of Risk Assessment to the Oil and Gas Industry	Risk	Environmental & Regulatory (4, 3, 7, 9, 14)
6. Integrated Energy and Environmental Assessments	Environment(al)	Development (33), Oil Processing & Refining (8), Environmental & Regulatory (4, 14)
7. Center for Material Science	Material(s)	Production (3), Deepwater Offshore (5, 8, 9, 16), Oil Processing & Refining (5, 12, 13)
8. Engineering Modeling in Support of Oil & Gas Programs	Model(s), Modeling	Deepwater Offshore (16, 2, 4, 5, 7, 9)
9. Materials Science Laboratory	Material(s)	Deepwater Offshore (16, 2, 5, 8, 9), Production (3), Oil Processing & Refining (5, 12, 13)
10. Sensor and Process Diagnostics	Process(es)	Environmental & Regulatory (10, 3, 14), Deepwater Offshore (1)
11. Integrated Subsurface Characterization	Surface, Subsurface	Development (6, 2, 25), Exploration (1, 11)
12. Transport Assessment Strategic Initiative	Transport(ation)	Development (4, 16, 21), Gas Gathering (2), Gas Storage (2), Environmental & Regulatory (5, 9)
13. Simulation of In Situ Groundwater Remediation Processes	Simulation	Environmental & Regulatory (9, 2, 6, 12)
14. Information Extraction, Optimization, and Adaptive Control	Control	Oil Processing & Refining (26, 3, 25), Development (28)
15. Catalysis Capabilities	Cataly(st), Catalysis	Oil Processing & Refining (1, 7, 9, 19)
16. Destruction of Oily or Contaminated Waste	Waste	Environmental & Regulatory (12, 2, 9, 11)

## National Institute for Petroleum and Energy Research

1. Exploration, Drilling and Risk-Based Management	Risk	Exploration (1, 2-7, 10, 12-16); Drilling & Completion (1, 2, 6, 9-13); Development (33)
2. Reservoir Characterization and Assessment	Reservoir	Development (1, 2-33)
3. Extraction Research		Production (25, 1-6, 8, 11, 12, 16-27); Gas Storage (1, 2, 3); Development (30); Arctic Region Activities (5)
4. Thermodynamics	Therm(al), Thermodynamics	Oil Processing & Refining (27, 24, 19, 28, 25, 20, 1)
5. Process Development, Heavy Oil Upgrading and Catalysis	Process(es)	Oil Processing & Refining (21, 7, 1-4, 6, 9-11, 16, 18-25, 27, 28)
6. Fuel Chemistry and Evaluation	Chemi(cal), Chemistry	Oil Processing & Refining (27, 28, 20, 24)
7. Natural Gas Processing and Conversion, Process Modeling and Analysis	Model(s), Modeling	Gas Processing (8, 1-4, 6, 7)
8. Fuels and Engine Testing	Test(ing), Testbed	Oil Processing & Refining (27, 28, 22, 24); Environmental & Regulatory (7, 9, 14, 15)

<b>Capability</b>	<b>Key Word(s)</b>	<b>Applicable Technology Need</b>
9. Waste Minimization	Waste	Environmental & Regulatory (10, 11, 12, 7, 9, 13-15)
10. Gaseous Emissions		Environmental & Regulatory (14, 13, 15, 7)
11. Liquid Discharges/Waste Water	Waste	Environmental & Regulatory (10, 1-4, 6, 7-15)
12. In Situ Remediation of Petroleum Contamination Using Microbial and Chemical Recovery Technologies	Chemi(cal), Chemistry	Environmental & Regulatory (12, 1-7, 9-11, 13-15)
13. Mitigation of Environmental Impacts	Environment(al)	Environmental & Regulatory (12, 1-4, 6, 10, 13, 14)
14. Groundwater Resource Assessment Using Reservoir Characterization	Reservoir	Environmental & Regulatory (6, 1, 4)

## Oak Ridge National Laboratory

1. Advanced Separation Processes	Process(es)	Production (2, 6), Processing & Refining (2, 4, 18, 19), Gas Processing (4, 5, 6, 8)
2. Bioprocessing and Biotechnology	Process(es)	Environmental & Regulatory (2, 10, 12), Oil Processing & Refining (4, 6, 17, 21, 22, 23), Production (1, 2)
3. Advanced Fluid Mechanics	Fluid	Development (1), Drilling & Completion (2), Production (7, 8, 22, 25), Deepwater Offshore (4, 5, 6, 15)
4. Simulation Models	Model(s), Modeling	Development (25-28), Drilling & Completion (3), Production (6-11, 25), Oil Processing & Refining (6, 22, 27, 28), Environmental & Regulatory (4, 6-10, 14, 15)
5. Sludge Processing	Process(es)	Environmental & Regulatory (2, 11-13, 15)
6. Waste Minimization	Waste	Environmental & Regulatory (1, 2, 4, 7-15)
7. Advanced Materials	Material(s)	Exploration (15), Drilling & Completion (4), Production (3, 4, 5, 7-10), Deepwater Offshore, Arctic Region Activities, Oil Processing & Refining (9, 10)
8. Environmental Risk	Environment(al)	Exploration (2), Development (4, 10), Oil Processing & Refining (8), Environmental & Regulatory (4, 8, 9, 14, 15)
9. Incinerator Monitoring		Environmental & Regulatory (7, 8, 14)
10. Wastewater Treatment	Waste	Production (1-4), Deepwater Offshore (1), Environmental & Regulatory (1, 2, 6, 9, 11, 12, 13)

## Pacific Northwest Laboratory

1. Process Science and Engineering Complex	Process(es)	Oil Processing & Refining, Environmental & Regulatory
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Capability	Key Word(s)	Applicable Technology Need
2. Environmental and Molecular Sciences Laboratory (EMSL)	Environment(al)	Environmental & Regulatory, Development, Oil Processing & Refining
3. Marine Sciences Laboratory		Environmental & Regulatory, Deepwater Offshore, Arctic Region Activities
4. Natural Gas Transmission and Distribution Facilities		Gas Gathering, Gas Storage

## Sandia National Laboratories

1. Solar Powered Systems	System(s)	Exploration (14), Production, Gas Gathering
2. Advanced Manufacturing Technologies	Manufacturing	Oil Processing & Refining (3), Production, Gas Gathering, Deepwater Offshore
3. Robotics	Robotic(s)	Drilling & Completion (13, 9), Deepwater Offshore (7), Arctic Region Activities, Oil Processing & Refining (14)
4. Information Surety	Surety	Exploration (15), Deepwater Offshore, Production
5. Intelligent Sensors	Sensor(s)	Oil Processing & Refining (4), Gas Processing
6. Combustion Science and Technology	Combustion	Oil Processing & Refining (24, 4, 11, 16, 25, 27), Gas Processing, Environmental & Regulatory (10)
7. Materials Aging and Reliability	Material(s)	Oil Processing & Refining (13)
8. Batteries		Arctic Region Activities, Exploration, Development, Production
9. Synthetic Aperture Radar Imaging		Exploration (8)
10. High-Consequence Operations and Surety	Surety	Oil Processing & Refining (15), Gas Processing, Deepwater Offshore, Production
11. Microelectronics	Micro(scop)y	Development, Production, Oil Processing & Refining, Gas Processing
12. Optoelectronics	Electro(nics), Micro-, Opto-	Exploration (15), Oil Processing & Refining
13. Safe and Secure Transportation	Transport(at)ion	Production, Oil Processing & Refining, Gas Processing
14. Risk Management	Risk	Oil Processing & Refining (8), Environmental & Regulatory, Deepwater Offshore, Arctic Region Activities (5, 6, 7), Environmental & Regulatory (14)
15. Nondestructive Testing	Test(ing), Testbed	Oil Processing & Refining (12), Gas Gathering (2)
16. Joining Technologies		Oil Processing & Refining, Gas Gathering
17. Systems Engineering and Integration	System(s)	Arctic Region Activities (7), Deepwater Offshore, Gas Gathering



## **Enabling Capabilities – Argonne National Laboratory**

Each national laboratory as part of its response to the National Petroleum Council Task Group on National Laboratory Capabilities, was asked to describe capabilities of their laboratory that might not be adequately reflected in the project-specific summaries. The following is an attempt to highlight activities at Argonne that might be of considerable interest in the petroleum community but did not have activity and funding levels that met the criteria for inclusion in the summaries.

**1. Site Characterization:** Argonne has focused on the development of advanced technologies for the characterization and control of the subsurface environment. The Laboratory is pursuing a parallel program of basic research to understand the fundamental processes associated with subsurface physical and chemical phenomena, transferring this basic knowledge into workable field technology as rapidly as possible. To accomplish its advanced research and technology objective, Argonne has developed a world class facility for investigating the physics of multiphase fluid flow and characterizing the subsurface environment. Specialized equipment includes a cone penetrometer for the rapid characterization of subsurface contamination and geology at depth, a supercomputing visualization facility for the interactive realization of subsurface structures, and a unique system for conducting three-dimensional quantitative visualization of flow phenomena in porous media. Argonne's technology achievements include (1) the development of a methodology for rapid characterization of near-surface geology (<150 ft), (2) the design and implementation of a new technique to restore of contaminated soils in the deep vadose zone, and (3) the conceptualization and design of a novel technique for the in situ cleanup of deep (<500 ft) DNAPL organic contaminants in fractured rock. These projects made the transition from the bench to the field in approximately three years. [Environmental & Regulatory (3)]

**2. Site Remediation:** In site remediation Argonne is working in a number of areas including: membrane assisted solvent extraction, phytoremediation, foams, electrokinetic soil processing, and resin adsorption technology. A membrane-assisted solvent extraction (MASX) system coupled with a membrane-assisted distillation stripping system (MADS) was evaluated for use in decontaminating groundwater. Volatile organic compounds (VOCs) in the groundwater are extracted in the MASX unit using sunflower oil. In the MADS, VOCs are stripped from the sunflower oil, which is then recycled to the MASX unit. Phytoremediation is an emerging cleanup technology based on the well-known ability of plants to take up and concentrate contaminants in their tissues. Hyperaccumulator plants are grown to "biomine" the contaminated soil, and are harvested and treated to further concentrate the contaminants prior to final disposal.. Argonne s innovative approach is in integrating the traditional phytoremediation concept with other technologies to enhance the bioaccumulation by irrigation, fertilization, alteration of the soil's chemical/physical conditions, and/or the use of nontoxic chelating agents. Compared with alternative technologies, enhanced phytoremediation offers the advantages of being truly in situ, lower capital and labor costs, retaining the functionality of the soil ecosystem, and minimal disturbance to the environment, and a higher public acceptance. The use of foams is being examined in bench-scale treatability studies as a means to release and mobilize dense nonaqueous phase liquids (DNAPLs) and to couple with bioremediation techniques. The foams can either be produced in situ or above ground and injected in the contaminated zone. Injection/production wells (either horizontal or vertical) can be used to assist in the delivery, transport, and monitoring

of foams through the subsurface. The foams should drive the contaminants upward, thereby minimizing the potential to drive the contamination off-site (whereas surfactant flooding drives the contaminants downward toward the groundwater). The technology can treat soils having either scattered contaminants or pools of contaminants and can be applied to both saturated and vadose zones. It has the potential to mobilize and biodegrade contaminants either simultaneously or sequentially. Electrokinetic soil processing technology can deliver nutrients in conjunction with in-situ bioremediation. The project has three primary tasks: (1) Efficient injection of nutrients across sandy, silty, and clayey soil exhibiting varying permeability and pore fluid conductivity, (2) Uniform distribution of nutrients across sandy, silty, and clayey soils, and (3) Directing nutrients across heterogeneities in layered and clayey soil. The project serves to demonstrate the proof-of-concept. ANL's role is to perform bench-scale proof-of-concept, 1-dimensional experiments, while Electrokinetics, Inc. will perform larger bench-scale experiments using a parallel plate apparatus (2-dimensional). This technology would significantly increase the potential of bioremediation at contaminated sites. The process will be applicable to wetlands, uplands, coastal regions, and locations that are relatively inaccessible (such as underneath existing buildings). Considerable quantities of volatile organic compounds (VOCs) are released to the atmosphere from contaminated sites. Barometric pressure fluctuations cause volatilization of VOCs to occur; DOE has estimated that 90% or more of the VOCs released can be attributed to boreholes because they provide a path of least resistance. Argonne is developing a polymeric resin adsorption technology to minimize the release of VOCs from boreholes. The project involves performing laboratory proof-of-concept experiments (Phase 1) and a field demonstration (Phase 2). [Environmental & Regulatory (12)]

**3. Environmental Control Technology:** Argonne is currently developing a high-frequency microwave-induced plasma process for destroying volatile organic compounds (VOCs) in off-gas streams. By using a plasma, we can generate the high concentrations of free radical species necessary for the destruction reactions to occur at a lower temperature than is required for incineration. The primary focus has been the destruction of compounds, such as chlorinated hydrocarbons, which are difficult to destroy by incineration. The plasma reactor is a continuous flow system and operates at atmospheric pressure. With this plasma reactor, low concentrations (as low as parts per million) of VOCs present in off-gas streams can be destroyed without the addition of auxiliary fuels or the need to concentrate the VOCs, as is often required for incineration. Also being developed is a HCl-recovery process utilizing electrochemical cells similar to those used in molten carbonate fuel cells. The gas stream that contains the hydrogen chloride is directed and comes in contact with the cathode of the electrochemical cell. At this electrode the following reaction occurs:  $\text{HCl} + \text{e}^- \rightarrow \text{Cl}^- + 1/2 \text{H}_2$  The chloride ions produced then enter the electrolyte, which is composed of metal chloride mixtures held in an inert membrane, and migrate to the anode, where the following reaction occurs:  $2 \text{Cl}^- \rightarrow \text{Cl}_2 + 2 \text{e}^-$  The chlorine gas thus produced is recovered and can be recycled to upstream chlorination operations or for other uses. The hydrogen produced can also be recovered and used in the hydrogenation reactors in the plant or for fuel. [Environmental & Regulatory (10)]

**4. Chemical and Physical Analysis:** Wavelength-tunable pulsed and continuous-wave lasers are used as fluorescence excitation sources from the ultraviolet into the near-infrared to investigate the photophysics of species present in gas, liquid, and solid phases at temperatures

ranging from 1.5 K to 1100 K. High sensitivity, gated and ungated, and single and multichannel photodetectors are used together with optical filters, monochromators, and spectrographs to isolate and record the emission wavelengths of interest. Digital data acquisition, signal averaging, and analysis are carried out for the species that emit light on time scales ranging from subnanoseconds to seconds. Radioactive and chemically hazardous materials can be investigated at sensitivities that can approach detection of a single atom or molecule. Current emphasis is on actinide-containing materials but the technology has broad applicability. The Laboratory has the unique analytical capability for nondestructive, element-specific elucidation of electronic, geometric, and magnetic properties of bulk solids and solid surfaces. We also have significant first-hand experience in solving commercially-sensitive problems regarding corrosion products of iron and its alloys and for identifying iron-bearing phases in oil reservoir formations and production solids. Capabilities are also available for amorphous and crystalline powders, foils, films, fibers, frozen solutions, etc. [Oil Processing & Refining (24)]

**5. Corrosion:** This program primarily involves fundamental studies of aqueous corrosion and of microporous materials. The overall goal of corrosion research is to provide experimental information against which theoretical models of the metal/water and metal oxide/water interface can be tested over a wide range of temperatures and in a variety of chemical environments. The research program couples in situ surface-sensitive spectroscopic methods with interfacial electrochemical techniques and with theory. The studies of microporous materials are driven by the fact that chemical reactions at solid-liquid and solid-gas interfaces are responsible for a wide range of phenomena having both basic and technological significance, including mechanisms of molecular-sieve crystal nucleation and growth, heterogeneous catalysis, gas-phase cluster formation, and chemical-vapor deposition (CVD) of compounds and thermodynamically unstable crystalline phases. [Production (3)]

**6. Geotechnical Modeling:** Within the oil industry, many tools currently exist to model various aspects of sedimentary basin development, including stratigraphy, geologic structure, heat flow, hydrocarbon generation and fluid flow. However, in general, these tools run independently, even though the processes that they attempt to simulate are known to operate concurrently with, and are dependent upon, other processes. An integrated, quantitative, dynamic geologic model could provide a solution to the geological system under investigation on the basis of the physical processes that actually produced it. This type of forward model would be iteratively tuned to incorporate all forms of available geologic information, including core and borehole data, petrophysical data, logs, and seismic interpretations. A fully integrated basin simulator that included structural, stratigraphic, heat flow, geochemical, and fluid-flow models would require processing speeds presently available only on parallel supercomputers. Nevertheless, estimates of the increase of processor speed indicate that such capability may be conceivable for relatively inexpensive, top-end workstations in the next five years. [Development (25)]

**7. Gas Production:** Argonne is developing simple, low-cost, plant-based bioreactors for the Gas Research Institute (Chicago, Illinois). Modeled on saline wetland ecosystems, bioreactors clean up saline water usually produced with natural gas. Bioreactors use hydroponic techniques to filter and sequester contaminants and reduce wastewater volume through enhanced evapotranspiration. These studies indicate that the ideal plant is a vigorous, salt-tolerant species, with a large surface

area of transpiring tissue and a dense, fibrous root system that functions as a biological filter. A prototype bioreactor using two plant species reduced the total volume of wastewater (8,800 gallons with a salt concentration of 1.5 percent) by 75 percent in fewer than eight days. [Production (2)]

**8. Fluid Dynamics:** The Laboratory has exceptional strengths in application of CFD to the simulation of flows and heat transfer in complex components of advanced energy systems, in particular, the Laboratory has developed methods applicable to a variety of slurry transport operations, fluidized bed flows, and gas/particulate transport systems. These computational methods, based on extensions of a general-purpose, three-dimensional code called COMMIX which was originally developed for nuclear reactor safety analyses, has been applied in numerous fossil energy component simulations to provide detailed design engineering and efficiency estimates. In an application of experimental and modeling capabilities the issue of phase separation inside a porous medium was studied. In order to determine the differences in the phase separation behavior of two liquids in the bulk as well as in the porous medium scientists from Exxon, Argonne National Laboratory, University of Pittsburgh and University of Maryland have conducted systematic small angle neutron scattering studies on water/lutidine mixture in vycor glasses. These studies clearly showed that the conditions under which the phase separation of the binary fluid occurs in the bulk are different from those in the confined geometries and the difference is mainly due to preferential wetting of lutidine. This was understood on the basis of a new theory and could not be explained by the classical Random Phase Ising Model. The unique capabilities of neutron scattering were essential for the success of these studies. [Oil Processing & Refining (25)]

**9. Chemistry and Catalysis:** Computational chemistry software capabilities at Argonne include programs for: (1) molecular graphics (used for understanding the size and fit of various molecules), (2) molecular mechanics (used for determining the three-dimensional conformation of molecules), (3) molecular dynamics (used in studying diffusional, absorption, and fluctuational effects), and (4) quantum mechanics (used for studying electronic excitations and the entropic and energetic constraints on reactions). These capabilities are now being applied in computational catalyst simulation to understand the nature of active sites in zeolite and clay based catalyst systems. Zeolites are the workhorse catalysts of the petroleum refining industry. In related work in-situ neutron diffraction data were collected on the powder diffractometers at IPNS by BP America scientists in order to understand the kinetics of industrial processes and to follow the structures of engineering materials as a function of temperature and/or other conditions. The unique properties of neutrons make studies of this kind well suited to explore structure/activity relationships in solid state materials. Three examples are given below. The thermal decomposition of iron titanates ( $\text{Fe}_{1-x}\text{Ti}_x\text{O}_5$ ), important commercial sources of  $\text{TiO}_2$ , was examined. The industrial synthesis of these materials utilizes a quench that results in the production of a thermodynamically unstable oxide. At elevated temperatures the kinetics and mode of decomposition of these oxides were determined via analysis of the neutron diffraction data. In another study, the synthesis of a vanadium antimonate catalyst, which is used for selective oxidation of hydrocarbons, was monitored to ascertain the role of added elements. In-situ neutron diffraction data collected at the calcination temperature showed that the primary purpose of the

additional elements is to affect the kinetics of oxidative decomposition of the catalytically active phase, and reduce the production of a non-selective phase [Oil Processing & Refining (1)]

**10. Computer Applications:** Currently Argonne operates a 128-node SP1 POWERParallel system through the Argonne High-Performance Computing Research Facility (HPCRF). This system has a peak performance of about 16 Gflops. The IMP POWERParallel System series provides a unique I/O-intensive environment for major parallel applications. In particular, the IBM system is the first scalable, parallel system to offer multiple levels of I/O capability. An upgrade to a 512-node (150 Gflops) POWERParallel system is planned. Argonne has extensive experience in the field of data visualization. Experts have developed ways to present data to analysts in a manner that is suited to the work being done. Graphical user interfaces have been developed to optimize pre- and post-processing of information during analysis. A variety of graphical tools has been developed to aid in viewing and editing data. Work has been done to extend geographical information systems for specific needs and to bring new visual capabilities to computer applications. Research includes a proof-of-concept prototype designed to present a methodology for selecting and comparing spectra for hyperspectral imagery. This effort incorporates neural network technology for aid in making comparisons. Argonne recently assisted the Department of Energy in a project to modernize the Tertiary Oil Recovery Information System (TORIS) maintained by the Bartlesville Project Office of DOE. This project included implementing a modern distributed hardware and software architecture, porting multiple TORIS simulation models to the new environment, implementing an intelligent graphical user interface and numerous database and utility applications. Staff with expertise in computer systems and staff with geoscience and reservoir engineering expertise teamed to provide a comprehensive solution. The Laboratory has developed a number of Engineering Mechanics computer codes, which continue to be actively developed and used in their traditional applications as well as being adapted for other industrially significant purposes. These codes address issues such as fatigue and failure analysis, structural analysis, dynamics of complex mechanical systems, vibration analysis, crash worthiness, earthquake analysis and response, fluid/structure interactions, seismic isolation, and piping systems analysis. These programs may be directly useful for simulation of complex structures such as deep-water-drilling and production platforms.[Development (25)]



