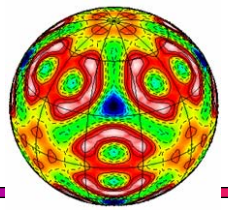


BASIC ENERGY SCIENCES –
Serving the Present, Shaping the Future
http://www.science.doe.gov/bes

DOE/BES Workshop on Clean and Efficient Combustion of 21st Century Transportation Fuels

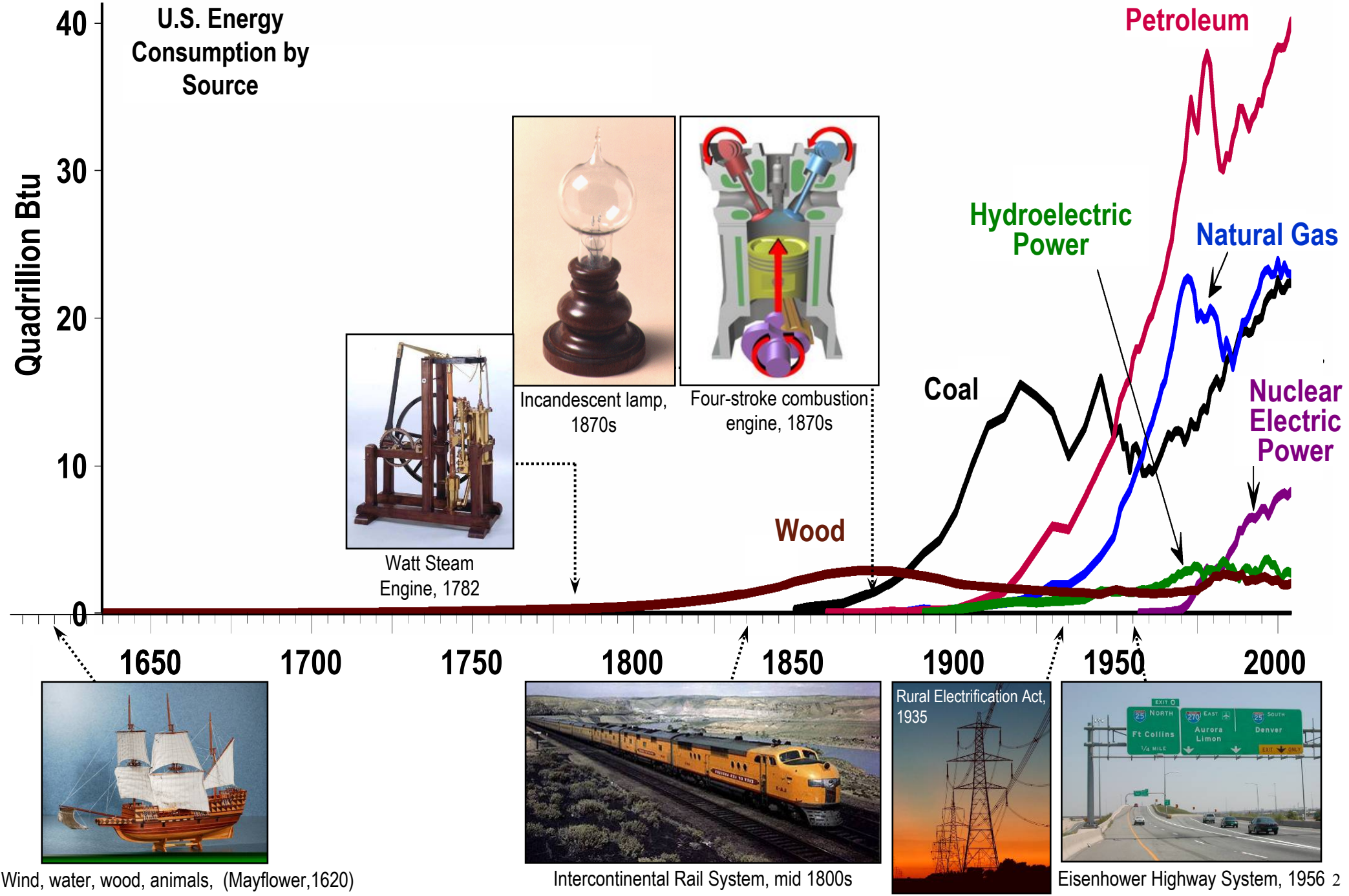
Eric A. Rohlfing
Director, Chemical Sciences, Geosciences, and Biosciences Division
Office of Basic Energy Sciences
http://www.sc.doe.gov/bes/bes.html