## **Enabling Capabilities – Brookhaven National Laboratory**

**1. The National Synchrotron Light Source:** The National Synchrotron Light Source (NSLS) is a user facility where scientists and engineers from industry, universities and government laboratories throughout the United States and abroad perform basic and applied research in many fields of science. The NSLS is currently the nation's largest user facility dedicated solely to the production of synchrotron light. This light consists of a continuous spectrum of electromagnetic radiation ranging from infrared to x-rays. The intensity of light in beams emitted from the NSLS synchrotrons is many orders of magnitude greater than conventional laboratory-generated light beams. Basic and applied research is conducted at the NSLS by scientists from a variety of disciplines including chemistry, geoscience, materials science and physics. Examples of applied research are surface studies designed to improve the performance of catalysts and to minimize corrosion. A sophisticated imaging technique known as computerized microtomography has been developed to provide 3-dimensional images of the pore structure of objects such as drill cores. This information has been coupled with modern computer modeling techniques to elucidate the pore structure of reservoirs. (Exploration; Development; Production, Oil Processing and Refining)

**2. High Flux Beam Reactor:** The High Flux Beam Reactor (HFBR) is one of the nation's major centers for neutron investigations in solid state and nuclear physics, chemistry, materials science and structural biology. It is designed specifically to provide intense external beams of thermal and sub-thermal neutrons for experimental purposes. The only research reactor in the U.S. with a liquid hydrogen neutron moderator, the HFBR supports a major program in sub-thermal neutron investigations. The unique capabilities of the HFBR and its experimental facilities are also being utilized in a wide range of neutron diffraction studies. For example, accurate structures determined for transition-metal hydrides are relevant to homogeneous and heterogeneous catalysis applications and complement current research on metal hydride reactivity patterns. Studies of gas clathrate hydrates promise to yield insight into the stability of these materials which comprise large reserves of methane and other low-molecular weight hydrocarbons in the Arctic regions. Most of the experimental facilities at the reactor are operated by Participating Research Teams consisting of Brookhaven scientists and regular users of the reactor from other government, industrial and university laboratories. Research at the HFBR is often complementary to that at the National Synchrotron Light Source, and projects that utilize both of these user facilities are welcome. (Oil Processing and Refining 1, 9, 24; Development 5, 9)

**3. Applied Physical Sciences Division:** Members of the Applied Physical Sciences Division are engaged in a broad range of research tasks in support of the mission of the Department of Energy. Programs related to the transportation sector include adsorbents for natural gas vehicle storage systems, and creation of organic sulfur in marine sediments, and three-dimensional imaging of drill core samples, leading to an improved understanding of the origins and properties of oil reservoirs. A third group of projects includes research on identification of impurities in coal combustion products and development of advanced materials coatings. New programs in environmental technologies address the physical and chemical science associated with waste management and contaminated sediments. Most of the research in the Division relies heavily upon the special capabilities found at the National Synchrotron Light Source, and at other special BNL facilities.

Photon, ion and neutron beams are utilized as needed to accomplish the required tasks, and new or improved microanalytical methods are developed when necessary. A large number of collaborators from other institutions participate in these Divisional programs. (Oil Processing and Refining 1, 22, 23; Gas Storage Exploration, Development )

**4. Materials Science Division:** The major efforts in the Materials Science Division were the investigation of properties of superconducting oxides with high critical temperatures; methods of superconductor fabrication including thin films, new materials, and composite conductors; the synthesis and characterization of electroresponsive molecular and polymeric systems; the investigation of mechanisms of corrosion; and the structure and properties of surface-modified materials and interfaces. Primary emphasis in these programs is on gaining an understanding of the microscopic and microstructural factors influencing the properties of the materials. Development of superconductors with high mechanical tolerance and with low ac losses for electric power systems applications are also carried out in collaboration with applied programs. A program to develop lightweight alloy hydrides for nickel-metal hydride batteries and to apply the facilities at the National Synchrotron Light Source for in situ characterization of metal hydride electrodes is now underway. Work has recently begun on a new program for Advanced Permanent Magnet Materials. The Materials Science Division also offers a wide range of material preparation and characterization services to the Laboratory and its users. (Production 3; Oil Processing and Refining 5)

**5. Biosystems and Process Sciences Division:** The Biosystems and Process Sciences Division (BPSD) supports DOE activities through research that is applied in the areas of fossil and renewable energy to energy-related effects in terrestrial ecology, botany, and biogeochemistry, to the development of bioprocesses for treating energy-related waste materials, to the effects of air pollution and to improving capacity for predicting responses of C-uptake by vegetation to atmospheric change. Energy-related industrial processes to which current BPSD studies are relevant include detoxification of geothermal energy production by-products, enhanced oil recovery, upgrading of heavy crude oils, recovery of commercially valuable metals from waste streams, conversion of organic wastes to new products such as detergents and adsorbents, etc., and the development of instruments and engineering for applications in the emerging biochemical technologies. BPSD is actively pursuing research in understanding the basic biochemical mechanisms involved in the microbial transformations of organic complexing agents of radionuclides and toxic metals; mobilization and stabilization of radionuclides and toxic metals commonly present in DOE wastes. Information derived from this study will aid in the environmental restoration and long-term management of DOE contaminated sites. BPSD develops specialized plant exposure systems such as the Free-Air Carbon dioxide Enrichment (FACE) array. The understanding gained by this program of large-scale field experiments is critical to evaluating the role of ecosystems in regulating global carbon dioxide concentrations in a warmer, CO<sub>2</sub>-enriched world. Molecular mechanisms regulating physiological responses of plants to CO<sub>2</sub> enrichment are studied in controlled, programmable growth chambers and in FACE experiments, providing a mechanism basis for the improvement of models of vegetation response to global atmosphere and climate change. (Production 18, 21)

**6. Energy Efficiency and Conservation Division:** This Division is composed of the Buildings Group and the Process Materials Group. The mission of the Buildings Group is to improve our understanding of thermal processes that take place in buildings and in the equipment that is used to heat and cool buildings, and to assist industry in the development of technologies that will permit buildings to be heated and cooled more efficiently. This mission of the Process Materials Group is to develop, study, and test polymer-matrix composites (polymer concretes) and cementitious matrix composites for a variety of applications, including geothermal energy systems, district heating systems, and civil-engineered structures. Basic studies furthering the development of stable, adherent protective coatings on steel and aluminum substrates are also conducted. (Oil Processing & Refining 16, 17, 18, 27)

**7. Chemical Sciences Division:** The six programs of the Chemical Sciences Division focus on the elucidation of fundamental chemical and physical processes which are relevant to energy conversion, production, utilization and storage. The programs span a wide range of experimental, structural and theoretical investigations addressing: The role of porphyrin derivatives in bioenergetic reactions (focusing on mechanisms by which light is converted to chemical energy) and in the mediation of nitrogen assimilation, hydroxylations and the conversion of carbon dioxide to methane. Fundamental aspects of the dynamics of electrode interfaces; modeling of electrochemical and photoelectrochemical processes. Correlation of structure and function in electrochemical processes. Reaction rates and reaction pathways of combustion-related reactions of fuels and intermediates over an exceptionally wide temperature range (200 to 2500 K). The thermodynamics, reactivity and structure of metal hydrides with particular regard to materials useful in hydrogen storage, battery applications and catalytic hydrogenation reactions. Synthesis and characterization of molecular sieves (e.g. zeolites and aluminum phosphates). The programs utilize unique Brookhaven facilities such as the National Synchrotron Light Source (NSLS) and the High Flux Neutron Beam Reactor (HFBR), and have developed and applied a number of specialized probes such as the flash photolysis-shock tube technique, discharge-flow photoionization mass spectrometry (using the UV ring of the NSLS), x-ray scattering and EXAFS structural characterizations (using the x-ray ring of the NSLS), and the laser-induced temperature jump. A wide variety of more conventional physical-chemical techniques are also employed, e.g.: x-ray and neutron crystallography (at the HFBR), epr, nmr and optical spectroscopy, and electrochemistry. Theoretical efforts address problems in molecular dynamics, molecular orbital theory, the phenomenology of electrochemical and photoelectrochemical processes, and reaction kinetics and mechanisms. The metal hydrides work is partially supported by funds originating from the CIA and subcontracted by Hughes Aircraft. One CRADA (with W.R. Grace) is about to begin, and several CRADA proposals have been submitted. The major support comes from the Chemical Sciences Division, U.S. Department of Energy. (Production 24; Gas Storage)

**8. Analytical Sciences Division:** The mission of the Analytical Sciences Division is the development and application of quantitative methods for the analysis of a diverse range of systems, ranging from mathematical models of physical systems to environmental and epidemiological data. There are three groups in the Division, each with its own major focus. Work in the Mathematical Sciences Group concentrates on the development of advanced numerical and computational methods. Current emphasis is on methods for partial differential equations, innovative approaches to parallel computing, and the use of visualization techniques

for the study of nonlinear systems and chaos. The Biomedical and Environmental Assessment Group is concerned with the provision of scientifically based quantitative estimates of health and environmental risk and damage from energy supply and use. Results are used in planning and formulating energy technology policy and in guiding energy-related biomedical and environmental research. The Scientific Information Systems Group is concerned with real time and archival information systems for environmental data. The group is involved in the design, implementation and management of environmental data bases and the design and implementation of environmental data acquisition and display systems. Members of the group also act as consultants on information systems to other DAS programs. (Exploration 1, 2; Development 2, 28, 33; Environmental and Regulatory 8)

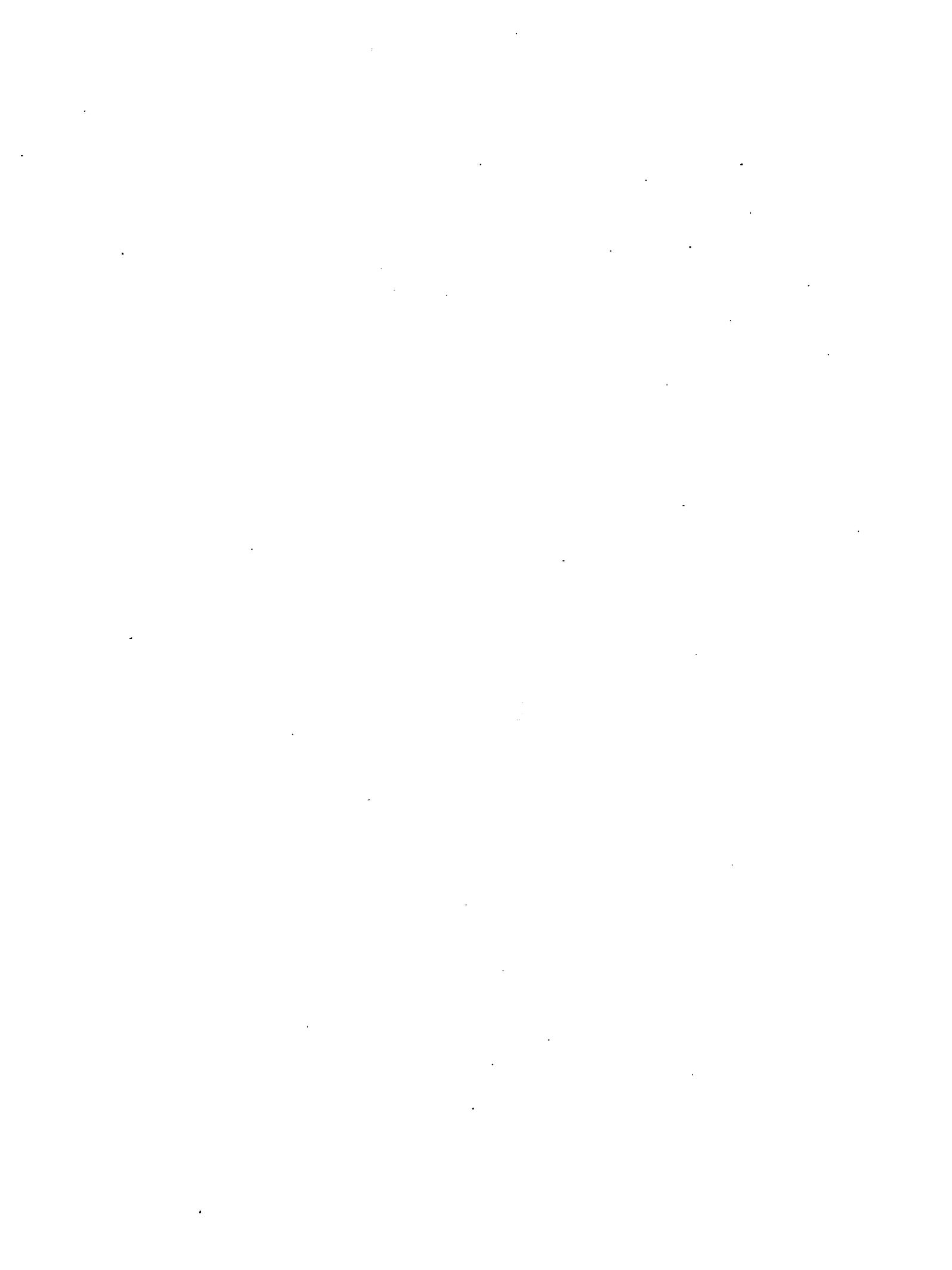
**9. Environmental Chemistry Division:** The Environmental Chemistry Division is engaged in a wide range of programs encompassing interpretive and theoretical studies, measurement methodology, laboratory experiments, and field studies. Areas of research include (1) development of methods and practical instruments for detection and real-time measurement of a variety of atmospheric constituents for use in field studies and laboratory experiments; (2) development and application of gaseous tracers applicable at extremely low concentrations for studies of atmospheric transport and dispersion, building air infiltration and ventilation, geophysics of oil and gas recovery from production wells, and leak detection in fluid handling systems; (3) theoretical, laboratory, and field studies directed at understanding the formation and behavior of aerosols; (4) studies of the formation, transport, mixing, and removal of gaseous and particulate pollutants in ambient air; (5) modeling of the kinetics of chemical reactions of atmospheric pollutants; (6) laboratory and field studies directed at the incorporation of sulfur and nitrogen oxides into cloudwater with the consequent formation of acid rain; (7) theoretical and observational studies of radiative transfer and fluxes in the atmosphere; and (8) analysis of data and development of parameterizations relevant to global climate change. (Development 4, 21; Gas Gathering 2; Gas Storage 2; Environmental and Regulatory 5, 10)

**10. Environmental and Waste Technology Center:** This activity is organized as a Division of the Department of Advanced Technology. Its principal mission is to identify, characterize, develop and demonstrate innovative strategies and technologies in order to solve hazardous, mixed and radioactive materials management issues that the federal government and private sector face today and in the future. Areas of technical competence in the Center include, but are not limited to, geochemistry, materials technology, risk assessment, barrier technologies and decommissioning and decontamination. Specific current programs include the experimental analysis and evaluation of geochemical processes which influence contaminant transport in soil and seabed environments. Work is also in progress to characterize and evaluate materials performance including corrosion testing, metallographic evaluations, mechanical testing, failure analysis (stress corrosion cracking, welding problems, erosion-corrosion), and nondestructive testing. The Center supports a strong program in the development and application of analytical and/or computational models to assess the impacts to people and the environment caused by the disposal of contaminants. This risk assessment expertise is being applied to investigations of ground water flow, contaminant transport, geochemical interactions and health effects. (Environmental and Regulatory 4, 9, 10, 14)

**11. Seismic and Structural Engineering Evaluation Programs:** Seismic programs within the Department of Advanced Technology provide seismic and structural engineering technical assistance to the Department of Energy(DOE) and the Nuclear Regulatory Commission(NRC). This assistance includes the development and application of advanced software and the evaluation of structural and aging behavior. The staff has broad experience in seismic analysis, structural response evaluation, soil mechanics, soil-structure interaction analyses and natural hazard assessment. This expertise is being utilized to perform seismic evaluations of DOE facilities. For example, probabilistic, site specific, seismic hazard evaluations are performed that include assessment of soil liquefaction, soil settlement after a seismic event and the seismic capabilities of existing structures. Related studies are conducted for the NRC and extend to the evaluation of the aging of structural and mechanical components in the commercial nuclear power industry as well as at DOE facilities. Mechanical engineering skills are also applied to evaluating the potential for thermal fatigue cracking in pipes, wear in components due to flow-induced vibration, and the effects of cyclic stresses induced by thermal stratification in pressurized piping. (Exploration 6; Development 3, 14, 28)

**12. New Infrastructure Technologies for the 21st Century:** The "state-of-the-art" scientific and engineering capability of Brookhaven National Laboratory and many other academic and industrial organizations in the New York region and throughout the country, have been mobilized into a consortium to meet the challenge of modernizing infrastructure technology and bringing it into the 21st century. Brookhaven and other consortium members have devised a range of breakthrough infrastructure technologies that will have a profound impact on present and future infrastructure. These include sophisticated devices for surveillance mapping and in-situ repair of weak points in underground gas pipes, water mains, sewer pipes, etc..In order to achieve these goals, Brookhaven is leading a National Infrastructure Center (NICEST).The primary thrust and purpose of this Consortium is to develop unique infrastructure techniques and products that will greatly enhance the presently ongoing research at Federal Agencies and in industry and academia. It is anticipated that the products of this broadly-based program will benefit many industries that operate sophisticated and complex facilities such as those found in the petroleum industry. (Oil Processing and Refining 3, 5, 6, 11, 13; Gas Gathering; Gas Storage 2, 4, 7)

**13. High Temperature Combustion Facility:** The High-Temperature Combustion Facility is operated by the Department of Advanced Technology of Brookhaven National Laboratory to support and promote research in the area of combustion science of high-temperature gaseous mixtures. The facility, designed and constructed as part of a joint research program between the United States Nuclear Regulatory Commission and the Japanese Nuclear Power Engineering Corporation, can accommodate combustion research activities encompassing the fields of detonation physics, flame acceleration and low-speed deflagration phenomena. A wide range of combustible gas mixtures at initial temperatures up to 700K and post-combustion pressures up to 100 atmospheres can be studied. Experimental combustion vessels designed to accommodate detonations, combustion instrumentation capabilities, data acquisition and control hardware and software, staff combustion expertise and a wide range of National Laboratory resources support the operations of this world-class facility. (Production 24)



## **Enabling Capabilities – Idaho National Engineering Laboratory**

**1. Engineering Mechanics, Fracture Mechanics, and NDE** - The INEL uses advanced computational methods and observational techniques to evaluate strength and lifetime parameters associated with piping, pressure vessels, and process equipment. There are strong economic and environmental incentives to extend plant life while conserving resources, protecting the public, and protecting the work force. Degradation of structural integrity due to corrosion, stress corrosion cracking, corrosion fatigue, thermal embrittlement, and creep are major considerations for extending plant life. Although such capabilities were developed primarily for the nuclear industry, they are applicable to gas processing facilities, refineries, and petrochemical plants. (Oil Processing & Refining 12, 13, 3)

**2. Advanced Materials and Processing** - The INEL conducts a broad range of advanced materials and processing research and development on metals, ceramics, and composite materials. The work emphasizes the design of microstructure and the control of fabrication processes to cost-effectively provide enhanced properties and meet performance requirements. Utilizing extensive capabilities in theoretical modeling, process diagnostics, and materials characterization, INEL advanced materials and processing is focused in the following areas: production of composite materials using particulate and whisker reinforcement to enhance strength and toughness of metal matrix and ceramic matrix composites; development of advanced welding technology for metals and alloys as well as techniques for ceramic joining; development of plasma processes for advanced extractive metallurgical and waste processing, ceramic synthesis, and coating technology; improved powder metallurgy techniques for fabricating metal and ceramic powders; and development of powder atomization techniques providing metallic materials with superior high temperature microstructure stability, strength, and corrosion properties. (Oil Processing & Refining 5; Deepwater Offshore 16)

**3. Advanced Manufacturing** - At the INEL, advanced manufacturing is focused on enhancing the competitiveness of U.S. industry by integrating research in the areas of materials, sensor development, and process control. Systems have been developed to provide real time feedback control for arc welding, to provide waste-stream free machining using pressurized liquid nitrogen for cutting, abrading, and drilling applications, and to provide knowledge based monitoring of equipment performance and health to improve manufacturing productivity and product quality. The INEL is currently working with U.S. auto makers to advance the concept of “intelligent manufacturing” via two CRADAs. This concept involves advanced systems that provide access controls, computer-aided design, robotics, flexible machines, automated decision making tools, and visualization tools networked through computers to provide engineers and operators with information to effectively complete tasks, handle manufacturing variations, and accommodate rapid production changes. (Oil Processing & Refining 5,14)