2007 Diesel Engine-Efficiency and Emissions Research (DEER) Conference
Detroit, MI
August 13, 2007

OFFICE OF SCIENCE U.S. DEPARTMENT of ENERGY

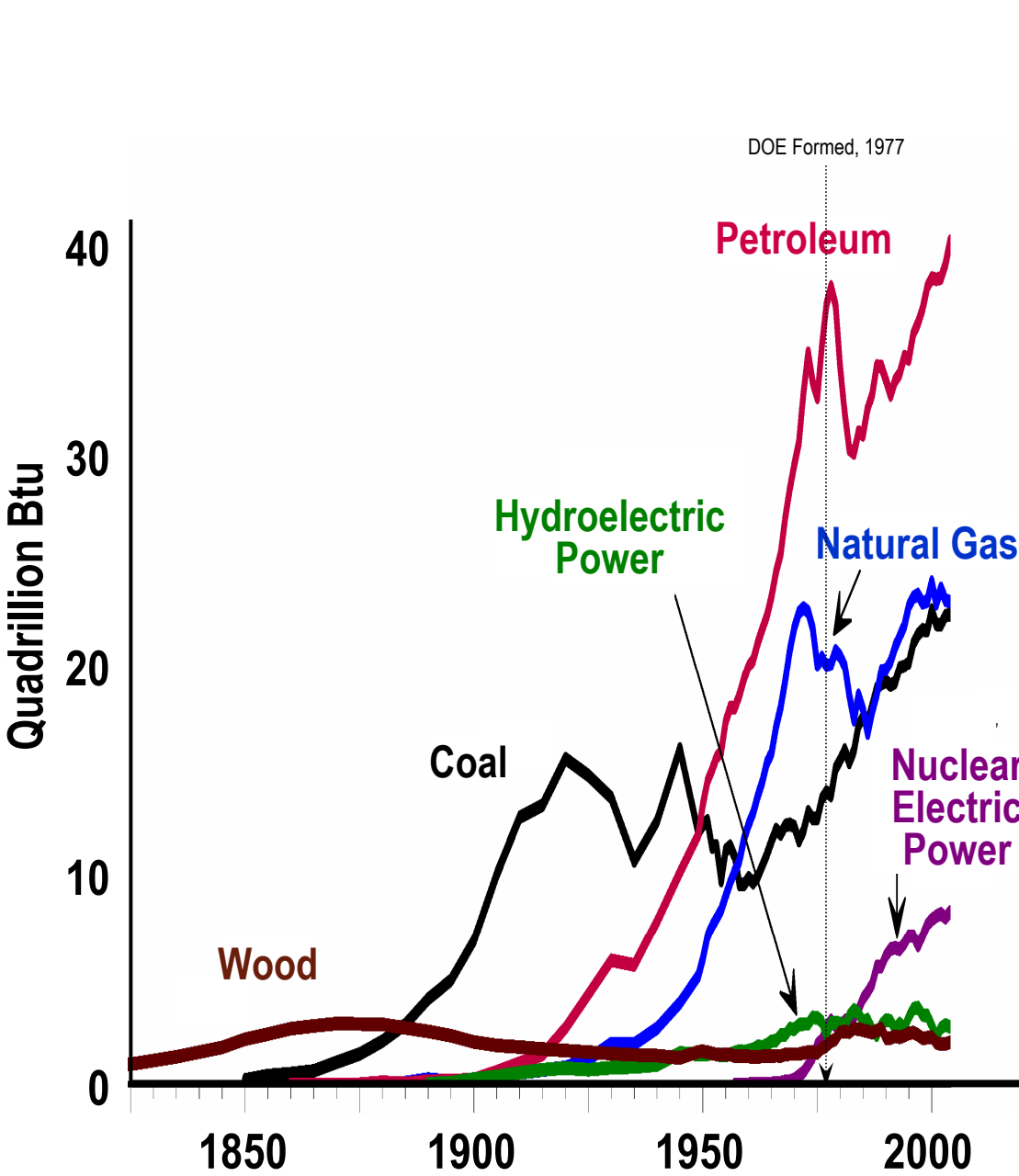
Technology, Energy, and Society are Inextricably Intertwined

Today's Energy Technologies and Infrastructures are Firmly Rooted in the 20th Century

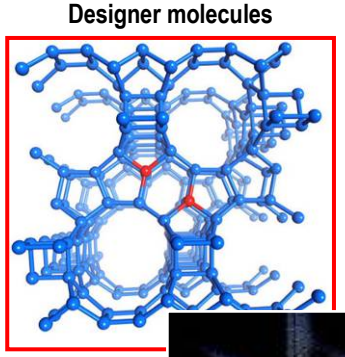


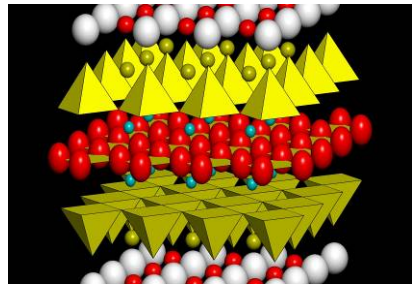
What Will the 21st Century Bring?

21st Century Science and Technology Will Exert Control at the Atomic, Molecular, and Nanoscale Levels



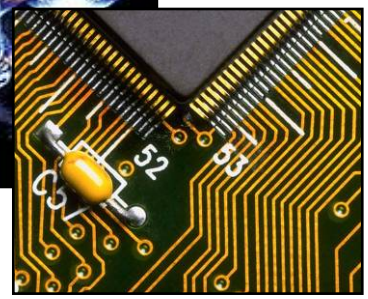
Designer molecules





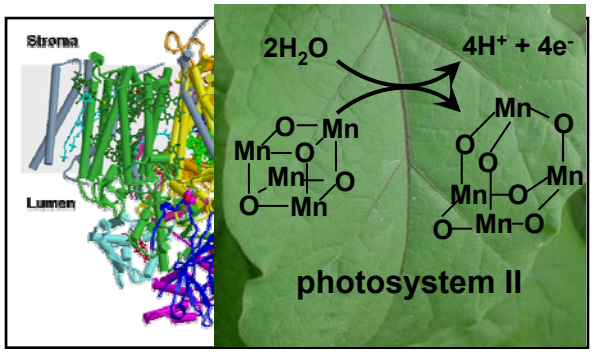
High Tc super-conductors

Solid-state lighting and many other applications of quantum confinement and low-dimensionality



Peta-scale computing

Bio-inspired nanoscale assemblies – self-repairing and defect-tolerant materials and selective and specific chemical reactivity.