**4. Sensors and Controls** - The INEL develops sensors and process control systems for application in harsh environments where remote sensing is required. Areas of expertise include acoustics, optical, microwave, and chemical technologies to sense the process state and resulting product of such processes as arc welding, plasma spray, nuclear reactors, cupola melting, hearth melting, ceramic sintering, and bioreactors. Robust, rugged, noncontacting sensors have been

melting, ceramic sintering, and bioreactors. Robust, rugged, noncontacting sensors have been developed for Babcock & Wilcox, the U.S. Navy and U.S. Army, Ford, Chrysler, General Motors, the American Foundrymen's Association, Chevron, Shell, and Exxon for diverse industrial applications. Sensor inputs integrated with standard control techniques, neural networks, expert systems, and fuzzy logic control methods are applied in industrial processes when expert knowledge or empirical operating data form the basis for process understanding. (Oil Processing & Refining 26; Deepwater Offshore 3)

**5. Robotics and Smart Systems** - The INEL has developed a broad range of intelligent systems that combine advanced computer systems, sensors, tracking systems, and data bases to perform sensing and surveillance functions in remote or hostile environments. Systems that have been utilized and developed at the INEL include pipe crawlers, pipe sleds, miniature cameras, miniature pan and tilts, hemispherical cameras and systems, sampling and characterization system sensors and underwater inspection vehicles. These systems have been utilized for internal inspections of a wide range and size of piping, vessels, basins, tanks, ventilation ducts, and storage wells. By combining robotics and smart control systems with the need for large base-load certifiable chemical analyses for environmental applications, the INEL has developed a number of modules (and necessary software) for analytical laboratory automation. Additionally, the INEL has developed sensor/software systems that provide real-time information on the current serviceability of various types of machinery including hydraulic pumps, HEPA filters, and lathes. This technology provides users with critical "pre-failure" information (Oil Processing & Refining 14; Deepwater Offshore 3)

**6. Reservoir Modeling** - The INEL performs extensive modeling of geothermal reservoir systems using the commercially-available general purpose code, TETRAD. This code can be used for three-phase (water, gas and oil) modeling of black oil systems. TETRAD also can be used in a multi-component mode to model processes such as miscible gas injection, solvent flooding, CO<sub>2</sub> flooding, and nitrogen injection. In a thermal mode, it can be used for studies of steam injection into an oil reservoir. And finally, it can be used for several types of geothermal applications and aquifer studies (Development 25)

**7. Computational Fluid Dynamics** - The INEL has an international reputation in developing and employing thermal-hydraulic/fluid dynamic systems analysis and special application codes. An INEL thermal hydraulics code (RELAP5) is used world-wide in the nuclear industry for safety assessment and complex simulation calculations. It is designed to model transient multiphase, multi-component flow and energy transfer in complex piping and vessel systems with additional models for system components such as pumps, turbines, valves, etc. The computational staff also maintains a suite of simulation codes for a variety of physical applications such as advanced multiphase flow modeling, plasma flow and combustion modeling, complex turbulent flow, fusion reactor plasma physics modeling, and underground transport of organic materials and contaminants. They are also engaged in computational research relating to solution methods, numerical discretization, and parallel algorithm development. Current and developing collaborations exist between the INEL computational staff and the heat exchanger industry, the nuclear power industry, and the automotive industry, as well as with universities, other government laboratories, and federal agencies. (Oil Processing & Refining 25; Production 22)

**8. AI/Expert Systems** - INEL has used artificial intelligence technology to solve many process control problems which are similar to those faced by oil refinery and gas processing system operators. One important application is an alarm filtering system developed for use in complex plants where a critical process monitoring system is employed. The computer package operates in the off-normal condition when multiple alarms could potentially overwhelm an operator with a mix of critical and trivial information. The routine prioritizes information and displays it to assist operators resume normal operations. This approach, which greatly enhances plant safety, is in use at an INEL nuclear reactor and chemical processing facility. (Oil Processing & Refining 26)

**9. Integrated Visualization** - The INEL has developed an Integrated Visualization Environment (IVE) which has proven extremely effective in several application environments. The IVE allows users to manipulate, analyze, display and interact with extremely large and disparate data sets. All the traditional visualization tools are available along with the capability to operate in an immersive environment. This allows the user to view the information in its true 3D form. There are also simulation and automatic analysis capabilities and the entire system resides on top of a high performance data base. This allows not only the data, but analysis, simulation and viewing procedures to be archived, and hence queried during subsequent data analysis tasks. (Exploration 13)

**10. Simulation Based Design** - The design, testing and construction of large engineered systems in an extremely complex and demanding task. It is often very difficult and expensive to develop and test the many possible alternatives for these large engineering projects, particularly in remote, hazardous locations. Simulation Based Design dramatically reduces these costs by allowing the design, testing and validation to occur entirely in software. Hence the effects of changing particular system parameters can be immediately conveyed to all concerned parties, and the design modified on the spot to incorporate new or modified features. The system can operate with users that are widely dispersed geographically and yet still facilitate interactive and concurrent design. The INEL leverages the substantial effort funded by ARPA in the ship building arena and is posed to expand these capabilities into new application areas. (Deepwater Offshore 7,16; Arctic Region Activities 6)

**11. Chemical Processing** - New and innovative chemical processes are an important component in the total system for solving problems associated with environmental issues, energy efficiency and conservation, and cost-effective manufacturing and waste recovery. At the Idaho National Engineering Laboratory, we design, model, develop, test, and prototype cost effective processes, which can enhance petroleum operations. Membrane technologies to address problems of separations in highly acid, basic, or corrosive environments involving either liquid or gas streams are being developed. A new family of intermetallic catalysts that are longer lived and resist poisoning offer opportunity for a three-way automotive catalytic converter for nitrogen oxides, carbon monoxide, and hydrocarbons. Since these catalysts are not poisoned by sulfur containing gases, they are a prime candidate for hydrogenation catalysts in the chemical process industry. This poison resistance also offers added opportunity as a selective deep oxidation catalyst for combustion of VOCs and halocarbons. We have developed a precipitation process for removal of zinc, copper, cadmium, and nickel to below national pollution discharge levels in aqueous waste

streams. This technology was field tested and implemented at Tinker Air Force Base. Secondary ion mass spectrometric methods have been developed to identify contaminants such as surfactants, indoor pollutants, and pesticides. Advantages of this technology are that it can analyze virtually any surface with no sample preparation. An inexpensive and reversible fiber optic-based chemical sensor is under development for characterization and monitoring of VOCs in air and water. Proof-of-concept experiments have demonstrated TCE detection of 100 and 700 ppm in water and air, respectively. INEL researchers study and fabricate composites to enhance characteristics and performance of structural materials against weather, mildew, UV deterioration, and fire. INEL has developed a process for destruction of halocarbons that is environmentally safe, operates at low temperatures, and is economical. (Environmental & Regulatory 11; Oil Processing & Refining 4, 1, 7, 11, 19)

**12. Biotechnology** - Bioprocessing research programs at the INEL are using microorganisms to solve several of our nation's environmental and energy problems. INEL developments in bioprocessing and biofilters are centered on thin-film, gas-phase processes to improve conversion. We have built bioreactors to convert methane to methanol and developed biofilters to degrade halocarbons, hydrocarbons, and combustion gases for environmental restoration. In situ bioremediation processes rely on the microbial population within a contaminated area to break down contaminants. We are developing methods to identify subsurface microorganisms by nucleic acid testing of sediments. In our goal of developing cleaner-burning fossil fuels, we are pursuing biological processes that can solubilize or depolymerize coal to liquid fuels or biologically remove sulfur from fuel. We have isolated coal depolymerizing bacteria and characterized the end products. We are testing bacterial cultures for their ability to remove sulfur from coal substrates and are investigating the use of these microbes for desulfurization of crude oil. Several of our researchers in oil recovery are inhibiting the souring ( $H_2S$ ) of oil in reservoirs by microbial sulfate reduction through the application of biocides. Enhancing oil mobility within a reservoir by microbial action to improve wettability of the reservoir is being studied to improve microbe capability. (Oil Processing & Refining 11; Environmental & Regulatory 12; Production 21)

**13. Risk and Reliability Analysis** - The INEL has over 50 professionals with expertise in performing risk and reliability assessments supporting the design and operation of complex facilities. The staff has particular strengths in risk assessment methodology and software development, practical applications of risk assessment (e.g., identification and ranking of design and procedural alternatives, risk-based inservice inspection and testing), and human reliability analysis. The staff is also involved in the development and teaching of short courses on risk assessment. Some relevant projects include Defining the Role of Risk Assessment in Oil Spill Prevention, Accident Sequence Precursor Modeling, Risk Impact of Advanced Technologies, and Aging Risk Assessment. INEL staff are participating on the ASME Research Committee on Risk-Based Technology, which is developing practical approaches for risk-based inservice inspection and testing of mechanical equipment. In addition, the INEL has excellent ties with major universities including direct working relationships with MIT, UCLA, and the University of Maryland. The university programs are investigating a number of key issues, e.g., the safety implications of process control software, and the impact of organizational factors on risk. (Environmental & Regulatory 14; Oil Processing & Refining 8).

**14. Human Factors** - INEL has extensive experience in the study of human error in complex operations. Our base experience is analysis (both qualitative and quantitative) of human error in the nuclear arena. Starting from this detailed background, we have developed tools for assessing human reliability and evaluating human error that can be applied to any complex system. We have also developed considerable expertise in the design and evaluation of advanced human-computer interfaces for the control of complex processes and applied it in the development of state-of-the-art control interfaces such as the Advanced Test Reactor at INEL. Recent projects include: (1) working with the U.S. Coast Guard to improve the gathering of human error data by Coast Guard investigators - applying this expertise to characterize the human error in oil transport operations will greatly reduce the risk of oil spills; (2) applying human factors principles to increase the efficiency of oil and gas operations, as in our study for British Petroleum to identify the causes of human errors that led to stuck pipe incidents in drilling operations on platforms in the Gulf of Mexico, that, when implemented by BP, led to significant decrease in the incidence of stuck pipe incidents; (3) our work with Exxon to perform a review of their processes for designing the human-computer interface for a natural gas processing plant; and (4) an ergonomics assessment of the control station of an offshore oil field diving ship used in the North Sea. (Oil Processing & Refining 3,15)

**15. Environmental Technologies** - The INEL is one of the nation's premier environmental laboratories with a full spectrum of related skills, ranging from monitoring and assessment methods in all media, through the development of novel remediation and prevention approaches. Hundreds of professionals are involved in these activities. The Center for Integrated Environmental Technologies at the INEL represents a core group of senior-level scientists and principal investigators supported by technical staff conducting research on the design, testing, and implementation of integrated environmental monitoring systems. A systems approach to environmental monitoring and assessment is employed for all of these studies. This approach includes: 1) evaluation of source-receptor relationships, 2) multimedia (i.e., air, water, soil, biota) monitoring of key contaminant pathways within the environment, 3) the use of selected ecosystem parameters to detect anthropogenic influence, and 4) the application of a systems conceptual model as a heuristic tool. The INEL can field a complete suite of pollution prevention and environmental remediation technologies. Interdisciplinary teams are formed with the optimum mix of scientific and engineering personnel to attack complex problems. Successful demonstrations of this capability have been made on large projects at the INEL, and other DOE labs, at military installations and for other government sponsors. (Environmental & Regulatory 4, 10, 11, 12, 14)

**16. Earth Sciences** - INEL has approximately 100 Earth Sciences professionals with a strong experience base in petroleum engineering, geology, geochemistry, hydrology, subsurface flow and transport modeling, and geophysics. Over the last few years, this group has pioneered capabilities in sterile drilling technology, subsurface remediation applications, field sampling procedures, shallow high-resolution geophysics, and aquifer characterization techniques. Geoscience personnel have expertise in contaminant plume modeling and field verification of model results, passive soil venting technologies, remediation of hydrocarbon-contaminated soils, and near real-time geophysical monitoring of subsurface wetting fronts. INEL researchers have developed

specialized radiological and nonradiologic methodologies and codes to model release and transport from a variety of airborne, surface spills and aqueous sources. INEL has conducted a series of North Slope studies at the request of DOE/FE. These include assessment of undiscovered oil and gas potential, development of five known but non-producing fields, and evaluation of natural gas conversion technologies for North Slope applications. (Exploration 7, 9, 15, 16; Development 2, 4, 8, 14)

## **Enabling Capabilities – Lawrence Berkeley Laboratory**

Lawrence Berkeley Laboratory (LBL) is a multiprogram national research facility operated by the University of California for the Department of Energy. Its fundamental mission is to provide national scientific leadership and technical innovation to support the DOE's objectives. The Director of LBL is appointed by the Regents of the University of California and reports to the President of the university system. LBL benefits from its close working relationship with the University of California, Berkeley, as well as other universities, laboratories, and industrial organizations. LBL's core research strengths and facilities with direct application to the needs of the oil and gas industry are listed below.

**1. Advanced Light Source (ALS) –** The Advanced Light Source (ALS) is a national user facility at LBL dedicated to scientific research and development in several areas pertinent to the U.S. oil industry. It produces extremely bright synchrotron radiation, resulting in high spatial resolution because of the focusability of the photons beam generated. Consequently, users can study materials, such as catalysts, from a microscopic, surface morphological, spectroscopic, or analytical approach. X-ray fluorescence microscopy, for example, has been used to study films of quaternary metal oxide catalysts valuable to the petroleum industry. This technique allowed users to view the dispersion of the metal ions in the films on micron-resolution spatial maps.

Contaminants in this system could be studied at the femtogram ( $10^{-15}$  g) level because of the high sensitivity of the x-ray fluorescence microprobe. Other experimental approaches available at the ALS include absorption, x-ray photoelectron, and other types of spectroscopies that can be used to study both materials and interfacial reaction phenomena pertinent to the petroleum industry. (Oil Processing & Refining 1, 5, 7, 9)

**2. Barrier Fluid Technology for Production Enhancement and Waste Isolation:** LBL has developed a subsurface barrier technology using specialty liquids, which can be used to enhance hydrocarbon production and/or the containment of contaminants. The barrier materials are liquid when injected into the subsurface and produce impermeable barriers through a very large increase in viscosity. Two general types of fluids are used. In the first type, the increase in viscosity is provided by a gelation process. In the second type, the increase in viscosity is caused by a vulcanization-like process that results in the cross-linkage of the injected substances and the formation of a matrix of infinite viscosity. Both types of barrier materials are environmentally benign and chemically and biologically inert. The LBL barrier technology alleviates the adverse effects of the chemistry of the subsurface, thus allowing the control of gel/crosslinkage times. Appropriate emplacement of these substances can seal thief zones in petroleum reservoirs and enhance traditional remediation technologies (such as pump-and-treat) by redirecting flow to inaccessible and difficult-to-treat, less-permeable zones. Alternatively, an inert impermeable "cage" is created to surround and isolate the contaminated area. Such a "cage" could enhance or even make possible remediation techniques (such as soil flushing) that currently face regulatory approval problems due to concerns about contaminants escaping into previously unaffected areas of the subsurface. (Production 16; Drilling & Completion 6; Environmental & Regulatory 12)

**3. Center for Atmospheric and Biospheric Effects of Technology (CABET)** -- CABET was established in 1988 as a resource to LBL, DOE, and other research institutions on matters pertaining to the atmosphere and biosphere. Its major research themes include combustion processes; atmospheric transport and transformation processes for combustion emissions, greenhouse gases, and air toxics; human and ecological exposure and risk assessment; and national and international energy and environmental policies. Advanced sensors, instrumentation, computer models and software, control technologies, and analysis methodologies are developed and applied in these areas. Energy-efficient strategies and technologies are developed and analyzed for their effectiveness in remediation of environmental problems and pollution prevention. (Environmental & Regulatory 7, 8, 10, 12)

**4. Center for Computational Seismology:** The Center for Computational Seismology (CCS) provides a wide range of computational tools to serve U.S. Department of Energy (DOE) Energy Research Programs. It is also a focus for the fundamental advances in seismic imaging needed for the DOE's Fossil Energy, Environmental Management, Nuclear Waste Disposal, and Energy Efficiency Programs. Research is carried out over the entire spectrum of seismology, from basic studies in earthquake source mechanisms to the applied work of reflection seismology. CCS provides the core environment for the development of new application codes (e.g., 3-D seismic tomography, seismic reflection processing, VSP analysis, cross-well EM data inversion, and subsurface monitoring). The cornerstones of CCS are the solid theoretical base provided by our involvement with the Department of Geology and Geophysics and the Department of Engineering Geoscience at UC Berkeley, and the hardware and software facilities found at a national laboratory such as LBL. The core of our hardware facilities is a distributed SPARC workstation environment with modern graphics and computational tools. We also have access to "compute engines" such as the Cray-based MFE and FSU computational centers and LBL's MASSPAR parallel-processing machines. The software base is built upon 12 years of our own efforts in coding internal analysis routines, in addition to modern commercially based processing packages such as 3-D DISCO (FOCUS, Cogneseis Inc.), SIERRASEIS (Halliburton Inc.), and AIMS (Geoquest Inc.). (Exploration 4, 6, 14, 16; Development 3, 10, 11, 12)

**5. Chemical Energy Research** -- Chemical energy research at LBL has revealed new reactions between transition metals, such as rhenium, and organic molecules that are important to the improvement of catalysis involved in coal-conversion processes. Continuing program areas focus on the fundamental chemistry of important environmental and fuel species, including aqueous and gaseous species of carbon and sulfur. Catalytic conversion of carbon monoxide and hydrogen to gaseous and liquid fuels is studied to develop more efficient catalysts for hydrocarbon production. (Oil Refining & Processing; Gas Processing,)

**6. Chemical Physics** -- Our extensive chemical physics research includes several major programs. One focuses on spectroscopic studies of the structures of reactive intermediates. Laser-induced fluorescence, multiphoton ionization, and negative-ion photodetachment are used to study reactive species such as free radicals and cluster ions that may be important in combustion processes, reactive plasmas, and high-technology manufacturing processes. Techniques such as the use of crossed molecular beams are used for advanced and novel studies of the dynamics of important reactions with the goal of understanding elementary chemical

reactions through single-collision conditions or laser excitation. (Oil Refining & Processing; Gas Processing)

**7. Combustion Science** -- Research activities focus on acquiring a fundamental understanding of the chemical and physical processes that occur during combustion for the purpose of optimizing tradeoffs between reducing emissions and increasing efficiency. Novel diagnostics are devised to characterize flows and to measure species concentrations. High-performance computing is used to explore chemistry/flow interactions in combustion systems. Advanced approaches include studies of photodissociation, laser spectroscopy methods, molecular-beam mass spectroscopy, and the use of unimolecular kinetics for the theoretical study of high-temperature reactions important to combustion. (Environmental & Regulatory 10, Oil Refining & Processing 16, 24, 28)

**8. Database Management** -- LBL has extensive experience in research and development of data management techniques for scientific, statistical, and image data. This work falls into four major areas: (1) data organization for efficient retrieval, (2) support for object-oriented data models atop commercial (relational) database systems, (3) data structures and operations for scientific applications, and (4) query optimization for parallel and distributed systems. The first area includes placement and retrieval optimization for large spatiotemporal datasets on tape storage and design and optimization of parallel image servers. The second topic includes development of object-level database design tools, query and browsing tools, and data-entry and display tools. The third area encompasses algorithms for processing temporal, spatial, sequential, and statistical summary data, and optimization for random sampling queries. (Exploration, Development, Drilling & Completion, Production, Environmental & Regulatory)

**9. Distributed Computer Systems and Networking** -- LBL staff has been extensively engaged in experiments with gigabit/second-speed computer networks and the design and development of improved flow-control algorithms for high-speed data communications. Ongoing work includes a cooperative venture with industry to develop high-speed, network-based, digital-video and image-processing systems based on massively parallel computer systems and an innovative program to use high-level languages to visualize complex data sets. Staff is also engaged in the design and development of a number of distributed computing applications, including distributed imaging and visualization. (Exploration, Development, Drilling & Completion, Production, Environmental & Regulatory)

**10. Drilling** -- Through the Petroleum Engineering Department at the University of California, Berkeley, LBL can offer experienced engineers who are engaged in developing improved drilling technologies, including drill-bit design, cryogenic drilling of horizontal holes in unconsolidated rocks, and electro-osmotic migration of bit-balling in shaley rocks. (Drilling & Completion 8, 13)

**11. Ecological Systems** -- Ecological systems research is concerned with developing new tools for risk assessment and site restoration. Bioassays and biophysical indices have been devised to elucidate the effects of environmental stress at the whole-animal and cellular levels. Bioremediation techniques are being developed for the removal of heavy metals from waste waters. (Environmental & Regulatory 14)

**12. Flue-Gas Chemical Research** -- Flue-gas research focuses on developing new processes for SO<sub>2</sub> and NO<sub>x</sub> removal, as well as for the destruction of volatile organic compounds. Flue-gas research includes experimental work all the way to pilot-plant testing and demonstration-scale evaluation. The PhosNOX process and iron-thiocholate processes have been shown to be promising techniques for the removal of flue gas from fossil-fuel power plants. A process employing a new catalyst has been shown to be highly effective for direct reduction of SO<sub>2</sub> by synthesis gas to elemental sulfur. (Environmental & Regulatory 10)