Strategic Planning in Basic Energy Sciences

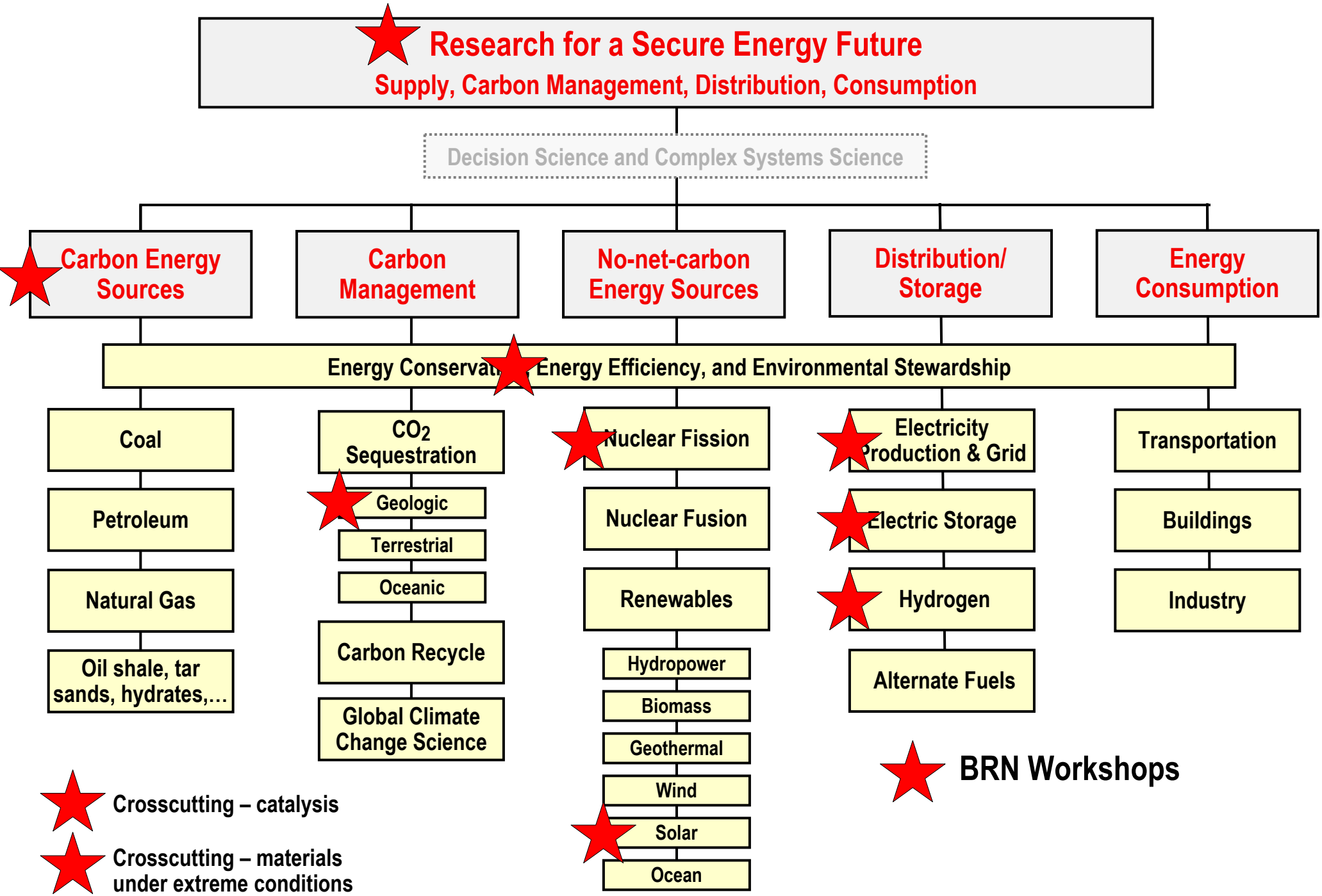
- **Phase I:** The Basic Research Needs workshop series.
  - Strategic planning for BES use-inspired (energy-relevant) research in coordination with DOE technology offices.
- **Phase II:** Basic Energy Sciences Advisory Committee (BESAC) Grand Challenges Report.
  - Strategic planning for BES grand-challenge/discovery research.
  - Report in preparation; update at BESAC meeting July 31.
- **Phase III:** BESAC panel(s) to summarize and connect scientific themes from Phases I and II, including "enabling tools"
  - BESAC just charged with this task…..

BESAC Chartered the First Basic Research Needs Workshop

RECOMMENDATION: Considering the urgency of the energy problem, the magnitude of the needed scientific breakthroughs, and the historic rate of scientific discovery, current efforts will likely be too little, too late. Accordingly, BESAC believes that a new national energy research program is essential and must be initiated with the intensity and commitment of the Manhattan Project, and sustained until this problem is solved.

February 2003

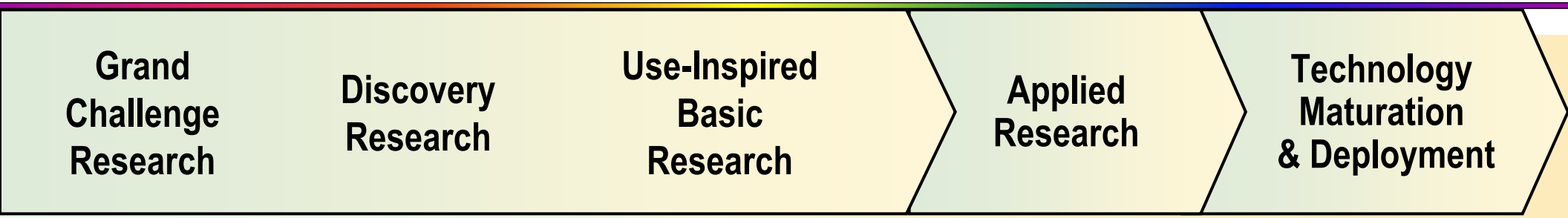
Past and Future BRN Workshops Address Many Elements Required for a Decades-to-Century Energy Security Strategy



The "Basic Research Needs" Workshop Series

- **Basic Research Needs to Assure a Secure Energy Future**
  BESAC Workshop, October 21-25, 2002
  The foundation workshop that set the model for the focused workshops that follow.
- **Basic Research Needs for the Hydrogen Econom**
  BES Workshop, May 13-15, 2003
- **Nanoscience Research for Energy Need**
  BES and the National Nanotechnology Initiative, March 16-18, 2004
- **Basic Research Needs for Solar Energy Utilization**
  BES Workshop, April 18-21, 2005
- **Advanced Computational Materials Science: Application to Fusion and Generation IV Fission Reactors**
  BES, ASCR, FES, and NE Workshop, March 31-April 2, 2004
- **The Path to Sustainable Nuclear Energy: Basic and Applied Research Opportunities for Advanced Fuel Cycle**
  BES, NP, and ASCR Workshop, September 2005
- **Basic Research Needs for Superconductivit**
  BES Workshop, May 8-10, 2006
- **Basic Research Needs for Solid-state Lightin**
  BES Workshop, May 22-24, 2006
- **Basic Research Needs for Advanced Nuclear Energy System**
  BES Workshop, July 31-August 3, 2006
- **Basic Research Needs for the Clean and Efficient Combustion of 21st Century Transportation Fuels**
  BES Workshop, October 30-November 1, 2006
- **Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems**
  BES Workshop, February 21-23, 2007
- **Basic Research Needs for Electrical Energy Storag**
  BES Workshop, April 2-5, 2007
- **Basic Research Needs for Materials under Extreme Environments**
  BES Workshop, June 10-14, 2007
- **Basic Research Needs for Catalysis for Energ**
  BES Workshop, August 5-10, 2007
- **Basic Research Needs – Final Wrap-up Worksho**
  BESAC, TBD

The Continuum of Research, Development, and Deployment



- Basic research to address fundamental limitations of current theories and descriptions of matter in the energy range important to everyday life – typically energies up to those required to break chemical bonds.

- Basic research for fundamental new understanding on materials or systems that may revolutionize or transform today's energy technologies

- Basic research for fundamental new understanding, usually with the goal of addressing showstoppers on real-world applications in the energy technologies

- Research with the goal of meeting *technical milestones*, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes
- Proof of technology concepts

- Scale-up research
- At-scale demonstration
- Cost reduction
- Prototyping
- Manufacturing R&D
- Deployment support

Goal: new knowledge / understanding
Focus: phenomena
Metric: knowledge generation

Goal: practical targets
Focus: performance
Metric: milestone achievement

The Continuum of Research, Development, and Deployment

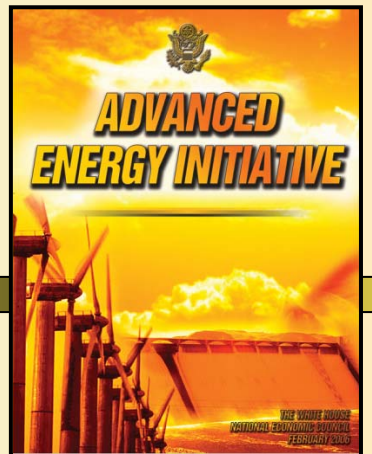
Grand Challenge Research	Discovery Research	Use-Inspired Basic Research	Applied Research	Technology Maturation & Deployment

(BESAC) Grand Challenges Panel

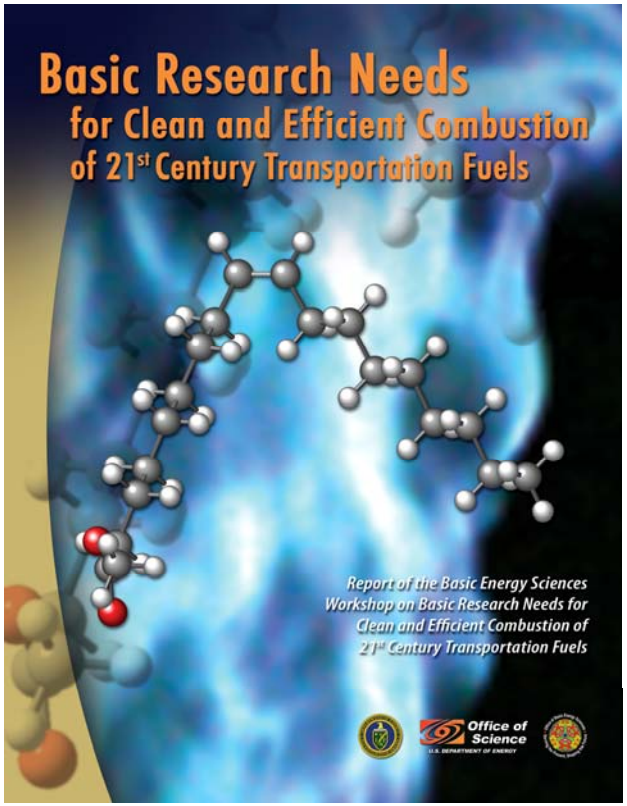
Technology Office/Industry Roadmaps

(BES) Basic Research Needs Workshops

(BES, BESAC, …) Tools and Facilities in Support of Research



Basic Research Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels



Organizing Committee

Co-chairs:

Andy McIlroy, Sandia National Laboratories
Greg McRae, MIT

Panel Leads

Novel Combustion:

Dennis Siebers, SNL
Volker Sick, Univ of Michigan

Fuel Utilization:

Phil Smith, Univ of Utah
Charlie Westbrook, LLNL

Crosscut Science:

Craig Taatjes, SNL
Arnaud Trouve, Univ of Maryland
Al Wagner, Argonne National Laboratory

Workshop held October 30 – November 1, 2006

Report now available in pdf format on BES website. Printed copies (limited) and CDs available.

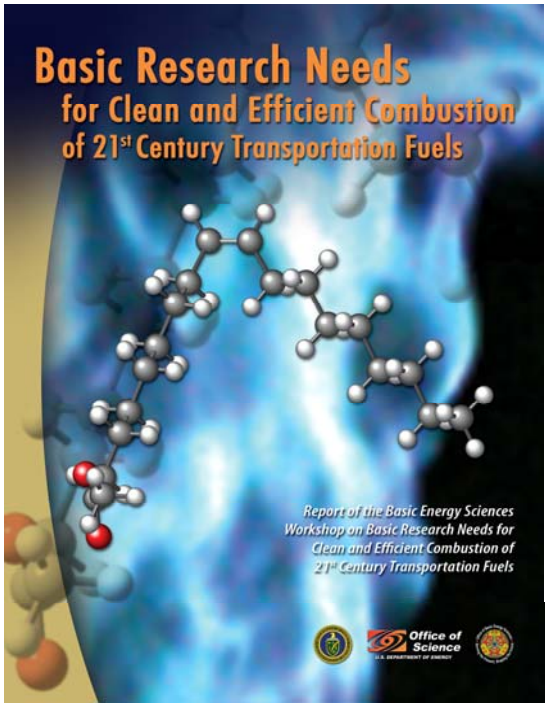
BES BRN Workshop Process

Before the workshop:

- Technical background document to set the background for the participants.
- Draft sets of key questions each panel should address.
- Warning to participants to come fully prepared in advance.

During the workshop:

- Plenary talks:
  - EERE perspective (James Eberhardt)
  - Industry perspective (Hukam Mongia, GE)
  - Economic effects (David Greene, ORNL)
  - Science challenges (Charlie Westbrook, LLNL)
- Breakout panels
- Interim report outs of progress
- Draft report writing



Following the workshop:

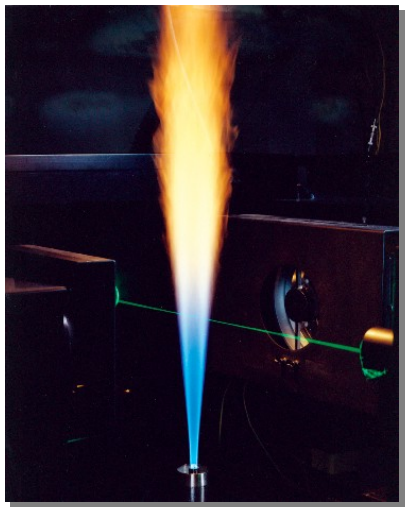
- Extensive reworking of the initial written output by core writers & panel leads
- Draft report completed 2/2007
- Final report released 5/2007
- Printed copies and CDs now available.