**13. Isotope Geochemistry** -- The Center for Isotope Geochemistry is one of the best equipped laboratories in the world for measuring the isotopic composition of the radiogenic elements (e.g., Sr, Nd, Pb, Ca), the light stable elements (H, C, N, O, and S), and the noble gases (He, Ne, Ar, Kr, and Xe) in rocks and fluids. The Center has additional capabilities for chemical isolation of the short-lived cosmogenic nuclides (<sup>10</sup>Be, <sup>14</sup>C, <sup>26</sup>Al, and <sup>36</sup>Cl) and for high-precision measurements of trace element concentrations. We use an isotopic approach complemented by numerical modeling to monitor geological processes at the appropriate length and time scales needed for a predictive understanding. (Exploration 1, Development 1, 4, 8)

**14. Materials Energy Research** -- There are several interdisciplinary research centers at LBL that bring DOE resources to bear on scientific challenges of national importance. Specific focus areas are surface science and catalysis, polymers and composites, high-performance metals, ceramics science, biomolecular materials, enzymatic synthesis, and high-T<sub>c</sub> superconductivity. The Surface Science and Catalysis Program focuses on studies of advanced catalysts for clean fuels, pollutant reduction, and methanol synthesis. This program also includes the development of advanced surface instrumentation and techniques, including nonlinear optical techniques, scanning tunneling and atomic-force spectroscopies, and advanced Raman spectroscopy. The High-T<sub>c</sub> Superconductivity Program focuses on basic science, including the theory, synthesis, and characterization of new materials, and thin films and their applications. LBL's research into multilayer, thin-film structures created by means of photolithographic and laser-deposition techniques has led to the development of high-T<sub>c</sub> superconducting magnetometers/magnetic gradiometers based on dc superconducting quantum interference devices (SQUIDs) that operate at liquid-nitrogen temperatures. Geologic applications for such devices include arrays of detectors in borehole sondes for the detection of fields associated with crosshole and surface-to-borehole electromagnetic tomographic imaging. (Oil Processing & Refining 1, 5, 7, 9; Exploration 16; Development 10, 12,)

**15. National Center for Electron Microscopy (NCEM)** -- The National Center for Electron Microscopy (NCEM) is a national user facility at LBL dedicated to high-resolution microscopy of materials and related reaction interfaces. Bulk lattice properties, films, and grain-boundary problems are all amenable to study by using the instrumentation of this facility. The Atomic Resolution Microscope has been especially important in keeping the U.S. (along with associated industrial users) on the leading edge of transmission electron microscopy, especially as it relates to materials science. These facilities are highly useful for studying catalysis, corrosion, fuel, and

other petroleum-related research and development problems. (Oil Processing & Refining 1, 3, 5, 6, 7)

**16. Neutron Source Development** – A team of researchers specializing in ion sources, gamma-ray spectroscopy, and earth sciences at LBL, in collaboration with faculty in the Nuclear Engineering Department, UC Berkeley, has developed a compact, long-life, 14-MeV neutron tube that has applications in borehole logging. The new neutron source uses an rf-generated-plasma ion source and a mini-electrostatic accelerator to attain much longer life and higher flux than tubes based on Penning ion sources. Higher flux translates into improved spatial resolution, as resolution is presently flux-limited. As with present 14-MeV sources, either thermal neutrons or gamma rays are produced by the interaction of neutrons with earth materials. Gamma-ray spectroscopy, done with a high-resolution, solid-state Ge detector, provides a means for quantitative elemental analysis. LBL is also pioneering the development of heavy lead-based inorganic scintillometers that have 10 times faster response and rate capabilities than the currently favored bismuth germanate (BGO) detectors. (Development 17)

**17. Reservoir Characterization** – LBL offers world-recognized capabilities in providing multidisciplinary teams, consisting of geologists, geophysicists, geochemists, hydrogeologists, and reservoir and drilling engineers for projects in reservoir characterization. A wide variety of forward and inverse algorithms are utilized for the co-determination of data through deterministic and stochastic modeling of flow and transport on scales ranging from core samples to interwell spacings and up to basinal dimensions. LBL also has developed a number of borehole hydrologic tools and tracer methods for mapping fractures. (Development 1, 4, 6, 14, 21)

**18. Reservoir Simulation** – LBL has an international reputation in mathematical modeling and numerical simulation of coupled mass and heat transport in porous and fractured rocks. State-of-the-art codes developed at LBL are being applied worldwide for the predictive modeling of multiphase, multicomponent, nonisothermal fluid and heat flow and reactive transport for natural gas and oil recovery and storage, geothermal reservoirs, nuclear waste isolation, and environmental problems. Coupled to laboratory studies on rock properties, reservoir studies include the effects of capillarity and vapor adsorption, the interplay of formation heterogeneities and hydrodynamic instabilities, and stress-strain changes within the flow regime (e.g., compaction and subsidence). (Development 25,26,28,30,33)

**19. Scientific Visualization** – LBL capabilities include innovative visualization in a distributed computing environment. Visualization of earth sciences applications have included display of 3-D seismic and reservoir data for reservoir characterization and display of model calculations of water/chemical flooding and 3-D seismic wave propagation. Recent work includes (1) coupling a data-flow visualization package and virtual reality technology with a reservoir simulator, and (2) coupling compaction-subsidence codes to model and visualize well failures. (Development 25, 30, 33)

**20. Subsurface Imaging** – The imaging program focuses on the development of instrumentation and associated computer codes for high-resolution seismic and electromagnetic imaging of subsurface heterogeneities between boreholes and from surface to borehole. LBL is also working

on the simultaneous inversion of seismic and electromagnetic data to quantitatively determine porosity and fluid composition. (Development 10, 12, 14, 15, 16, 17)

**21. Surface Reactivity** – The program in reactivity at surfaces and interfaces will involve molecular studies of interfacial phenomena using new techniques in laser spectroscopy and x-ray scattering. The program is designed to gain an understanding of chemical reactivity in key areas of energy science, including nearly all catalytic reaction systems, solar-energy conversion technologies, light-assisted chemical syntheses, electrochemical energy-conversion technologies, and corrosion phenomena. (Oil Processing & Refining 3, 5, 7, 8, 9, 11)

## **Enabling Capabilities – Lawrence Livermore National Laboratory**

**1) Materials Testing and Advanced Materials:** Materials Science and Materials Engineering is a key technology area at LLNL. The Materials Engineering and Mechanics Section has state-of-the-art capabilities and facilities for studying the mechanical response of materials, components, and assemblies under various conditions of load, deformation and environment. Advanced capabilities exist for material characterization, fracture mechanics studies, high strain-rate behavior, design of composite materials and superplastic forming of metals. These capabilities have application in virtually any industrial process where high performance and reliability of material behavior is of paramount concern. We also have a strong effort in the synthesis, development and description of new materials. We design and synthesize new materials in an iterative process, where molecular design calculations on the expected characteristics of the new material, as well as actual performance characterization, drive the synthesis. Of special interest are carbon, organic, and inorganic aerogels, which are used in new catalyst systems, insulation, and energy storage; laminated metal composites, which combine various layers to achieve both corrosion and erosion resistance while improving strength and toughness; metal matrix composites, materials with significantly greater strength and stiffness which can be made to near-net form. We emphasize engineered materials with specific properties that can be fabricated through novel processing techniques. We model the overall process to improve the manufacturability and cost effectiveness of the material. [Drilling and Completion 8, 12; Production 3; Deepwater Offshore 7, 8, 9, 16; Oil Processing and Refining 5]

**2) Mass spectrometry:** Mass spectrometry (MS) has played an important role in many laboratory programs. Gas and liquid analysis for the fossil energy and environmental programs over the past 20 years used a variety of instruments, including pioneering work in the early 1980's in computer-controlled tandem MS. A current area of active research is analysis of solvent-swollen residua by matrix-assisted laser desorption/ionization (MALDI) time-of-flight mass spectrometry. ICP-MS is used for the fossil energy, environmental, nuclear test, and laser isotope separation programs. Isotope MS has been an important diagnostic method for the nuclear test program throughout its history, and these facilities have been used more recently to study NORM for DOE and groundwater sources and movement in California via oxygen isotope measurements. The largest instrument on site is an accelerator MS, which produces the majority of the carbon-14 radio-dating measurements in the world. Isotopic measurements are done for other elements as well, and I-129 is being explored as a method for absolute age dating of oil samples. [Exploration 7; Development 4, 21; Oil Processing and Refining 24; Environmental and Regulatory 10, 15]

**3) System and Decision Sciences Capability:** This capability enables the evaluation and optimization of processes and decisions. It finds diverse applications across the petroleum industry as it has in nuclear energy and in guiding decisions at the national laboratories (nuclear waste disposal, nuclear and hazardous transportation, nuclear reactors, laser-isotope separation, nuclear weapons, and space-based defense). The 30 staff members include broad industrial/academic backgrounds in operations research, statistics, mathematics, economics, psychology, engineering and physical sciences. They are well represented in the peer reviewed literature and have continuing support. Of particular interest to petroleum industry are:  
**Probabilistic risk assessment:** Assessment of the risks and consequences of low probability,

high consequence accidents using event trees, fault trees, human factors, and simulation models. The technologies could be applied to oil tanker operations and hazardous materials and reservoir management. **Reliability analysis:** Component failure rates and models of system structure are used to estimate the reliability of the system as a whole, and to identify cost effective means of improving reliability in large scale systems involving complex interactions between the plant, safety systems, human operators, and the environment. Can be used throughout the industry. **Technology choice:** Technology options for a wide range of missions are evaluated by applying decision models to estimate the risks associated with the pursuit of new technologies, the potential value of R&D efforts, and the sensitivity of decisions to key assumptions and value judgments. Developed to guide national lab decisions in technology development. **Economic simulation models:** A computer package has been developed for modeling markets permitting an analyst to build a network model of an economic system and find equilibrium prices and quantities over time. It includes representations for natural resources, conversion processes, markets, and demand centers as well as interactions that affect production, pricing, and capacity expansion decisions. **Environmental impacts of hazardous materials disposal:** An upper level systems model was developed that coordinated the operation of corrosion, geochemistry, and hydrodynamic sub-models to forecast leakage rates from a proposed nuclear waste repository. It is capable of characterizing the risks from a collection of tanks of hazardous materials and a decision model was developed to aid monitoring and clean-up activities. [Exploration 2; Development 28, 33; Oil Processing and Refining 3, 8, 11, 13, 15; Environmental and Regulatory 4, 14]

**4) Scientific Basis for Risk-based Regulation:** LLNL capabilities to assist the oil and gas industry comply with federal and state endangered species acts (ESAs) include developing risk-based approaches to evaluating proposals for listing species; assessing project effects; streamlining regulatory compliance; and developing a nation-wide database designed to assist in project planning. The capability is based on 15-years of experience supporting projects at the Naval Petroleum Reserves, California (NPRC) and LLNL/Site 300. These programs have published over 90 technical reports and articles. This capability has direct application to the oil and gas industry because it will provide improved scientific information and access to information that may guide development of policy and regulations by federal and state resource agencies. We have considerable experience preparing integrated health-risk assessments of organic and inorganic contaminants released into the environment. We are known nationally for our pioneering work in the development of multi-pathway, multi-media exposure models. For example, we have completed two assessment models for the California Environmental Protection Agency, one dealing with air toxics and the other for hazardous waste sites. Our research has also focused on characterization of the variabilities and uncertainties in health-risk assessments. A growing area of research involves quantification of the ecological effects associated with contaminant releases to the environment. [Environmental and Regulatory 4, 7, 14]

**5) Nondestructive Evaluation:** LLNL has built a world-class nondestructive evaluation facility over the last 20 years to service internal programs. NDE encompasses material characterization, in-service inspection, periodic monitoring and other activities related to safe operation of structures and machinery. We have developed innovative NDE solutions for complex applications using the synergism between physics and engineering. Current work has focused on the transfer

of NDE technology to commercial applications for the auto, aerospace and heavy machinery industries. Extensive capabilities in ultrasonic inspection, radiography, computed tomography and infrared imaging enable LLNL to offer multiple solutions to a variety of industrial problems, including process monitoring, material characterization, corrosion detection, site characterization and environmental monitoring and assessment. One new technology is an extremely low cost, compact micropower radar system. The radar is several cubic inches in volume, is capable of battery operation for months at a time, is of extremely robust construction, and has ground penetrating ranges of several feet. Imaging systems based on this technology are currently underdevelopment. The technology is currently being licensed for a number of applications ranging from stud finders to burglar alarms and be evaluated for such applications as bridge inspection and military mine detection. [Development 5, 12, 15, 22; Drilling and Completion 11; Production 10; Deepwater Offshore 7, 16; Oil Processing and Refining 12, 13]

**6) Parallel Linear System Solvers and Adaptive Numerical Methods:** Our expertise in parallel linear system solvers and adaptive numerical methods has been applied to many industrial applications, including environmental remediation, combustion, plasma etching, and nuclear well logging. Our iterative linear solvers can solve systems having more than one million unknowns in just a few seconds on parallel computing platforms. Our adaptive numerical methods allow one to concentrate computational effort where it is most needed, and typically require 10-100 times fewer spatial zones than a comparable uniform mesh. These capabilities can be brought to bear on several applications of interest to the petroleum industry, including borehole tool design and data analysis, oil reservoir simulation, and modeling of fixed bed catalytic reactors. [Exploration 1; Development 15, 16, 17, 25; Production 8, 11; Oil Processing and Refining 6, 25; Environmental and Regulatory 6]

**7) Atmospheric Modeling:** LLNL has an exceptional capability in atmospheric modeling, with components in emergency preparedness and response, dense-gas dispersion, cloud dynamics, pollutant dispersion, cloud dynamics and microphysics, atmospheric modeling, and global atmospheric and climate change modeling. One particularly unique capability is the Atmospheric Release and Advisory Capability, (ARAC) which has a 30 person staff to provide around-the-clock on-call, worldwide emergency response assessment within 60 minutes for radiological and toxic chemical accidents for DOE. Example applications were the COSMOS satellite burnup over Canada, Three-mile Island and Chernobyl accidents, Kuwait oil fires, and Mt. Pinatubo eruption. Research activities in support of ARAC and other applications include modeling the affect of complex terrain on atmospheric currents. We also have developed models for atmospheric chemistry, including ozone depletion, and lead a comparison of various general circulation models for atmospheric change calculations. [Environmental and Regulatory 7, 8]

**8) Systems Engineering for Complex Industrial Systems:** The national labs have been asked to solve complex U.S. industrial problems which require the integration of expertise in multiple disciplines. For example, the U.S. Enrichment Corporation recently announced its intention to commercialize the Atomic Vapor Laser Isotope Separation (AVLIS) technology by authorizing the LLNL to conduct the first large scale transfer of modern technology from a research environment to industrial production. Also, a recent CRADA has been established to develop advanced numerical control technologies to compete with foreign machine and robotics industries

Many other collaborations of this nature are in progress. The magnitude and complexity of these projects require the deployment of advanced technologies for controls and information processing. The requirements will include operational, financial, political, environmental, and regulatory issues. Balancing these requirements within the constraints of cost and schedule is a key to successful implementation. The systems engineering approach provides the means to examine the problems, evaluate the requirements, identify the risks, formulate the scope of work, examine the management structure, and provide a structured manner of executing these projects. [Production 14; Oil Processing and Refining 2, 3, 6, 8, 11, 14; Environmental and Regulatory 7, 10, 11]

**9) Computer Simulation of Mechanical and Thermal Processes:** Over the last 20 years, LLNL has developed a suite of world class finite element codes in the areas of computational mechanics (DYNA, NIKE), heat transfer (TOPAZ), and fluid dynamics (HYDRA). This suite of codes is under active development (e.g., porting to parallel computers) with funds being leveraged between DOE Defense Programs, CRADAs, LLNL directed research and development, and the extensive collaborators program with industry. There are many potential applications for these tools in the petroleum industry. These programs are ideally suited to the nonlinear analysis of structures subjected to extreme loading such as blast, earthquakes, and impact. Computational fluid dynamics capabilities can be utilized to model flow around deep water platforms and the dispersion of pollutants from stacks and around buildings. These codes also form the framework for modeling the physical processes involved in basin evolution to deal with the fully-coupled processes of multicomponent multiphase flow in porous media, conductive and advective heat transfer, and mechanical deformation, including fluid flow in faults and fractures. Simulation of fully coupled fluid, thermal, and mechanical processes in earth systems has applications in hydrocarbon exploration and recovery, radioactive waste disposal, geothermal systems, and mineral exploration. [Exploration 1; Development 2, 25; Production 8, 11; Deepwater Offshore 6, 9, 16; Oil Processing and Refining 3, 13]

**10) Electromagnetics:** The LLNL has a distinguished toolset in electromagnetics, both experimental and computational, extending from d.c. to microwave. In the lower range up to hundreds of kHz, many of the techniques are applied and/or are applicable to the problem of subsurface remote sensing. Some techniques, such as electrical resistance and electromagnetic tomography, were developed specifically for subsurface detection and imaging for geophysical applications, while other techniques such as those based on computer tools for frequency and time domain analysis, were directed towards full-wave analysis for em interactions at high frequencies but are easily extensible to the geophysical regime. The activities have had a reasonably even distribution between electromagnetic geophysical techniques and advanced higher frequency and time domain methods. The geophysical applications for ERT and EMT are already well known. An additional LLNL capability involves highly regarded higher frequency codes that can be used to accurately solve forward problems for propagation in the complex subsurface medium. These efficient solutions obtained using integral equation methods in very efficient algorithms can be used with efficient inverse problem solvers to create a map of the subsurface region. [Development 10, 15, 16, 17, 18, 30; Drilling and Completion 11; Oil Processing and Refining 12; Environmental and Regulatory 5]

**11) Micro Technology Capability:** The LLNL microtechnology capability is focused on activities in devices, instruments, or systems which require microfabricated components, including electronics, photonics, micro-structures, and microactuators in applications for global security, global ecology, bioscience, and national industrial competitiveness. For example, our personnel have designed and fabricated silicon-based microaccelerometers for kilo-g and for micro-g accelerations, circular-cross-section capillary channels in silicon wafers which have cleanly separated a mixture of industrial gases, sub-mm adjustable-position bimorphic actuators which function in air or in water, thin-film shape-memory-alloy actuators, and clear ultralow stress silicon nitride films 100-nm thick with 1-cm<sup>2</sup> area, and many other microstructures. The above items represent opportunities for in-situ sensing, microminiature sensing devices (microsensors) and microminiature sample dispensation (micro-pumps, -valves, etc.). [Development 34; Oil Processing and Refining 12; Gas Processing 5, 8; Environmental and Regulatory 10]

**12) High-powered lasers:** LLNL is recognized by many government and industrial organizations as the world-leader in high-power advanced laser-based systems. The most recognized laser is the Nova laser, used for inertial confinement fusion experiments. We have also developed high-powered dye laser systems for uranium isotope separation, including the ability to transmit high power levels through fiber optics, and we have developed numerous other laser systems for the Department of Defense. Activities with industry include biomedical applications, laser machining and materials processing, and analytic remote sensing. [Exploration 8; Gas Storage 2; Environmental and Regulatory 5, 10]

**13) Neural Networks:** During the last 6 years, our Imaging and Vision Team in the Signal and Image Processing Research Group has developed an excellent capability in neural networks, automatic target recognition (ATR), sensor data fusion, remote sensing, computer vision, pattern recognition and parallel processing architectures. This capability is in addition to our core capabilities in signal and image processing, estimation, and control developed over 20 years. Our research efforts include work in hierarchical scale space decompositions (Gabor transforms, wavelets, etc.), probabilistic neural networks and general regression neural networks, development of a computer vision software package, and feature selection research. We do fundamental and applied research to develop advanced algorithms and software on computer work stations for a wide variety of applications, with over 40 publications over the last 5 years. These capabilities can be used for seismic processing (e.g., lithology estimation, velocity analysis, and event tracking). [Exploration 1, 3, 4, 12; Development 11, 14, 28, 33]

**14) Rock Mechanics:** LLNL has an extensive capability in laboratory, theoretical and modeling studies of the geomechanical behavior of rock and rock like materials at conditions ranging from those found at the surface to several kilometers depth. This rock mechanics capability at LLNL was developed over the last 25 years to address questions associated with many projects deemed to be in the national interest, including, but are not limited to, defense-related rock mechanics, nuclear waste disposal at Yucca Mountain, Nevada, oil and gas exploration and production, and basic research into rock behavior. LLNL is recognized as a world-class center for rock mechanics/geomechanics, with extensive laboratory capabilities that are unmatched in breath and depth of capability. We have more than 100 publications in the past

5 years, and several of our staff are recipients of national and international research awards. [Exploration 1, 9, 16; Development 3, 5, 9, 12, 18]

**15) Large Scale Plant Process Control System:** LLNL has developed large scale process control systems for various large-scale experiments and is now enhancing the control system for the new billion dollar Atomic Vapor Laser Isotope Separation (AVLIS) facility. A sophisticated control system is required that provides real-time integration of all the elements and field devices (currently estimated to be 100 thousand input/output points) to the highest layer of the plant management system. The control system is comprised of computer systems providing functionality for the plant management through detailed control of feed, enrichment, and product operations. The computer systems provide reliable, safe, fully integrated process control systems for real-time data acquisition and control of most essential plant processes and support activities. These processes and activities include operator control of process systems, data archival and retrieval, alarm processing, access control, logging, refurbishment, and data display. Automation will be provided to maximize the production throughput and to minimize the need for maintenance personnel in areas such as testing, diagnostics, trouble-shooting and refurbishment. In addition, a Plant Information Management System provides functions relating to health and safety monitoring, security management, trending, performance calculations, report generation, inventory control, production planning, business services, and human resource management. This type of process computer systems can also be applied to large scale petrochemical facilities. [Oil Processing and Refining 25, 26]

**16) Computational Earthquake Initiative:** Over the past three years the Lawrence Livermore National Laboratory has committed substantial resources to research new techniques for estimating earthquake ground motion and predicting the earthquake response of soils and structures. This research has resulted in new methods of developing site-specific earthquake ground motion estimates based on site measurements of frequently occurring micro-earthquakes. Advanced, nonlinear finite element computational tools are employed to numerically model the response of soil and structural systems. In addition to the methodologies developed, this project has formed the nucleus of a multidisciplinary team of seismologists, geotechnical engineers and structural engineers addressing all elements of seismic response computations. The methods developed under this research have potential application to any major structure subject to earthquakes, including offshore platforms and industrial facilities such as refineries and major pipelines. Elements of this research are being applied in a U.S. Minerals Management Service sponsored seismic hazard evaluation for offshore platforms in the Santa Barbara California region. [Deepwater Offshore 16; Environmental and Regulatory 14].