Workshop Details

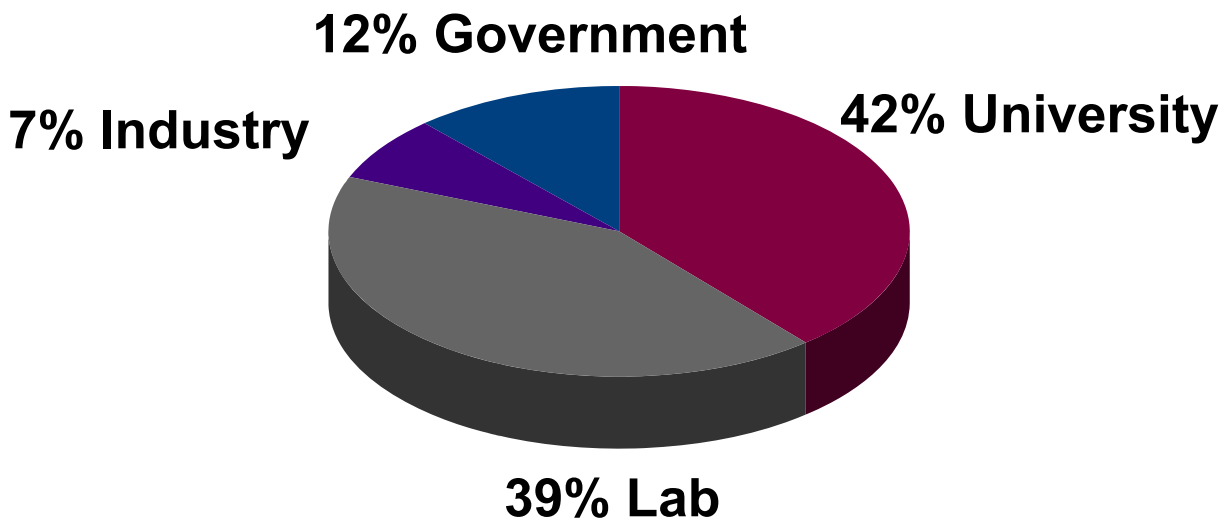
Novel Combustion

Fuel Utilization

Crosscut Science

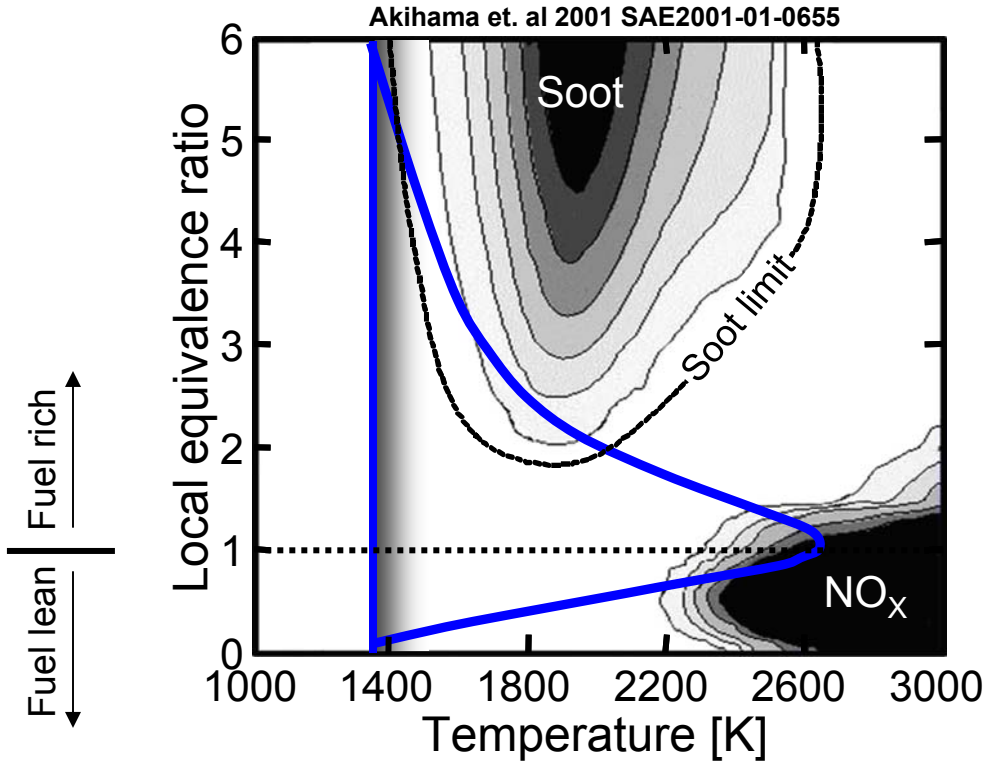


95 Participants



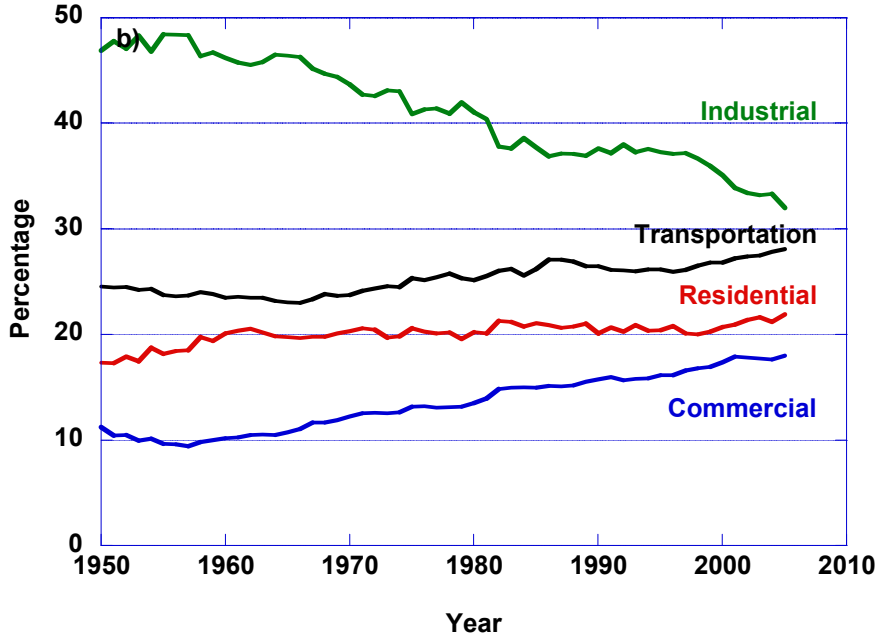
Transportation Combustion Challenges

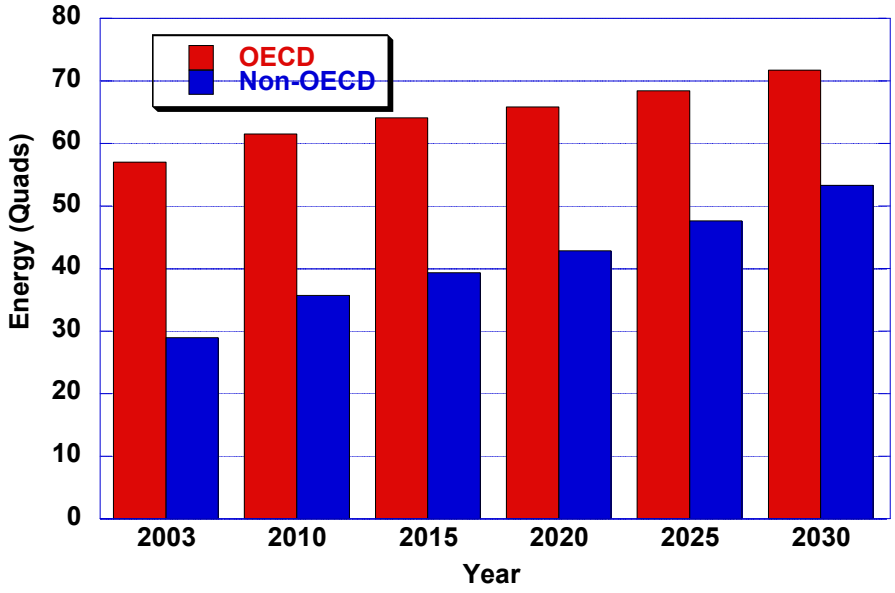
- **Efficiency & cleanliness difficult to achieve together**
- **Diesels are efficient, but difficult to make clean**
  - No throttling losses
  - High compression ratio
  - Continuum of rich to lean
  - Soot and NOx often anti-correlated
- **Spark ignited engines are 'clean,' but less efficient**
  - Stoichiometric burning
  - Little soot, 3-way catalyst eliminate NOx
  - Throttle losses
  - Low compression ratios



Motivation: Transportation Sector Key to Energy Use

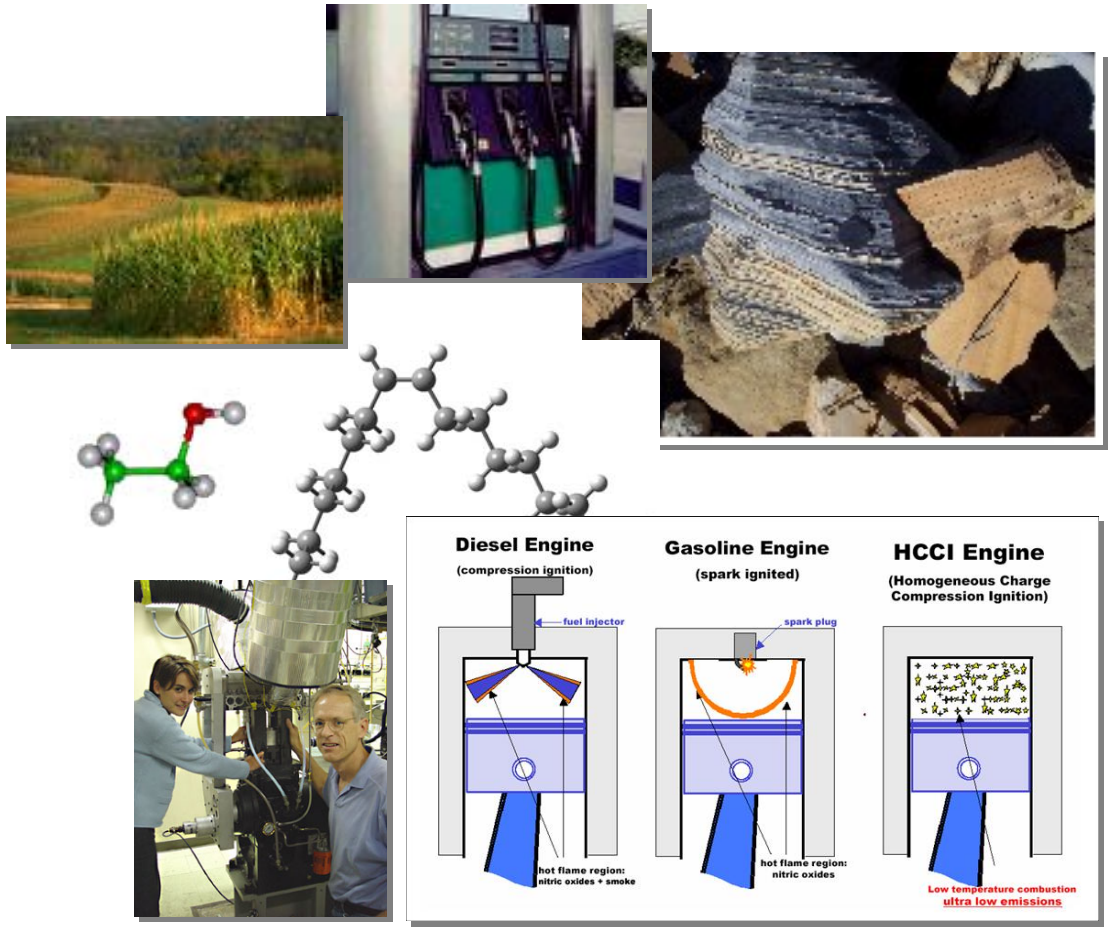
- Transportation accounts for ~1/3 of energy use
- When electricity generation is factored out, transportation dominates
- Demand projected to increase
- 97% of transportation energy from petroleum
- Relatively small number of technologies are employed
- Transportation sector energy use has significant import for national energy security and the environment





Motivation: Changing World of Fuel and Engines

- **Fuel streams are evolving rapidly**
  - **Heavy hydrocarbons**
    - Oil sands
    - Oil shale
    - Coal
  - **Renewable fuel sources**
    - Ethanol
    - Biodiesel
- **New engine technologies**
  - **Direct injection (DI)**
  - **Homogeneous Charge Compression Ignition (HCCI)**
  - **Low-temperature combustion**



Workshop Charge and Objectives

To explore basic research needs in the areas of gas-phase chemistry, combustion diagnostics, and combustion simulation that will enable the use of transportation fuels derived from non-traditional sources in a manner that optimizes engine efficiency and minimizes pollutant formation.

- Non traditional fuels are defined as those derived from carbon-neutral, renewable resources, such as biodiesel or ethanol, and those derived from non-traditional fossil fuel reserves, such as heavy crude oil, tar sands, oil shale, and coal.

- The output of the workshop will seek to define a set of basic, priority research directions (PRDs) that would employ and expand the current broad expertise base in gas-phase chemistry and combustion research into the realm of non-traditional fuels.

Priority Research Directions

1) Combustion Under Extreme Pressure
2) Understanding and Exploiting Surface Chemistry in Transportation Systems
3) Breakthrough Discovery Tools
4) Multi-scale Modeling
5) Basic Research Needs for Smart Engines
6) Physical and Chemical Properties for Combustion of 21st Century Transportation Fuels
7) Automated Discovery of Fuel Chemistry Kinetics
8) Spray Dynamics and Chemistry for New Fuels

Predictive Modeling of Combustion in an Evolving Fuel Environment

- **Predictive modeling is the key to combustion optimization in a non-linear parameter space**

- **Challenges:**

9 orders of magnitude in space and time

Complex chemistry, varying with fuel evolution

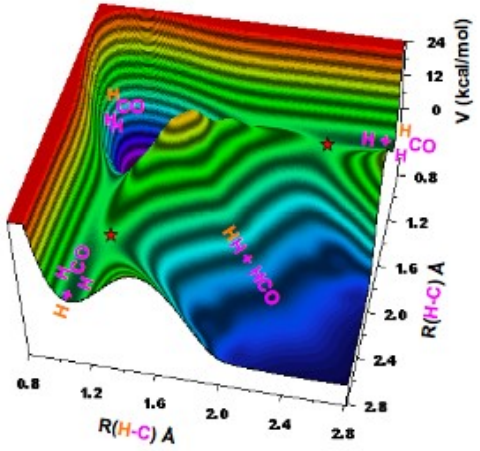
Work needed in:

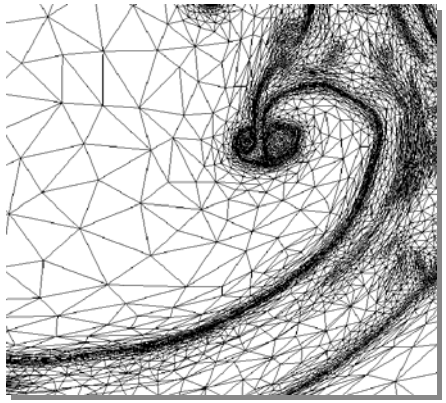
Chemical mechanism development

Turbulence-chemistry interaction

Algorithm development

Large dataset analysis

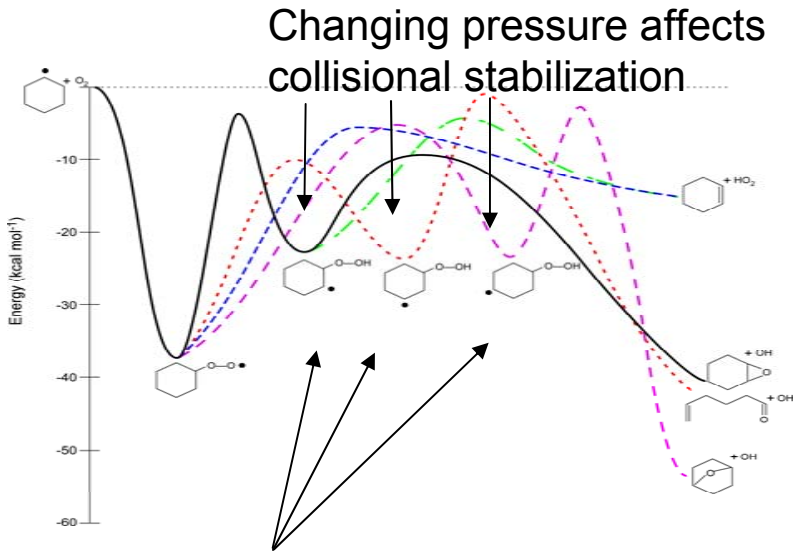




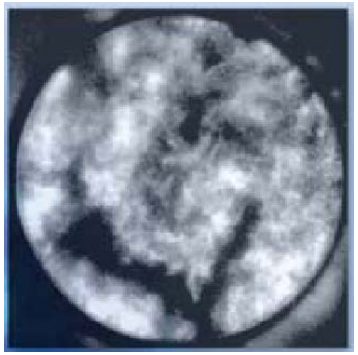
PRD 1: Combustion Under Extreme Pressure

Summary

- Advanced engines operate at higher pressures, but both physical and chemical properties are poorly understood at high pressure
- Prediction of ignition and propagation at high pressure is critical for design of new engines
- Knowledge of combustion phenomena at high pressure will enable new high-efficiency, low-pollution engines operating with traditional and alternative fuels