**17) Robotics for Hazardous Materials Handling:** Traditional teach and playback robots do not have the sophistication necessary to apply them in unstructured environments or control them remotely in hazardous environments. Commercial products are often not flexible or robust enough for hazardous environments. LLNL has been researching industry expertise and working with them to develop more modular, remote controllable and autonomous systems (more sophisticated control programs based on sensor information). LLNL, with IBM and Cimetrix, have developed a more environmentally hardened robot with a graphical model based control system for use in hazardous environments. LLNL has developed advanced control algorithms for

computer 3D vision interpretation, automatic path generation, collision avoidance and remote control of manipulators. Industry involvement has been accomplished through a variety of mechanisms including contract support to LLNL, product updates based on LLNL product evaluations and critiques, and collaborative developments. Several prototype systems have been developed at various levels of maturity, including a multi-legged walking platform that will be inserted through 12 inch risers into storage tanks but stand several feet tall and a gantry robot that is being delivered by IBM for production use. Two systems are currently being designed and built for use in waste facilities. Telerobotic and advanced control technology, coupled with innovative mechanical structures extends an operator's reach into hazardous environments without increasing the tedious nature of the task. [Oil Processing & Refining 14]



## **Enabling Capabilities -- Los Alamos National Laboratory**

**1. Computational Testbed for Industry:** The extensive supercomputing resources of Los Alamos National Laboratory are now available to in industry and small business. As part of an ongoing Department of Energy program designed to enhance US industrial competitiveness, Los Alamos established the Computational Testbed for Industry. The Testbed gives US-owned corporations and small businesses quick and easy access to the Laboratory's vast array of high-performance computational tools and experienced technical staff on a cost-shared basis. It also gives both beginning and advanced industrial users an opportunity to solve real-world problems with powerful computational tools. These tools offer the ultimate in visualization, data storage, and networking. The Computational Testbed for Industry takes full advantage of the Laboratory's computing environment and wealth of computational expertise in many areas, including environmental modeling and remediation, materials and molecular dynamics, seismic imaging and reservoir management, semiconductors and electromagnetics, computational biology and biotechnologies, stochastic and deterministic particle transport, computational fluid dynamics, reactive flows, combustion, computational chemistry, economics and business simulation, and advanced manufacturing. The Computational Testbed for Industry is a Department of Energy User Facility. (Development 25, 2, 27; Exploration 3, 4, 6, 13; Environmental and Regulatory 8, 9)

**2. The Advanced Computing Laboratory:** The Advanced Computing Laboratory is committed to providing a state-of-the-art computational environment that couples novel high performance computer architectures with the best in advanced workstation technology and high speed networking capabilities. By exploiting the unique strengths and capabilities of each technology to address particular aspects of complex computational challenges, this heterogeneous environment enables us to take on some of the largest scientific computations ever attempted. **Thinking Machines Corporation's Connection Machine Model 5:** The CM-5 has made practicable the simulation of extremely large-scale, complex systems that have been previously unachievable. The CM-5 is currently configured with 1056 processing nodes, 4224 vector units, 32 gigabytes of main memory, 440 gigabytes of on-line high-speed disk storage, and four 100-megabyte per-second HIPPI interfaces coupling it with other available computing resources. **Cray Research, Inc.'s T3D:** With its powerful node level processors coupled to a very fast, low latency interprocessor interconnect as well as the I/O resources of the YMP front end, the T3D provides an effective environment for traditional message-passing programming models as well as for distributed shared memory programming. **IBM Power2 Risc System/6000:** Equipped with both HIPPI and ATM network interfaces, the Power2 has played a significant role in ongoing research in the application of high-speed networking capabilities to the solution of complex distributed computational problems. **Silicon Graphics, Inc., Onyx:** The Silicon Graphics, Inc., Onyx, with two 75-megahertz MIPS R8000 processors, 512 megabytes of main memory, an extremely powerful Reality Engine 2 graphics pipeline, and two RM-4 raster managers, is a focal point for most of the data visualization activities taking place at the ACL. (Exploration 4, 3, 6, 13; Development 2, 25, 27; Environmental and Regulatory 8, 9)

**3. The High Performance Parallel Processor Program:** Under the Industrial Computing Initiative Agreement between the Department of Energy and seventeen leading industrial companies, Los Alamos is a partner in major efforts that include the advancement of massively

parallel computing and its applications in industry. The agreement is part of the DOE's High Performance Parallel Processor Program, also known as "H4P." Signatories to the three-year program include Los Alamos, Livermore National Laboratory, Cray Research, Inc. (CRI), Thinking Machines Corp., and several other industries. The DOE is paying half of the \$52 million agreement, and industry is contributing the other half. **Oil and Gas Exploration:** CRI and Los Alamos are helping Amoco Production Company to develop their reservoir simulation software to run on the Cray T3D system. The Amoco software is a proven, field-tested tool for simulating oil and gas reservoirs. Development of the software to run on a massively parallel processing machine will give the resulting model higher resolution and the ability to deal with greater geologic complexity. Simulations that normally take several days or weeks will run in less than an hour. **Chemical Processing:** Los Alamos and CRI are teaming with Exxon Research and Engineering Company to take advantage of the speed and memory of massively parallel systems. Models co-developed will help make it possible to accurately model and improve the efficiency of multiphase chemical reactions that occur in many industrial processes. (Development 25, 14; Oil Processing and Refining 6, 11, 21, 24, 25; Environmental and Regulatory 9)

**4. Multiphase Flow Computer Code Library:** Our multiphase flow research effort at Los Alamos has been directed for the past several years toward advancing the state-of-the-art in computer simulation of reactive multiphase flows. Our goal has been to explore new methods for using the most modern supercomputers available to efficiently and accurately simulate large-scale reactive multiphase flows of interest to both Industry and the Department of Energy. Such a capability could be used to optimize industrial processes such as Fluid Catalytic Cracking and Ebullated Bed Resid Hydrocracking found in petroleum refining, for example. Our research has components in multiphase flow theory, numerical methods and applied computer science. The vehicle for our research is a multiphase flow computer code library called CFDLIB. The work on multiphase flow theory connected with CFDLIB includes the development of comprehensive models for multiphase turbulence and for exchange of mass, energy and momentum among phases. We are also incorporating a multi-species heterogeneous chemical reaction package. The numerical methods employed by CFDLIB are state-of-the-art and enable robust large-scale simulations of multiphase flows in complex two and three dimensional geometries. We have carefully structured the CFDLIB computer codes to solve multiphase/multispecies flow problems on a variety of computing platforms including most conventional UNIX workstations, Cray YMP supercomputers, clusters of IBM workstations, and massively parallel supercomputers such as the new Cray T3D. (Oil Processing and Refining 25, 6, 21, 24; Production 22)

**5. Applications of Risk Assessment to the Oil and Gas Industry:** Risk assessment tools for human health and damage to ecosystems have been developed by Los Alamos for organic chemicals, metals, and radioactive materials. Application to the potential environmental transport paths from production, refining, and use of oil and gas products is another possible use of the tools. The risk assessment tools for accidental releases, environmental restoration, waste management, and environmental monitoring address the hydrological, atmospheric, biological, and geological or soils fate of contaminants. Screening models for rapid evaluation of contaminants in the environment and the human or ecological risk implications have been developed. If the screening models indicate a potential for exposures in excess of environmental standards, more detailed risk assessment models are used to determine if the initial estimates are realistic. The

same types of models are used to develop screening concentration limits for contaminants in soils, water, or air. If needed, risk assessment models are used to derive cleanup levels for environmental media such as air, water, or soils. The same models are used for comparisons of alternative technologies and to provide risk level input into decisions where risks, costs, and regulatory factors must be considered. In each case, an estimate of the uncertainty in risk estimates is provided so decision makers are aware of the potential for challenge and can select the level of confidence needed. (Environmental and Regulatory 4, 3, 7, 9, 14)

**6. Integrated Energy and Environmental Assessments:** A huge gap often exists between the results of science and technology and what is needed by policy makers for making decisions. For example, measurers make measurements and modelers develop and run models, but the significance of these measurements and model results need to be made useful to decision makers. Los Alamos has developed a science-based energy and environmental assessment capability--merging measurements, modeling, and analysis--to assist policy makers in decision making. This capability allows policy makers to consider the environmental, economic, social, political, and institutional impacts of energy production and use. One example of where this tightly coupled approach has been successfully applied is in the area of urban air quality, where the results are being used by municipal planning offices to reduce atmospheric pollution. This integrated assessment capability can be applied by Los Alamos to a wide array of oil and gas production and end use scenarios. (Development 33; Oil Processing and Refining 8; Environmental and Regulatory 4, 14)

**7. Center for Materials Science:** The Center for Materials Sciences (CMS) is the focal point for a growing intellectual community in materials science that extends from basic research in condensed matter physics to applied materials technology. Members of the CMS team are leaders in topical areas of materials research, they collaborate with Los Alamos staff and the external materials science community, and they contribute to the development of new research capabilities. CMS facilities contribute to many Laboratory programs. The center's Scanning Tunneling Microscopy Laboratory captured images of the spiral growth mechanism of high-temperature superconductor thin films and continues to be a major player in applied superconductivity programs. The Electron Microscopy Laboratory supports a community of users pursuing interests in ceramics, metals, semiconductors, composites, and polymers. The Ion Beam Materials Laboratory has contributed to research involving materials analysis, geosciences, materials synthesis and processing, radiation effects, and surface science. (Production 3; Deepwater Offshore 5, 8, 9, 16; Oil Processing and Refining 5, 12, 13)

**8. Engineering Modeling in Support of Oil & Gas Programs:** Los Alamos National Laboratory possesses a comprehensive engineering analysis capability that could be used to support Oil and Gas initiatives. The capabilities of experienced analysts and state-of-the-art software are coupled to advanced computing hardware to solve engineering problems that have recently included heat treat distortion in gears, superplastic forming, impact analysis of composite fan blades, structural acoustics, drill stem dynamic modeling as well as a host of design problems in the nuclear weapons program. The problems we solve are generally characterized by complex geometries requiring a very large number of equations to simulate accurate response, advanced material models (e.g., heat transfer, stress and metallurgical transformations in a single

calculation) or large deformations typical of superplastic forming or impact. (Deepwater Offshore 16, 2, 4, 5, 7, 9)

**9. Materials Science Laboratory:** The Materials Science Laboratory (MSL) is a focal point for integrating Los Alamos National Laboratory's broadly based capabilities in materials science to address the evolving needs of defense, energy, and basic science and to aid the transfer of related technologies to U.S. industry. The MSL is a user facility with all of its resources readily available to external sponsors and collaborators. In addition to experimental programs in mechanical behavior, materials processing, synthesis, and characterization, the facility provides access to the Laboratory's extensive computing capabilities for programs in modeling and simulation. The MSL supports 20 distinct materials research topics: advanced materials synthesis, corrosion compatibility, dynamic testing, electron microscopy, high-temperature superconductivity, laser processing, machining research, materials and process modeling, mechanical testing, micromechanics and nonindentor, microwave processing, optical metallography, organo-metallic chemistry, polymer synthesis and characterization, pulsed laser deposition/CVD, single crystal synthesis, spectroscopy, surface science, thermomechanical processing, and x-ray. These research topics are grouped into four focus areas; mechanical behavior in extreme environments, materials processing, advanced materials development, and materials characterization. (Deepwater Offshore 16, 2, 5, 8, 9; Production 3; Oil Processing and Refining 5, 12, 13)

**10. Sensor and Process Diagnostics:** The increasing demand in both the industrial and military sectors for sensitive, rapid, reversible and cost efficient sensors has generated a number of technical efforts that use to advantage the well established synthetic chemistry, materials science, theoretical modeling, and device fabrication capabilities at the Laboratory. In one instance, the covalent bonding of bucket-shaped organic hosts to surface acoustic wave substrates has allowed the ppb level detection of chlorinated hydrocarbons, aromatics (benzene, toluene) and other pollutants with reversible and reproducible responses. Non-invasive diagnostics that can allow sensitive, real-time detection of process stream constituents have also been developed at Los Alamos. Optical probes from the infrared through the visible have been coupled to fiber optics to allow spectral detection of condensed or gas phase analytes. Vibrational spectroscopy has been used to provide "fingerprint" detection of individual species within a complex mixture while absorption methods can also provide rapid measurement of sample composition remotely, safely and with relatively moderate expense. (Environmental and Regulatory 10, 3, 14; Deepwater Offshore 1)

**11. Integrated Subsurface Characterization:** From the modeling perspective, both the emerging environmental industry and the more mature petroleum industry lack a coherent view of the earth's interior, that is, a self-consistent earth model. Presently there are structural models based primarily on geophysical measurements, lithological/stratigraphic models based on petrophysical measurements, and hydraulic models based on petrophysical and engineering measurements. Additionally, there are geological models which, through the increasing use of geostatistical techniques, integrate geophysical and petrophysical measurements. By contrast, petrophysical and engineering data have not yet been fully integrated. As a result, different earth science professionals use two different and incompatible earth models to address the same problem of developing hydrocarbon reservoirs. Los Alamos is working to integrate the various

earth models used by petroleum professionals. The recent development by the Petrotechnical Open Software Corporation (POSC) of an industry-wide data model, **epicenter**, for exploration and production measurements provides a foundation for this effort. The initial focus is to reconcile the use of various types of measurements in the large intersection between geological and hydraulic modeling. Current practice in geological modeling gives very little or no weight to engineering measurements. Stochastic approaches provide statistical techniques such as co-kriging and conditional simulation that may be used to address scaling and other problems which must be solved in order to integrate engineering measurements with those more traditionally used in geological modeling. (Development 6, 2, 25; Exploration 1, 11)

**12. Transport Assessment Strategic Initiative:** The transport assessment initiative will support improved efficiency of oil, gas, and mineral production by applying chemical principles and techniques to assess fluid flow and chemical transport in complex natural systems. The approach is to build an interdisciplinary, multi-organizational team to investigate the interaction of dissolved chemical species with mineralogically and hydrologically complex media. The intended result is: (1) *Improved production* through better oil and gas reservoir characterization; (2) *Assured gas supply* through decreased loss from underground storage reservoirs; and (3) *Reduced waste generation and pollution* from produced waters in oil and gas fields. The initiative merges existing strengths in chemical tracer technology, sorption & surface chemistry, chromatography, use of natural chemical tracers, and multi-phase transport modeling in geologically-complex environments. The transport assessment initiative benefits from the leverage of related work on:

- Heterogeneous catalysis to minimize energy use and waste generation in chemical processes.
- In-situ leaching studies for environmental remediation of heavy metals in soils.
- Geochemical and hydrogeochemical characterization for environmental restoration of waste sites.
- Advanced chemical sensors for in-situ, real-time measurement in chemical processes.

(Development 4, 16, 21; Gas Gathering 2; Gas Storage 2; Environmental and Regulatory 5, 9)

**13. Simulation of In Situ Groundwater Remediation Processes:** Los Alamos Earth and has developed computer codes that can address simple and complex *in situ* groundwater remediation problems. These codes are designed to simulate fully 3-D non-isothermal, multiphase flow in heterogeneous and fractured media. They include modules to analyze chemical reactivity, biokinetics, horizontal, vertical and angled well systems, air sparging and barometric effects. In addition, we have coupled the flow and transport codes with advanced grid generation tools which include the ability to generate realistic meshes directly from hydrostratigraphic data. We have applied these tools to a variety of problems, including performance assessments for novel remediation techniques (e.g., *in situ* air stripping and *in situ* bioremediation using horizontal wells), determining effectiveness of remediation scenarios, designing monitoring activities, and predicting potential contaminant migration. (Environmental and Regulatory 9, 2, 6, 12)

**14. Information Extraction, Optimization, and Adaptive Control:** A number of capabilities exist at Los Alamos centered around information extraction, optimization, and adaptive control. These capabilities arise from basic and applied research in modern methods such as neural

networks, fuzzy logic, genetic algorithms, and model-based prediction and control. Complex problems are attacked through integration of these methods. For instance, relevant portions of a data stream from a process are first located using feature extraction techniques or expert knowledge. It is then feasible to create a model from the data (e.g., a neural network) which mimics the process behavior. Such a model can be used to optimize, control, or identify faults in the underlying process. These models are frequently designed to be amenable to adaptation in order to exploit on-line data. Typical applications include fraud detection in the financial industries, automotive engine and braking control, and industrial process control. (Oil Processing and Refining 26, 3, 25; Development 28)

**15. Catalysis Capabilities:** Capabilities at Los Alamos for the study of catalysis include a wide array of state-of-the-science techniques and instrumentation for examination of solid catalysts, gas phase reactions, and gas-solid interactions. These include neutron diffraction for structural studies of catalysts and inelastic and quasielastic neutron scattering for obtaining structure and dynamics of adsorbates on catalyst surfaces, a variety of beam technologies with high spatial and depth resolution for the characterization of solid catalysts including depth profiling techniques, high field solid state NMR spectroscopies, and a variety of optical and electron spectroscopies for *in situ* diagnosis of catalysts and catalytic reactions. Areas of active research in catalysis include shape selective oxidation catalysis including novel zeolite synthesis and characterization, NO<sub>x</sub> abatement, catalysis in supercritical fluids, homogeneous catalysis with lanthanide complexes, zeolite and metal membrane fabrication for separations, reactive separations, process sensors, and the use of microwave fields for catalysis using a variety of frequencies and energy densities. (Oil Processing and Refining 1, 7, 9, 19)

**16. Destruction of Oily or Contaminated Waste:** Complex wastes are characterized by the presence of one or more hazardous organic components and bulk materials. Current storage practices are a great expense and are in violation of storage and handling regulations. The presence of bulk materials in a heterogeneous mixture prevent treatability of the waste stream by any single technology. However, the order of application of new or current treatment options and the interfaces between them must be ascertained and a methodology for selection must be developed. Los Alamos is developing an integrated treatment train that combines proven technologies of bioremediation and chemical treatment (i.e., chelation, pretreatment) with: a modular approach, tailor made to the waste stream; cost effective engineering design; environmentally benign processing; waste minimization with 50% bulk reduction; and effective treatment of an array of waste streams. It is also clear that presently-used methods for cleanup of solvent-contaminated groundwater are ineffective. Therefore, Los Alamos has embarked upon an effort to develop and demonstrate a series of methods for dealing with such situations - ranging from *in situ* stabilization techniques for contamination at low levels to *ex situ* treatment of organics. (Environmental and Regulatory 12, 2, 9, 11)

## **Enabling Capabilities – National Institute for Petroleum and Energy Research (NIPER)**

Due to the diversity of its facilities and staff, its industry, lab and university partnerships and its close proximity to its customers, NIPER has developed and maintained a highly respected portfolio of oil and gas research programs throughout its long history. Serving domestic and international governments and petroleum industries, NIPER is solely an oil and gas research facility, and has been since its establishment in 1918. Considering the oil and gas experience of the personnel on staff and the facilities at hand many capabilities exist which enable NIPER to move beyond its current petroleum R&D program. Unique, designed and built on-site equipment, and a staff consisting of chemical, petroleum, and mechanical engineers, chemists, geologists, geophysicists, physicists, biologists and other scientists and engineers give NIPER the capability to be one of the few petroleum R&D facilities of its kind in the world and the only federally owned, fully integrated petroleum lab in the Nation.

**1. Exploration, Drilling & Risk-Based Management:** Exploration, Drilling & Risk-Based Management focuses on identification and recovery of additional hydrocarbons from mature fields, considering exploration, drilling, environmental & regulatory risk. Geologists and engineers at NIPER are applying sequence-stratigraphy, tectonic analysis, source rock evaluation, and analysis of thermal maturation, hydrodynamics, and migration pathways to refine basin models. Testing of new or emerging exploration and geoanalytical technologies is accomplished through cost-shared field projects. Additional or expanded capabilities exist in areas of reservoir petroleum geology, geochemical surveying using non-evasive collection of surface samples, surface iodine anomalies, fluorescence anomalies derived from the fused aromatics, and spectral gamma aerial radiometric interpretation; seismic technology; geophysical research; petroleum geohydrology and hydrodynamics characteristics of aquifers and aquitards; petroleum geochemistry including isotropic characterization of subsurface fluids; remote sensing data analysis and surface fracture analysis of surface lineaments, fracture traces, circular and arcuate anomalies; drilling and completion including underbalanced drilling for energized drilling fluid, gas lift design, artificial lift, slimhole and coiled tubing drilling; coalbed methane resource assessment, numerical simulation, drilling and completion. (Exploration 1, 2-7, 10, 12-16; Drilling & Completion 1, 2, 6, 9-13; Development 33)

**2. Reservoir Characterization & Assessment:** Reservoir Characterization is critical to successful application of any technology to improve oil recovery. A combination of geologists, petroleum engineers and physicists, and specialized on-site equipment allows computerized tomography, nuclear magnetic resonance imaging and petrographic image analysis to be accomplished at NIPER. A team of skilled geologists and geophysicists enable NIPER to study sedimentologic and geologic heterogeneity and their potential effect on oil recovery through field studies of outcrops and geophysical exploration. Divided into three sub-groups; Geoscientific Measurement, Reservoir Description, and Reservoir Modeling, the Reservoir Characterization and Assessment team is skilled in the areas of seismic interpretation, well logging, well testing, geochemistry, crosswell imaging, petrophysics and core analysis, rock mechanics, remote sensing, reservoir architecture, postdepositional modification, formation and basin scale studies, geological modeling and reservoir simulation. Additional areas include: Inversion methods for reservoir parameter estimation including the gradient method, the reparameterization and subspace

methods, and the inverse solution algorithm; catholuminescence microscopy for the determination of pore-filling minerals and fabrics; fluid inclusion analysis including homogenization and freezing point depression; electron microprobe analysis for elemental composition of diagenetic and allochemical components of rock in conjunction with secondary electron image or backscattered electron imagery provided by the scanning electron microscope, stable isotope analysis of C and O; and biostratigraphic analysis; NMR measurements in the low-field regime; imaging of fluid distributions in porous media using X-ray CT imaging and 2-D X-ray scan imaging; and rock-fluid and fluid-fluid interactions; coalbed methane reservoir characterization, natural fracture detection and modeling; and coalbed methane field operations. (Development 1, 2-33)

**3. Extraction Research:** Extraction Research at NIPER is focused in three areas: Improved Oil Recovery (IOR), Advanced Oil Recovery (AOR) and Simulation of Extraction Processes.

Chemical, microbial, gas and thermal oil recovery processes, (AOR), have the potential for recovering significant amounts of oil. Waterflooding, Pressure Maintenance, Sweep Improvement, Completion, Stimulation, Horizontal and Infill Wells, and Field Pilots fill out the NIPER capabilities in IOR, while the areas of Process, Reservoir, Economic, and Tracer Model Development highlight the capabilities in Simulation of Extraction Processes. The NIPER staff is conducting research in fields such as mixed surfactant systems; alkaline-surfactant-polymer (ASP) flooding; microbial oil recovery technology to optimize performance; bioremediation technologies; gas and thermal recovery methods; measuring interfacial tensions (IFT) between two phases of water-oil-gas systems; and specialized physical models to test performance of additives for improving sweep efficiency. Additional areas are: Tight gas sands and stimulation technology including fracture fluid polymer stability and degradation, polymer breaker characterization and selection, proppant selection, formation damage potential from stimulation fluids, fluid flow under darcy and non-darcy flow regimes and proppant embedment measurements and prediction; natural gas well testing, natural gas gathering, processing, metering and pipeline transmission; natural gas underground reservoir storage; design criteria for gas gathering line sizing; and coalbed methane production and reservoir management research. (Production 25, 1-6, 8, 11, 12, 16-27; Gas Storage 1, 2, 3; Development 30, Arctic Region Activities 5)

**4. Thermodynamics:** NIPER houses the only fully integrated thermodynamics lab in the world generating complete thermochemical and thermophysical data on a range of chemical compounds needed in chemical process technology. Using unique state of the art equipment and software which were built on-site, NIPER researchers have lead the way in the study of exotic fuel systems for U.S. Space Program and military needs. Current R&D in areas of oxygenates for reformulated fuels and ambient vapor pressure measurements for special State of California requirements are two examples of thermodynamic and thermophysical studies ongoing at NIPER. Rotating Bomb Calorimeters, Twin Ebulliometers and an Inclined-Piston Vapor Pressure Apparatus highlight the uniqueness of the NIPER Thermodynamics laboratory. (Oil Processing & Refining 27, 24, 19, 28, 25, 20, 1)

**5. Process Development, Heavy Oil Upgrading and Catalysis:** A full range of experimental capabilities for bench-scale and pilot-plant development and evaluation of process technologies exists in NIPER's labs. NIPER has the expertise, capabilities and equipment to develop technology related to heavy oil upgrading, including the understanding of the fundamental

chemistry and thermodynamic properties of heavy crude oil and residua. Improved methods of separating heavy fractions of crude oils while minimizing product degradation, supercritical extraction, fixed bed and fluidized bed catalytic processing especially in the areas of hydrotreating, hydrocracking and catalytic cracking and thin-film distillation to evaluate various feedstocks and catalysts are part of the on-going Process Development research at NIPER. The synergism of NIPER's experience in catalyst development, understanding of petroleum chemistry and expertise in the analysis of catalysts and products of reactions offers an exceptional opportunity for development of new catalysts, understanding of catalytic processes and developments, and offers the potential for breakthrough in developing catalysts by design. (Oil Processing & Refining 21, 7, 1-4, 6, 9-11, 16, 18-25, 27, 28)

**6. Fuel Chemistry and Evaluation:** Researchers in these areas work together to solve processing and environmental problems. Fuel chemistry and evaluation provides comprehensive chemical and physical property analyses on crude oil quality and potential problems of commingling, compatibility and contamination of crude oil. It also includes causes of processing problems, and components which contribute to toxicity, instability, and other problems associated with process streams and final products. (Oil Processing & Refining 27, 28, 20, 22, 24)

**7. Natural Gas Processing and Conversion, Process Modeling and Analysis:** Having an extensive understanding of the processes and fundamental chemistry relating to petroleum and natural gas conversion processes, the staff at NIPER has been directly involved in the development and application of technology for the extraction of natural gas liquids from natural gas either produced directly or in association with crude oil, and the conversion of natural gas to liquids such as methanol. Utilizing this knowledge in process simulations can enhance existing process efficiency and speed the development of new processes. NIPER's historic involvement with the oil and gas industry and its overall understanding of total refinery configurations provides a unique basis for contributions in this area. (Gas Processing 8, 1-4, 6, 7)

**8. Fuels and Engine Testing:** Fuels and Engine Testing performs procedures required by state, federal and industrial entities. Temperature and computer controlled chassis dynamometers are used to perform EPA federal test procedures. Conventional and specialized emissions analyses, along with octane determination, drivability, acceleration testing, in-cylinder combustion analysis, and wear-analysis are among the core capabilities on site at NIPER. (Oil Processing & Refining 27, 28, 22, 24; Environmental & Regulatory 7, 9, 14, 15)

**9. Waste Minimization:** NIPER has extensive experience in the application of waste minimization technology, such as solvent recovery technology. The "Used Oil and Solvent Recycling Management Plan" developed at NIPER for the U.S. Navy can be effectively applied at government and industrial sites. (Environmental & Regulatory 10, 11, 12, 7, 9, 13-15)

**10. Gaseous Emissions:** Gaseous emissions are becoming a serious challenge to the refining industry as well as many other industries; from air pollutants such as oxides of nitrogen coming from industrial boilers and process units such as fluid cat cracking units to evaporative emissions of hazardous hydrocarbons such as benzene. NIPER's extensive experience in the sampling and

analysis of auto emissions can easily be extended to the analysis of gaseous emissions from refineries or from other industries. (Environmental & Regulatory 14, 13, 15, 7)

**11. Liquid Discharges/Waste Water:** NIPER has developed unique sampling and analysis capabilities for hydrocarbon streams and for soil contaminants. These techniques could be extended to the analysis of liquid discharges from refineries and other industries. Once these contaminants are identified NIPER has the expertise to determine to not only identify the source of these contaminants, but to develop ways to minimize waste stream pollutants. (Environmental & Regulatory 10, 1-4, 6, 7, 7-15)

**12. In Situ Remediation of Petroleum Contamination Using Microbial and Chemical Recovery Technologies:** NIPER provides technical and management support for the environmental aspects of the DOE Oil Program. Geologists, biologists, chemists, certified groundwater hydrogeologists, and registered environmental professionals deal with environmental problems ranging from oil spills and subsurface waste disposal to groundwater contamination. (Environmental & Regulatory 12, 1-7, 9-11, 13-15)

**13. Mitigation of Environmental Impacts:** Mitigation of environmental impacts of oil activities is an important facet of the Fossil Energy Research and Development Program. A multi-disciplined, in-house research effort at NIPER can assume the lead role in developing environmentally safe methods for remediation of petroleum contamination caused by crude oil production. Potential technologies that could be developed from this in-house research include: Gelled-polymer technology; application of surfactant technology for combined remediation and containment; phenolic resin technology for barrier information; microbial plugging technology; application of conformance control technology; modeling of contaminant flow in the subsurface; modeling of microbial transport in the subsurface; and use of imaging capabilities to evaluate fluid movement. (Environmental & Regulatory 12, 1-4, 6, 10, 13, 14)

**14. Groundwater Resource Assessment Using Reservoir Characterization:** NIPER has the capabilities to conduct environmental research in the areas of groundwater resource assessment and modeling, subsurface contaminant transport, and groundwater remediation. Expertise exists to characterize and simulate groundwater resources where complex geological characterization is required. In the area of Reservoir Characterization numerical simulation is directly transferable to the groundwater area. (Environmental & Regulatory 6, 1, 4)

## **Enabling Capabilities – Oak Ridge National Laboratory**

**1. Advanced Separations Processes** – Within the laboratory there exists state-of-the-art capabilities in all phases of inorganic ion exchange technology. Research and development activities have been conducted over the past ten years regarding selection of ion exchange materials for specific wastewater treatment applications. Laboratory and bench scale evaluations have been performed to evaluate performance to allow process design and scaleup. Evaluation of operational aspects of these systems has also been performed. This testing has produced improved designs for sliceable ion exchange columns and has led to operating strategies that maximize column life and removal efficiency. Capabilities exist to test processing for treating wastewater; selecting economical, practical flowsheets; and demonstrating the operability of the process on a pilot or full scale. (Production 2, 6; Processing & Refining 2, 4, 18, 19; Gas Processing 4, 5, 6, 8)

**2. Bioprocessing and Biotechnology** - Within the Bioprocessing Research and Development Center of Oak Ridge National Laboratory considerable competence has been established in the use of biotechnology to process fossil fuels. This includes the conversion of coal to liquids and gases, the removal of sulfur and nitrogen from petroleum products and coal-derived liquids and the clean-up of wastewater contaminated with organic compounds from fossil materials. In most cases, process development is being carried out on a small engineering bench-scale. (Environmental & Regulatory 2, 10, 12; Oil Processing & Refining 4, 6, 17, 21, 22, 23; Production 1, 2)

**3. Advanced Fluid Mechanics** -- There are available general Navier-Stokes solvers that have been developed in-house for solving steady and transient flow problems with and without free boundaries. Typical applications include: coating flows (as in making photographic or X-ray films), polymer processing, flow on trays in distillation columns, problems encountered in general chemical reaction or process engineering, and low-gravity processing or positioning of materials. Laboratory equipment for high speed videos (1,000 to 12,000 frames per second) is available to analyze flows and events that occur on the millisecond time frame, e.g. atomization and droplet formation. (Development 1; Drilling & Completion 2; Production 7, 8, 22, 25; Deepwater Offshore 4, 5, 6, 15)

**4. Simulation Models** -- The fuels modeling capability addresses availability, quality and use. The forecasting system consists of a world petroleum distribution model and the Oak Ridge National Laboratory Refinery Yield Model (regional petroleum refinery linear programs). This system has been used to study world oil disruptions; fuel specifications; jet fuel conversion; ultra low sulfur diesel fuel; gasoline reformulation and fuel effects on jet engine performance. Model applications include determination of conservation opportunities, the effects of fuel use policies and measuring progress in meeting energy use targets. Also, Oak Ridge National Laboratory scientists have developed computer models to assist in several issues regarding the Strategic Petroleum Reserve (SPR). Issues addressed include optimal size of inventory, draw down and distribution capabilities, regional product reserves versus centralized crude storage, crude oil mix, financing and the economic effects of market disruptions. (Development 25-28; Drilling &

Completion 3; Production 6-11, 25; Oil Processing & Refining, 6, 22, 27, 28; Environmental & Regulatory 4, 6-10, 14, 15)

**5. Sludge Processing** -- Dewatering of sludge wastes is a technique to minimize the volume of waste to be shipped or stored. In addition, it may be integrated with other treatment steps to prepare the waste for final disposal. Dewatering technologies include filtration, centrifugation, and thermal drying. The Laboratory is working with the private sector to apply this technology to reduce the volume of a mixed waste presently contained in several thousand deteriorating drums. Laboratory-scale support included the identification of the appropriate test protocol to determine the acceptance moisture content and the dewatering techniques that were capable of meeting this criterion. (Environmental & Regulatory 2, 11, 12, 13, 15)

**6. Waste Minimization** -- There exists substantial capabilities in terms of personnel, computer hardware and software and equipment for the development of analytical tools to support waste management activities. The personnel consist of chemical engineers with expertise in both theoretical and computer modeling. This group has experience in the development of relational data bases, interfacing and integration of data bases with other computer applications and artificial intelligence/expert system front end applications, such as user-friendly interfaces to data bases, including natural language interpreters to relational data bases. (Environmental & Regulatory 1, 2, 4, 7-15)

**7. Advanced Materials** -- Using state-of-the-art corrosion testing facilities and equipment studies have been conducted on the occurrence and rates of corrosion processes. From these studies advanced corrosion resistant materials have been developed as well as the ability to predict the onset of corrosion activity. Oak Ridge National Laboratory has extensive experience and has developed considerable expertise in the study of corrosion problems in conventional and advanced power systems. Through the Fossil Energy Materials Program, engineers have studied both fire-side and water-side corrosion in conventional coal-fired power plants, and they have been involved in evaluating materials and examining corrosion failures in fluidized bed combustors, coal gasification facilities, coal liquefaction plants, and Clean Coal-sponsored low NO<sub>x</sub> boilers. A state-of-the-art facility for studying structural materials and fracture mechanics has been developed. Relationships between micro structure fracture performance have been developed. Studies can be carried out in varied service environments as well as temperatures ranging from cryogenic to high. (Exploration 15; Drilling & Completion 4; Production 3, 4, 5, 7-10; Deepwater Offshore; Arctic Region Activities; Processing & Refining 9,10)

**8. Environmental Risk** -- Members of the Oak Ridge National Laboratory technical staff have experience and capability at analyzing electricity production technologies and their associated fuel production and waste management systems and identifying their impacts upon society (also called "externalities"). Assessment capabilities for electricity production and fuel cycle technology include impacts from construction, operation, waste disposal, and decommissioning operations as well as potential accident scenario impacts. The types of impacts we examine can span a wide range including health impacts from emissions and accidents, regional employment benefits, transportation, impacts upon recreational assets, etc. Impacts can be economically valued and converted into dollars, or mils/kWh in order to permit comparisons of dissimilar impacts and

tradeoff studies. (Exploration 2; Development 4,10; Oil Processing & Refining 8; Environmental & Regulatory 4, 8, 9, 14, 15)

**9. Incinerator Monitoring --** The Oak Ridge K-25 Site operates the sole licensed mixed waste TSCA incinerator in the United States. This facility provides technical support in the understanding and characterization of particulate and gaseous emissions during the combustion of high-organic content liquid wastes from wastewater treatment. Documentation of the chemical nature and size distribution of particulate from various sampling locations provides information to assist in evaluating mass balance calculations, efficiency of air pollution control equipment, stack emissions and environmental risk factors. (Environmental & Regulatory 7, 8, 14)

**10. Wastewater Treatment --** Within the laboratory there exists state-of-the-art capabilities in all phases of inorganic ion exchange technology. Research and development activities have been conducted over the past ten years regarding selection of ion exchange materials for specific wastewater treatment applications. Laboratory and bench scale evaluations have been performed to evaluate performance to allow process design and scaleup. Evaluation of operational aspects of these systems has also been performed. This testing has produced improved designs for sliceable ion exchange columns and has lead to operating strategies that maximize column life and removal efficiency. Capabilities exist to test processing for treating wastewater; selecting economical, practical flowsheets; and demonstrating the operability of the process on a pilot or full scale. (Production 1-4; Deepwater Offshore 1; Environmental & Regulatory 1, 2, 6, 9, 11, 12, 13)



## **Enabling Capabilities – Pacific Northwest Laboratory**

**1. Process Science and Engineering Complex:** Facilities and equipment required for petroleum processing and energy technologies are readily available at the Pacific Northwest Laboratory. The majority of the work in this area is conducted in the Process Science and Engineering Complex including the Physical Sciences Laboratory (PSL), the Chemical Engineering Laboratory (CEL), the Chemical Process Development Laboratory (CPDL), the Process Development Laboratory (PDL), and the Chemistry and Metal Sciences Laboratory (CMSL).

The PSL contains a biochemical engineering laboratory which houses a broad range of bioprocessing related research. The biochemical engineering laboratory contains most of the fermentation and separation equipment used to support process development activities. The CEL is a 900 sq ft laboratory which houses facilities and analytical equipment to support bench and large scale processing equipment. Outside the CEL are two gasification/pyrolysis reactors. Located inside a high-pressure bay in the CEL is a fixed-bed 1-liter catalytic hydrotreater used for upgrading pyrolysis oils and synthetic liquid fuels. This hydrotreater is used to process up to 1 liter/h of liquid feedstock at 400 C and 135 atm. The CPDL is a 1000 sq ft building that has the heavy duty laboratory space appropriate for high-pressure, high-temperature experimental studies. The CPDL, which is used for separations and thermochemical conversion process development activities, houses analytical equipment, a fume hood, and three high-pressure reactor systems. The PDL contains several bench-scale experimental systems. A fluidized-bed gasification system is used to study gasification/pyrolysis of wood and other residues, tar cracking, and catalysis. The MPL houses several materials processing and engineering scale-up activities. Current pilot systems include processing and engineering scale-up activities. Current pilot systems include the Hydrothermal Processing and the Superplastic Forming pilot plants. The Hydrothermal Processing pilot plant is used to study large scale operations in waste treatment, materials synthesis, separations, and supercritical fluids. The CMSL contains 6 general purpose chemistry laboratories used for separations and process chemistry. (Oil Processing & Refining, Environmental & Regulatory)

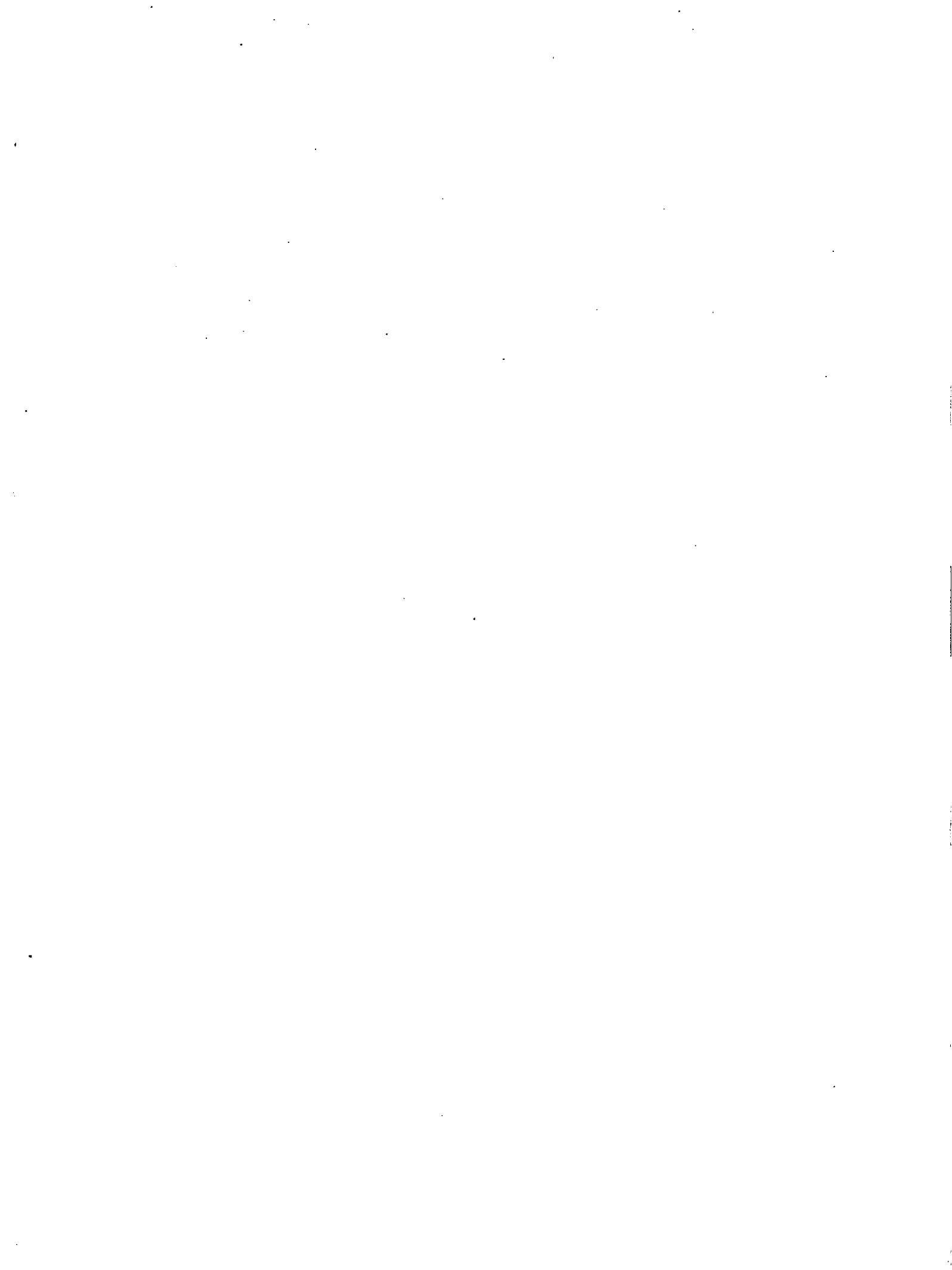
**2. Environmental and Molecular Sciences Laboratory (EMSL):** EMSL is a new facility that will greatly enhance PNL's basic research capabilities. EMSL is a national collaborative research laboratory where scientists from the U.S. and other countries can gather to conduct basic research that will contribute to the development of permanent, cost-effective solutions to complex technical problems. EMSL research results will be the scientific basis for evaluating a number of social and technical factors associated with cleanup activities--factors such as the health effects to cleanup workers and the public, the economic impacts of cleanup, the transport pathways and fate of contaminants in the groundwater as it moves through the soil. Information from EMSL research will also be used in risk assessment activities that will, in turn, be the basis for making rational decisions about the course of cleanup efforts. EMSL will be the keystone of PNL's environmental research portfolio. The new laboratory will house 250 resident and visiting scientists in a 200,000 sq ft building located at PNL. The EMSL's special resources will enable scientists to apply advanced experimental and computational capabilities to research in areas such as contaminated soils, and groundwater, waste processing, waste minimization, analysis and characterization, advanced processing, and health effects.

The initial complement of research equipment and general laboratory infrastructure will support scientific research across a broad spectrum of molecular phenomena critical to solving DOE's environmental problems. Major EMSL program areas will include: 1) high-performance computing to model molecular-level processes relevant to cleanup; 2) molecular structure and dynamics to study the chemistry of toxic wastes and chemical processes in the environment; 3) structural biology to study biological processes, bioremediation, and health effects; 4) advanced materials for use in new chemical and process control sensors, new separations techniques, and new waste storage forms, and 5) theory, modeling, and simulation to predict and better understand the behavior of molecular systems. (Environmental & Regulatory, Development, Oil Processing & Refining)

**3. Marine Sciences Laboratory:** Pacific Northwest Laboratory's Marine Sciences Laboratory (MSL) on Sequim Bay in western Washington was established in 1966 to provide research and development assistance to government agencies and industries engaged in protection of the marine environment, development of marine technologies, management of fishery resources, and operation of coastal utilities. A primary focus of PNL/MSL's research is in the characterization of sources, fates, and effects of chemical contaminants on marine ecosystems. Projects conducted at MSL include studies on global climate change, wetlands restoration, aquatic toxicology, ocean disposal, oil spill mitigation, and damage assessment. PNL offers complete services for all phases of assessment: field logistics, surveys, sample collection, analytical chemistry, ecological risk assessment, and database management. Support for field sampling program design in terrestrial, coastal, and riverine settings: PNL's scientists and engineers supporting these efforts are highly experienced in design of statistically valid environmental surveys and the use of advanced field data acquisition systems for efficient field programs. We are involved in all aspects of physical, chemical, and biological field activities required to record fate, effects, and recovery of oil-impacted environments. The MSL has facilities for real-time aqueous hydrocarbon measurements to monitor the extent of oil movement and dispersion for exposure assessments during aquatic spills or during countermeasure testing. Critical to oil spill characterization is extremely accurate chemical analysis, characterization, and identification of fugitive products in water, soil, sediment, and biological tissue (hydrocarbon fingerprinting).

PNL's MSL offers a world-class facility for detailed ecological risk evaluation and assessments of petroleum-impacted sites. In addition the lab offers environmental management programmatic research in the areas of: Design and supervision of NRDA Type B site assessments, including coordination of multi-component activities to optimize program productivity, Complete field and programmatic data management services in support of litigation activities, State-of-the-art geographic information system (GIS)/database services for the production of detailed maps of temporal and affected terrestrial/aquatic resources, and rapid preparation of event-specific Standard Operating Procedures to provide guidance to contractors in the conduct of spill assessment, cleanup, and long-term monitoring. (Environmental & Regulatory, Deepwater Offshore, Arctic Region Activities)

**4. Natural Gas Transmission and Distribution Facilities:** Pacific Northwest Laboratory, in conjunction with Battelle Memorial Institute operates several major natural gas research programs and facilities such as a number of major research programs on in-line inspection for the Gas Research Institute and for other clients. The objectives of these programs are to develop and improve inspection capabilities for gas-transmission pipelines. As part of the programs, Battelle manages the GRI Pipeline Simulation Facility, which includes an inspection laboratory for carefully controlled experiments and analyses, a pull rig for tests on full size inspection equipment in unpressurized pipe runs - where pipe runs contain removable defect sections containing metal loss, mechanical damage, and stress corrosion cracking. Recently commissioned, a 24-inch-diameter 4,700-foot long flow loop, which closely simulates an operating pipeline and allows research and development on a wide range of pipeline maintenance, operation, and rehabilitation topics in a safe and controlled environment, without risking the integrity of an operating pipeline. (Gas Gathering, Gas Storage)



## **Enabling Capabilities -- Sandia National Laboratories**

- 1. Solar Powered Systems** -- Sandia conducts research and development of advanced solar thermal components, dishes, heliostats, and receivers for dish and central receiver systems, and also designs, analyzes, and tests components and systems. In photovoltaics, Sandia's work is centered on developing cost-effective, reliable system technology produced by U.S. industry and used worldwide. We operate a Design Assistance Center that promotes the use of solar thermal and photovoltaic technologies at home and abroad through services to manufacturers, operators, and decision-makers, as well as educational outreach. In a joint venture with industry, Sandia is developing the first commercial dish-Stirling system, which promises to have great utility as a power source for remote locations. (Exploration 14; Production; Gas Gathering)
- 2. Advanced Manufacturing Technologies** -- Sandia has become the leader among DOE laboratories for advanced manufacturing technologies as a consequence of our responsibilities in systems and design engineering, production process development, intelligent machine research and development, and oversight of the performance and reliability of nonnuclear weapon components over the last forty years. Its Center for Advanced Manufacturing Technology provides a forum for collaborative work with industry on hybrid microcircuits, thin films, printed circuits, ceramics, plastics, and rapid prototyping capabilities. Its Integrated Manufacturing Technologies Laboratory conducts collaborative R&D in materials and processes, process simulation, engineering design, and manufacturing technology support. Current work focuses on metal removal and welding, weld process simulation, composites fabrication, high-speed communication of manufacturing data, and on-line monitoring and control. A specific focus is prototype fabrication and demonstration techniques for agile manufacturing. Finally, Sandia has a lead role in moving the DOE production complex toward environmentally conscious manufacturing for nonnuclear components. We have developed and introduced substitutes for materials and processes that required or generated hazardous materials. Such developments include lead-free soldering and CFC-free cleaning solvents for integrated circuits. (Oil Processing and Refining 3; Production; Gas Gathering; Deepwater Offshore)
- 3. Robotics** -- Sandia's Intelligent Systems and Robotics Center is a fully integrated research-to-development-to-application program that provides technologies for intelligent and agile manufacturing and operations in remote and hazardous locations. Areas of development include design for manufacturing and assembly, work environment design, systems engineering and integration, process modeling and simulation, precision machining, joining, assembly, automated inspection, integration frameworks, software engineering, artificial intelligence, expert systems, robotics, machine/cell/process control, and sensors/sensor fusion. The center is the focal point for Sandia's work in information-driven processes has more than forty in-house laboratories available for collaborative research and development. (Drilling and Completion 13, 9; Deepwater Offshore 7; Arctic Region Activities; Oil Processing and Refining 14)
- 4. Information Surety** -- Information surety is concerned with protecting information from unauthorized access, unauthorized accidental modification, and loss of access. This field is an essential discipline for Sandia's responsibilities in command and control of nuclear weapons. Consequently, we have developed extensive capabilities in design and analysis of cryptographic algorithms and protocols; adversarial analysis of hardware, software, and total systems; design

and analysis of access control systems; development of high-speed communication network security systems; development and fielding of use control systems; development and testing of tamper-resistant technologies; testing of biometric identification techniques; and development of computer security techniques. (Exploration 15; Deepwater Offshore; Production)

**5. Intelligent Sensors** -- Advanced sensors are the means by which intelligent processors monitor and control the operation of systems and manufacturing processes. Sandia has developed families of novel sensors that sense a range of chemical, thermal, electrical, physical, and mechanical properties for defense and commercial applications, including monitoring environmentally hazardous chemicals and controlling production processes. Such sensors, have broad new applications in remote monitoring, industrial process improvement, and real-time control. Commercial applications include assessing the quality of vehicle engine oil, identifying the presence of environmental pollutants, tracking physical features in manufacturing processes, and indicating the presence and concentrations of explosive gases. (Oil Processing and Refining 4; Gas Processing)

**6. Combustion Science and Technology** -- DOE's Combustion Research Facility (CRF) at Sandia's laboratory in Livermore, California, is chartered to conduct a broad range of fundamental and applied R&D in combustion science and technology. Research is conducted in collaboration with visiting scientists and engineers from industry, academia, and federal laboratories. The CRF conducts cooperative research with the coal, petroleum, natural gas, and fuel cell industries. Advanced experimental techniques emphasizing laser-based diagnostics and computational models are used in projects that enhance our ability to burn fuels cleanly and efficiently. The CRF's special capabilities are also used in such areas as environmental remote sensing, waste processing, and materials processing. Novel sensors and computational models from the programs are in active use in major U.S. industries. (Oil Processing and Refining 24, 4, 11, 16, 25, 27; Gas Processing; Environmental and Regulatory 10)

**7. Materials Aging and Reliability** -- Experimental and theoretical tools are available to study structural defects and impurities in solids and on surfaces. The experimental tools are high-resolution transmission electron microscopy, high- and medium-energy ion scattering facilities, video low-energy electron diffraction, surface analytical tools, scanning tunneling microscopy, and low-energy electron microscopy. Theoretical tools developed and employed include quantum chemistry codes, local density approximation/ pseudopotential methods, the embedded atom method, and cluster functional methods for large-scale atomistic computer simulations. These experimental and theoretical capabilities are used to study grain boundaries, interfaces, and surfaces in metal alloys and intermetallic compounds; impurity segregation to these boundaries; and interactions with dislocations, gas bubbles, and defect clusters. Many of the results from this research are used in concurrent development and engineering projects at Sandia and other national laboratories. In addition, results are disseminated to materials science programs at universities and industrial research and development laboratories via the Sandia visiting scientist program in computational materials science. (Oil Processing and Refining 13)

**8. Batteries** -- Sandia is working with industry to develop advanced rechargeable battery systems for utility energy storage applications as part of the DOE utility battery storage systems program. Sandia has served as lead laboratory for DOE-sponsored engineering development of

rechargeable batteries for almost ten years. Cost-shared contracts with industry partners develop both components and systems. Sandia's technical expertise is used to analyze the benefits of battery storage in utility systems, evaluate prototype batteries, and conduct applied research. (Arctic Region Activities: Exploration; Development; Production)

**9. Synthetic Aperture Radar Imaging** -- Sandia has developed synthetic aperture radar systems for a wide variety of treaty verification and nonproliferation applications. We are also exploring the integration of synthetic aperture radar with other imaging data and automated data analysis to handle the large volume of data from such systems. Synthetic aperture radar will be used for all-weather and day-and-night aerial inspection. Our SAR test bed has recently been modified to include a three-dimensional terrain mapping capability called interferometric SAR (IFSAR). An operational IFSAR system will permit real-time production of highly accurate topographic maps. A key to this capability is the imaging enhancements made possible by state-of-the-art high performance computing. (Exploration 8)

**10. High-Consequence Operations and Surety** -- Sandia conducts considerable research on the deformation of inelastic structures under extreme conditions of shock and temperature. One of Sandia's primary responsibilities is to understand the behavior of warhead systems during accidents. Crashes, drops, and fires must be understood and analyzed. Research is conducted in several aspects of mechanics and thermodynamics, including the development of equations and computational methods for modeling such phenomena. The design of nuclear weapon structures for their intended functioning and for behavior in severe accidents is conducted using analysis and materials modeling tools developed at Sandia. The design of safing systems relies heavily on our thermal analysis capability. Shipping containers, fuzes, and components are also designed using these tools. We have extensively tested nuclear power plant electrical equipment and components during simulated accident conditions. Sandia has conducted an extensive analytical and experimental containment integrity program. Testing has evaluated the hazards of turbine and external missile impacts. As needed, evaluations of seismic and fire risks are conducted in conjunction with testing. Test facilities have been developed for quantitative measurements of fire behavior and the effects of smoke and combustion products. (Oil Processing and Refining 15; Gas Processing; Deepwater Offshore; Production)

**11. Microelectronics** -- Sandia's electronics capabilities and programs integrate the entire electronic-component realization process at a single site. Our capabilities in this arena are unique among US government facilities. We apply our resources to developing custom components for specialized DOE and other federal agency applications as well as precompetitive technologies for industry. Sandia's Center for Microelectronics Technologies is being accessed by industry through a five-year, \$100 million cooperative research and development agreement (CRADA) with the U.S. semiconductor industry SEMATECH consortium, as well as through CRADAs with individual companies. The center is supported by a large range of semiconductor and microelectronics capabilities. Sandia's Microelectronics Development Laboratory (MDL) is a 74,000-square-foot facility that includes 30,000 square feet of clean-room space with 12,500 square feet of class- 1 clean space in twenty-two separate clean rooms. It contains the equipment and technology for state-of-the-art submicrometer silicon-integrated-circuit research and development line. The laboratory's design provides maximum flexibility for new processing equipment and device technologies and is uniquely configurable to support contamination-free

**manufacturing.** The MDL equipment supports the total semiconductor development cycle, including research, design, fabrication, test, prototype delivery, qualification, and technology transfer. (Development; Production; Oil Processing and Refining; Gas Processing)

**12. Optoelectronics** -- Photonics is an emerging technology that uses visible-light energy for functions normally performed by electrical energy. Because of their inherent immunity to electromagnetic interference and their tolerance to the effects of ionizing radiation and intense pulses of electromagnetic radiation, photonic/electronics devices can offer unique advantages over traditional electronic devices for a wide variety of applications. Optoelectronics will provide the hardware for the information highways that crisscross the United States in the twenty-first century. Optoelectronic elements will provide high-data-rate communication links between remote sites. Over shorter distances, optoelectronics will become the means by which computers communicate with storage and output devices and even among multichip modules that will provide the intelligence within computer workstations in the future. Sandia's achievements in optoelectronics include a revolutionary advance in the efficiency and manufacturability of vertical-cavity surface-emitting lasers. (Exploration 15; Oil Processing and Refining)

**13. Safe and Secure Transportation** -- Since its inception, Sandia has been the lead DOE laboratory for transportation technologies associated with the safe, reliable, and monitorable movement of defense hardware. This historical role includes infrastructure issues in geographic information system tracking of trucks, full vehicle system design and production oversight, and reliability and safety integration. For nearly twenty years, we have held a similar lead role for transportation systems for radioactive and hazardous materials for both DOE and the Department of Transportation. This role has involved infrastructure issues, including the geographic information system, cask design and certification, safety, performance assessment, and manufacturing. These two missions have also allowed Sandia to play important roles internationally in transportation of special materials in the former Soviet Union and in ocean and air transport of reactor fuel around the world. (Production; Oil Processing and Refining, Gas Processing)

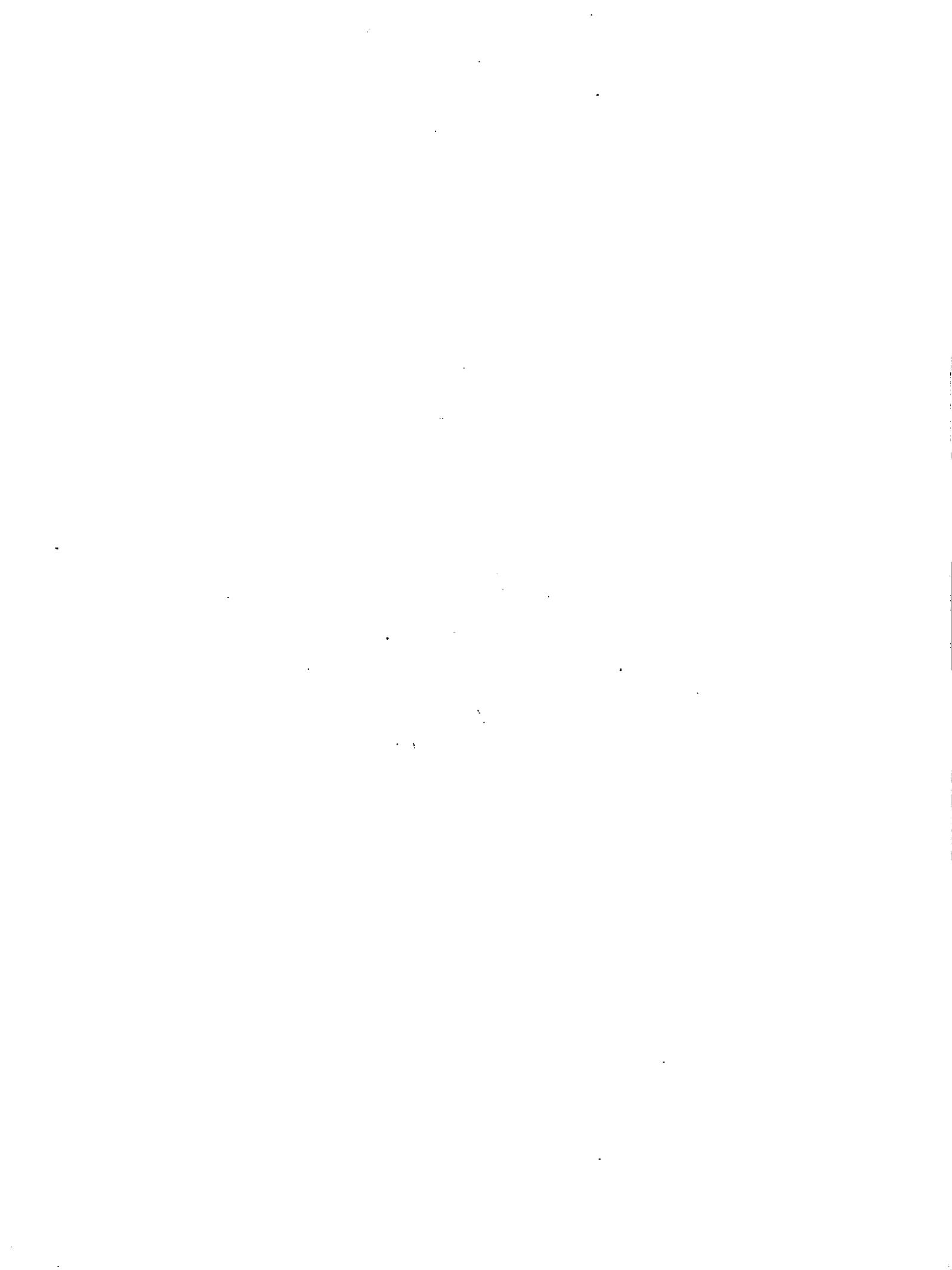
**14. Risk Management** -- Sandia is the originator of probabilistic risk analysis methodologies for nuclear power systems and nuclear weapons. Since 1973, Sandia has conducted a broadly based research program for the Nuclear Regulatory Commission in probabilistic risk assessment, severe accidents in nuclear reactors, reactor safety research experiments, engineering technology, low-level waste management, and safeguards and security. We have performed many of the risk assessments sponsored by the commission, developed state-of-the-art methods, participated in major technology transfer efforts, and addressed important regulatory issues amenable to solution by risk assessment. We have developed methods to analyze power plant systems, operations, human performance, accident processes, transport of radioactive materials, and health and economic impacts. (Oil Processing and Refining 8; Environmental and Regulatory; Deepwater Offshore; Arctic Region Activities 5,6,7; Environmental and Regulatory 14)

**15. Nondestructive Testing** -- Sandia has extensive capabilities in nondestructive testing (NDT) to analyze material properties, locate and characterize flaws within materials and joins, monitor the internal operation of complex mechanisms, and determine the integrity of bonds between

materials. Capabilities include x-ray tomography, ultrasonics, coherent optics, thermography, Raman spectroscopy, and other techniques. (Oil Processing and Refining 12; Gas Gathering 2)

**16. Joining Technologies --** Sandia has made a study of the science and art of joining technologies for many years. Nuclear weapons have very demanding requirements for long-lived integrity of joined surfaces, welds, and soldering joints. Consequently, Sandia has acquired a substantial understanding of the fundamentals of joining processes. Conventional arc welding during fabrication of some high-performance alloys exposes these materials to temperature cycles that can degrade the mechanical properties sufficiently that their utility is degraded. We are developing advanced joining technology for these materials using high energy-density welding processes. We are also exploring novel joining technologies for advanced ceramic and alloy structural materials. Emphasis is placed on developing new approaches to joining and sealing dissimilar materials that have particular relevance to advanced packaging. SMARTWELD, a recent Sandia product, is an integration of modeling, simulation, and sensors with actual welding processes to allow fabrication of critical components without extensive development time and costs. (Oil Processing and Refining; Gas Gathering)

**17. Systems Engineering and Integration --** As an engineering laboratory with a can-do ethic, we excel at providing a systems approach utilizing a broad range of capabilities towards solving a technical challenge. An example which has been discussed with industry addresses the threat posed to offshore structures by icebergs. The following weapons-related technologies could be applied: threat analysis and risk assessment tools, high-resolution synthetic aperture radar (SAR), earth penetrating radar, radar tags, remote sensors, ice penetrators, data collection, analysis, and assessment workstations, various telemetry methods, ocean circulation modeling on massively parallel computers, and munition technology. These would be used to detect, characterize, monitor movement, assess the threat, and, if necessary, design and execute mitigating tactics. (Arctic Region Activities 7; Deepwater Offshore; Gas Gathering)



**PART III**  

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**HISTORICAL LEGACIES**



## **Historical Legacy – Brookhaven National Laboratory**

Brookhaven National Laboratory was established in 1947, in the post -World War II era, for the purpose of bringing together the resources of academia and government to design, build and operate major user facilities and carry out research that would be beyond the means of a single university. The primary purpose then, as it is now, was to advance science in all frontier areas of interest to universities, industry and government.

In the intervening years, and especially since the formation of the Department of Energy, the Laboratory has continued to strengthen its ties to the U.S. industrial community. Through its Office of Technology Transfer , its open access policy for its user facilities, and its staff of highly-qualified scientists and engineers the Laboratory has been able to build a strong record in support of its mission: to support the basic Department of Energy activities through its leading-edge user research facilities, its research and technology development, its educational efforts and industrial involvement.

The Laboratory is organized in a manner that resembles a university in that it conducts its research within a group of scientific departments. While each of these departments nowadays has some interactions with industry, perhaps the two most active in this regard are the Department of Applied Science and the Department of Advanced Technology. This is not surprising inasmuch as those two departments evolved from a common parent, the former Department of Nuclear Engineering. Activities in both departments have expanded through the years to encompass all of the activities that are relevant to the mission of the DOE. Their common heritage is an understanding of the industrial community and its need to establish well-defined objectives for R&D programs that are consistent with a strategic plan. Together, these two departments perform about one hundred million dollars worth of research for the DOE, the Nuclear Regulatory Commission, other federal agencies and for numerous industrial customers under work for others agreements. Cooperative Research and Development Agreements cover other collaborations with industrial partners when appropriate.

The broad experience gained over the years by the Laboratory in managing the design, construction and operation of major user facilities has created a large cadre of scientists and engineers who possess skills that are relevant to the petroleum industry. This is readily discernable in the more detailed Project Summaries elsewhere in this report. Perhaps the most shining example can be found at Brookhaven s National Synchrotron Light Source, where for more than a decade, hundreds of industrial users have worked singly or in groups to perform proprietary and nonproprietary research of direct benefit to their companies and to the U.S. economy. It need only be restated here that the Laboratory and its staff stand ready to work closely with industry representatives to define the most effective ways to funnel their talents into specific collaborative projects.

## **Historical Legacy – Idaho National Engineering Laboratory**

The government established the 890 square mile INEL site in the late 1940s, when the Atomic Energy Commission needed a location for conducting nuclear research, development, and engineering. The southeastern Idaho desert location was ideal because it was remote, large and unpopulated. The initial nuclear-related mission for the INEL led to the creation of a large talent base, with strong capabilities in design, system integration, project management, and many related engineering and scientific disciplines. As the nuclear mission of the INEL began to wind down in the 1980s, the government found the INEL's technical skills could be easily moved into other important mission areas. New laboratory and engineering facilities were constructed in the City of Idaho Falls, and this infrastructure now supports many programs in a wide range of energy technologies. New focus areas in the environmental field have also emerged in support of DOE's need to assess and remediate their national laboratory and production sites.

The tie between inherent INEL capability and the fossil energy community has grown out of work in related energy fields. For example, large INEL Geothermal programs have created expertise in drilling and reservoir engineering, now being applied to borehole seismic and enhanced oil recovery projects. The development of advanced, energy-efficient manufacturing techniques have led to unique plasma processes for converting heavy oil or methane to higher value products. Instrumentation and materials research supporting nuclear plant safety and lifetime extension programs now are being applied to similar petroleum refinery issues. Bioprocessing skills developed for alternative energy programs and DOE environmental restoration programs are now finding applications in enhanced oil recovery projects and hydrocarbon contaminated soil remediation. Basic energy science sponsored research in materials has provided unique capability in membranes and catalysts which are being explored for application in numerous fossil energy areas. A host of environmental projects for DOE and other sponsors range from remote sensing and site characterization to treatment system development. INEL has grown to be a national leader in environmental technologies and is well positioned to transfer much of this expertise to the fossil energy community.

The application of these INEL technologies to petroleum industry problems has been largely facilitated by key personnel acquired from a downsizing petroleum community. These individuals have been able to recognize opportunities for improvement in their former industry and direct existing INEL laboratory capabilities toward these needs.

## **Historical Legacy – Lawrence Livermore National Laboratory**

Lawrence Livermore has been involved with activities related to oil and gas production since the late 1950s as a part of the Plowshare program, which evaluated the use of nuclear explosions for stimulation of Western tight gas sands and retorting of Green River oil shale. Subsequently, more conventional mining, drilling, and rock fracturing approaches to in-situ oil shale recovery, underground coal gasification, and tight gas recovery were initiated in the early 1970s. Many of the current oil and gas activities can be traced back to these beginnings.

The underground coal gasification project investigated ways to effectively recover unmineable (deep and low grade) coal resources, including several large-scale field experiments. The project produced the most effective method to date: the Controlled Retractable Injection Point (CRIP) process. This process used horizontal drilling before it was common in the oil and gas industry as a way to control underground chamber growth during the gasification process. Personnel in this project are currently investigating gasification of municipal solid waste with Texaco.

The oil shale project explored in-situ oil shale retorting with laboratory experiments, process modeling, and pilot retorts, and it provided technical support to the Rio Blanco in-situ experiments in the early 1980s. Subsequently, it examined aboveground retorting for 10 years, with an emphasis on a recycled hot solids process. The last two years included a CRADA with Amoco, Conoco, Chevron, and Unocal prior to cancellation of the national oil shale program.

The tight gas sands activities in the late 1970s and 1980s included experimental, modeling, and sensor development support of DOE field experiments. The LLNL activity produced the most detailed model of hydrofracturing to date, with the ability to model the transport of fluids in existing fractures and propagation of fractures across fracture and lithographic interfaces.

Diagnostic needs for in-situ experiments initiated geophysical tomography research at LLNL in the 1970s, which evolved to two successful techniques: electrical resistance tomography and electromagnetic tomography. These have been used most recently to monitor steam injection for environmental cleanup and heavy oil recovery, respectively.

The need for accurate chemical kinetic expression for modeling in-situ oil shale retorts led to a petroleum geochemistry project that derived kinetic models for geologic genesis of oil and gas. This project ultimately received \$1M in direct industry funding through last year. Oil shale and petroleum geochemistry activities spawned current activities in heavy oil upgrading. Expertise from the coal gasification and oil shale projects were combined in the late 1980s to co-develop a twin-screw coal pyrolysis process with Coal Technology Corp.

Throughout the 1970s and 1980s, Lawrence Livermore had an active group in energy modeling, including the tracking of world oil and gas production and resources. The group developed equilibrium models of the entire energy sector which could be applied on a regional as well as national basis. These models are now used on personal computers to model the penetration of new technologies into the marketplace.

## **Historical Legacy – Los Alamos National Laboratory**

For nearly 30 years Los Alamos has been a national resource of scientific and technical capabilities in the earth and environmental sciences in areas related to the DOE missions in energy, national defense, and environmental concerns. The scope of geosciences activities at Los Alamos expanded into energy research as a result of the oil crises of the 1970s and into environmental research as a result of DOE concerns over the effects of its activities on human health and ecosystems.

Solid-earth geosciences research began in earnest at Los Alamos as a result of the Limited Test Ban Treaty signed in 1963. This treaty required that all nuclear tests be carried out underground and that no radioactive debris be allowed to escape from the test area. A major investment in geological characterization and hydrodynamic modeling was necessary to ensure that all tests were "contained." The scope of geosciences activities broadened in the early 1970s when Los Alamos scientists and engineers originated the hot dry rock concept, which involves extracting thermal energy on a large scale from the hot but impermeable rock that underlies much of the United States and other continental land masses. In the late 1970s Laboratory scientists were requested to further broaden the scope of their efforts by assisting the Department in evaluating the Yucca Mountain area of the Nevada Test Site as a candidate for an underground repository for high-level nuclear waste. During the same period Los Alamos collaborated with other national laboratories in the National Uranium Resources Evaluation Program to quickly collect, analyze, and interpret hundreds of thousands of geochemical samples from a third of the United States. In the early 1980s, the Department increased its basic research activities in geosciences at Los Alamos to support the Department's continental scientific drilling effort. Los Alamos also began a program with the U.S. Agency for International Development to provide assistance to Caribbean and Central American countries in developing their indigenous energy and mineral resources.

Los Alamos has for decades been at the forefront of scientific computation and, most recently, the development of the supercomputer. Scientists at Los Alamos are in an excellent position to exploit supercomputers using numerical codes, high speed networks, and graphics systems developed at Los Alamos. Application of computational techniques to geologic, hydrologic and atmospheric phenomena is one of the most rapidly growing areas in the natural sciences. Along with observations from space, one of the most exciting changes in the earth sciences during the past thirty years has been the addition of predictive capabilities to previously descriptive disciplines. Natural systems are extremely heterogeneous and complex. Simulation of the often nonlinear processes in such systems requires substantial computational resources, and Los Alamos has been in the forefront of scientific computing since the invention of the computer. Solid and fluid mechanics capabilities developed in the weapons missions are now finding application in all aspects of the geosciences. These predictive tools are now integrating experimental and observational earth sciences with theory in sufficient detail to allow scientists to obtain both qualitative and quantitative answers to energy, environmental and other geophysical problems.

Strength in the above areas added to the breadth and depth of our years of experience mean we can continue to help solve many of the problems now facing the nation. Foremost among these problems are oil and gas production, other energy supplies, disposal of hazardous waste, and verification of nuclear testing treaties.

## **Historical Legacy – National Institute for Petroleum and Energy Research (NIPER)**

Founded as the U.S. Bureau of Mines Petroleum Experiment Station in 1918, the National Institute for Petroleum and Energy Research (NIPER) is the Nation's only federally owned fully integrated petroleum laboratory. Located in the middle of the "Oil Patch" and at the forefront of the ever-evolving domestic petroleum industry since its inception, NIPER researchers have been instrumental in the development of technology utilized by the petroleum industry over the past 77 years and are currently reaching into the future to solve tomorrow's petroleum needs.

Technology research areas which have evolved to meet the needs of the petroleum industry are summarized below:

- 1920s - Exploration, production, gas utilization, loss prevention
- 1930s - Production, processing, refining, drilling, completion, oilfield devices
- 1940s - Fuel analysis, refining, synthetic rubber, thermodynamics, water disposal, distillates for TNT
- 1950s - Secondary production, waterflooding, production, water disposal, metal corrosion, core and water analysis, radioactive tracers, oilfield devices, stripper wells, gas condensates
- 1960s - Waterflooding, production technology, drilling and coring, oil shale, gas condensates, gas hydrates, petroleum composition, air pollution, tracers, gas production stimulation, fuel stability, gas well delivery
- 1970s - Oil and gas production, enhanced oil recovery, heavy end distillates, production surveys, emission controls, advanced secondary recovery, improved oil recovery, process simulation, reservoir simulation, imaging technology, environmental projects, processing and thermodynamics, fuel chemistry, fuels and engine testing, DOE Crude Oil Database
- 1980s - EOR studies, field projects for EOR, gas production stimulation, "tight" gas sands, engine oil recycling, resource characterization, tar sands, engines testing, systems integration, synthetic fuels
- 1990s - Extraction research, reservoir characterization, drilling, exploration, risk-based management, field demonstration projects, environmental research, fuel chemistry, thermodynamics, refining and evaluation, planning and analysis, technology transfer, gas and oil technology partnerships

## **Historical Legacy – Oak Ridge National Laboratory**

Historically, the Oak Ridge Complex has been a separations and chemical processing center, and work has continued in this area throughout its history. Present day programs range from the most fundamental to demonstration projects. Initially, the challenge was to purify the crude uranium and separate isotopes more recently this expertise is used to solve difficult environmental problems. From the initial missions Oak Ridge has developed expertise and technical leadership in the areas of energy production and use, biological sciences and environmental technology, advanced materials and neutron based science and technology.

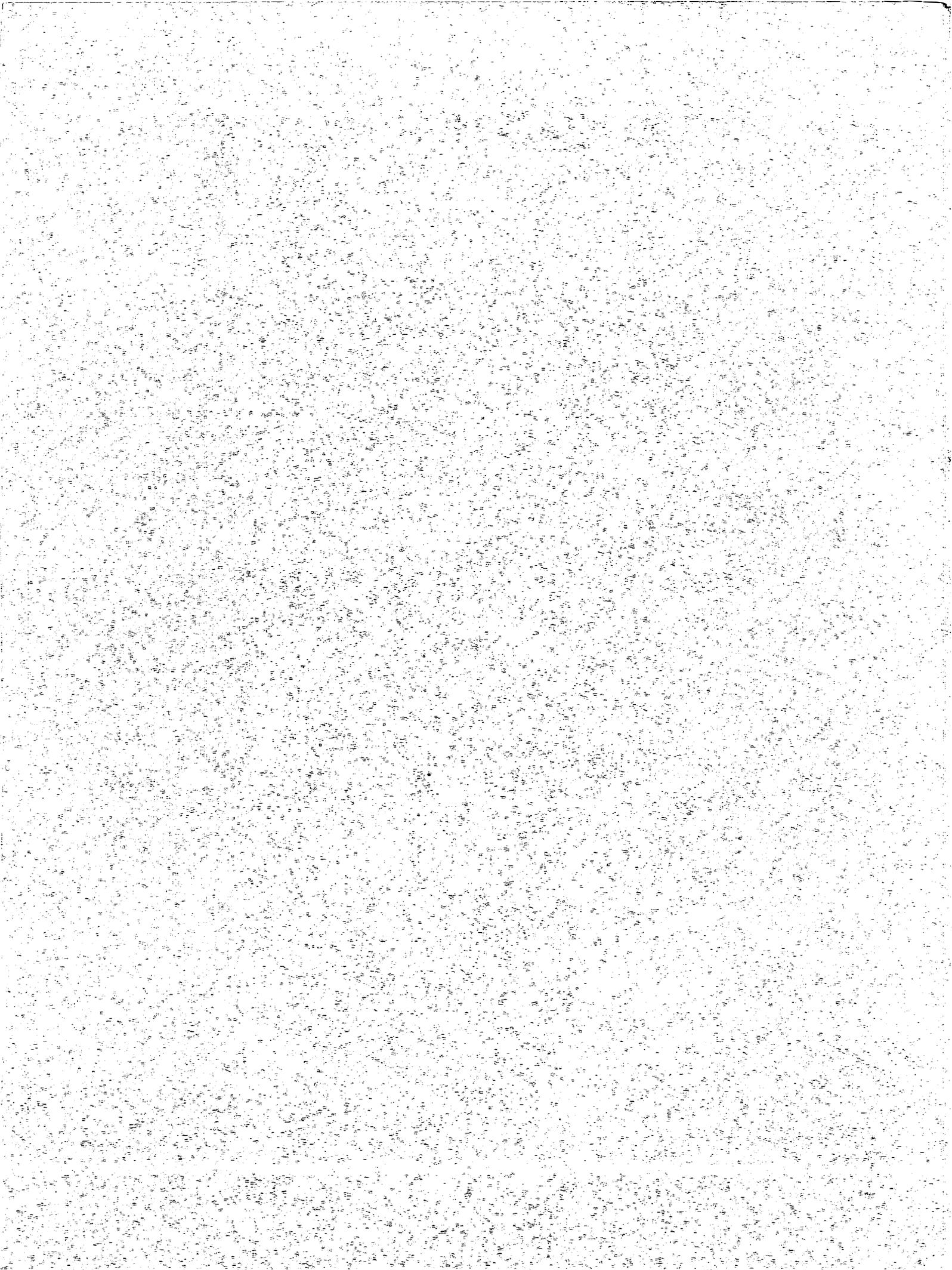
A broad spectrum of disciplinary foundations (biology, chemistry, computational sciences, ecology, engineering, geology, hydrology, physics, and toxicology) are integrated into programs aimed at solving major environmental problems associated with energy development, production and use. Technologies involving reactors, precision manufacturing and measurement, power conversion cycles, refrigeration systems, heat pumps, building systems, transportation, motor technology and energy storage are strongly represented. The demand for materials with enhanced capabilities in nuclear applications made Oak Ridge a premier provider of advanced materials and materials technology. These materials technologies include, ceramics, metals and alloys, surfaces and thin films, polymers and composites, superconductivity, and materials processing and characterization.

## **Historical Legacy – Sandia National Laboratories**

Over the years, Sandia has developed a rich history, broad capabilities, and outstanding staff in many, large programs which have produced technical capabilities of value to the petroleum industry: underground nuclear testing and verification, nuclear reactor siting, nuclear waste management (in salt at the Waste Isolation Pilot Plant (WIPP) and in volcanic tuff at Yucca Mountain), geothermal energy, geotechnical responsibility for the nation's Strategic Petroleum Reserve, wide-range of environmental programs and applications, and many different fossil energy programs. In the last area, Sandia has worked together with the petroleum industry since the early 1970's in such programs as in situ coal gasification, in situ oil shale retorting, enhanced oil recovery, unconventional and enhanced natural gas recovery, coal liquefaction, conversion of natural gas to liquid fuels, and combustion research.

There have been several underlying themes to these efforts: (1) Advanced instrumentation from the use of seismic, electromagnetic, and other geophysical methods for characterizing geologic media and mapping processes occurring 10's to 1000's of feet below the earth's surface through methods of determining the behavior and properties of complex hydrocarbon mixtures and processes. (2) Geomechanics applications aimed at understanding the complex, changing relationships between earth stresses, rock and rock mass properties, natural fractures, sedimentology and reservoir architecture, and multi-phase fluid flow in geologic media as oil and gas are produced. (3) Technology development with industry partners, such as developing significant, 10-fold improvement in insulated tubing used in steam injection, and playing a key role in the development of polycrystalline diamond compact drill bits and downhole steam generators for thermal recovery processes. Sandia also played a unique role in developing today's hydraulic and propellant fracturing technology through in situ instrumented experiments and mine-back observation in a deep mine at DOE's Nevada Test Site. (4) Integration of research, development and application as evidenced by key roles in managing and conducting large projects such as DOE's Multiwell Experiment (1980-88, \$38 million), and by projects which integrate Sandia capabilities with those of industry's to develop new technologies. (5) Basic research in geomechanics, geophysics and geochemistry, often in conjunction with universities, which provides a strong foundation for projects and technology development. (6) Advanced catalyst and process research, development, and testing for the conversion of coals to liquids and light hydrocarbons to alcohols, and where catalysts were developed with conversion activities exceeding the best commercially available materials for hydrocracking, denitrogenation, and desulfurization reactions. (7) Computer molecular simulation, utilizing advanced codes and massively parallel computers, for catalyst and membrane design and for modeling the properties of complex hydrocarbons and kinetics of refining processes. (8) Combustion research and science conducted since 1980 in a major DOE designated user facility which features advanced experimental techniques, laser-based diagnostics, advanced computational methods, and collaboration with visiting scientists and engineers from industry, academia, and other laboratories. (9) Technology transfer resulting from close collaboration with industry and epitomized by the Natural Gas and Oil Technology Partnership. Founded in 1988 with Los Alamos, the Partnership has pioneered a new paradigm of Industry-Department of Energy-National Laboratory interactions by bringing the capabilities of the Labs to the petroleum industry, by fostering innovative, flexible responses to industry needs, and by ensuring an industry-driven program.







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