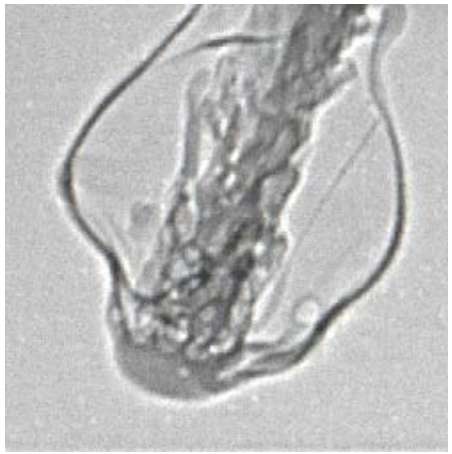


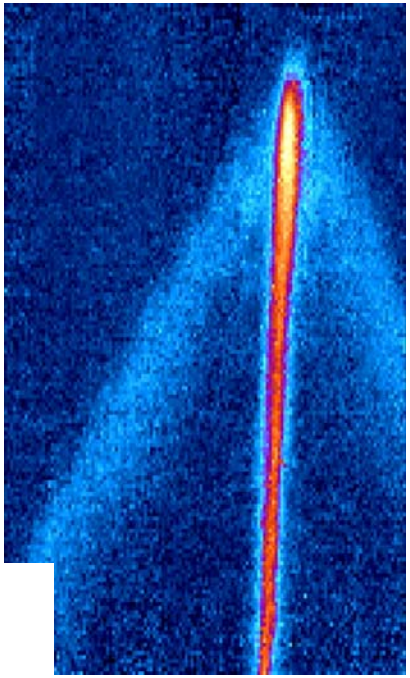
Isomerization produces chain branching species

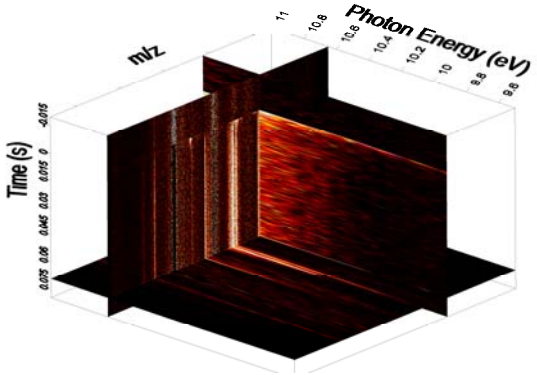


PRD 1: Combustion Under Extreme Pressure

Scientific Challenges







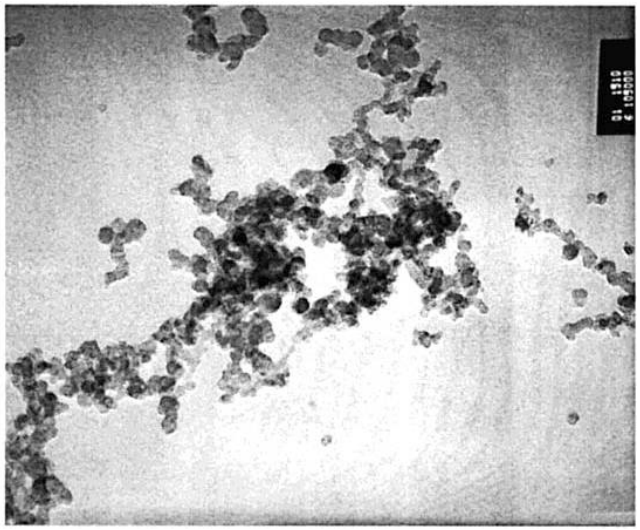
- Algorithms and theories to couple fluid mechanics to chemistry when separation of timescales no longer holds
- Accurate theory and computation for intermolecular potentials, collisional energy transfer, and non-statistical reactions
- Spatially and temporally resolved measurement for high-pressure, multi-phase reacting flows
- High-pressure chemical kinetics measurements with isomeric specificity

PRD 2: Surface Chemistry in Transportation Systems

Summary

• Problem: Inability to measure and control surface chemistry under engine conditions

• Impact: Soot, NOx, hydrocarbon emissions mitigation, increased fuel efficiency, better heat management



Approach:

• Advanced measurements and multi-scale models of soot growth and evolution under engine conditions

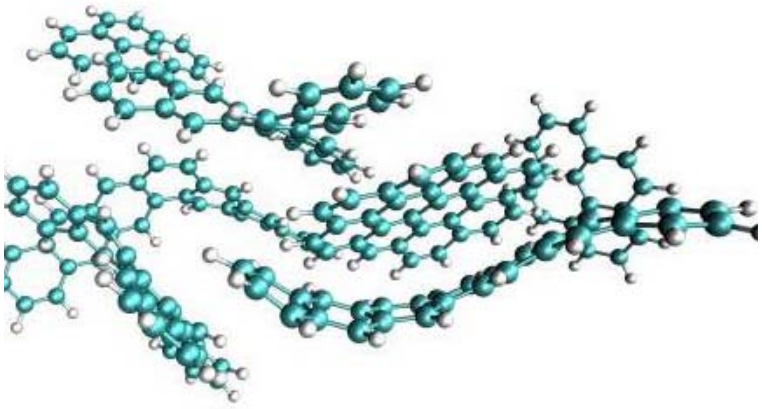
• New methods to study and control surface properties for better heat management and hydrocarbon emission

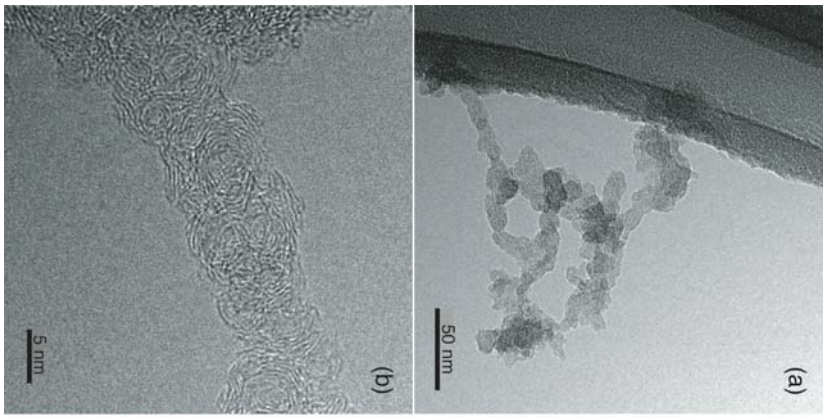
• Novel surface techniques to design after-treatment systems

PRD 2: Surface Chemistry in Transportation Systems

Scientific Challenges

- Soot modeling techniques need to be developed to span large spatial and temporal scales
- Methods to measure particle size, shape, composition, and precursors at high pressure need to be developed
- Techniques to measure surface chemistry under high pressure/high temperature conditions are needed

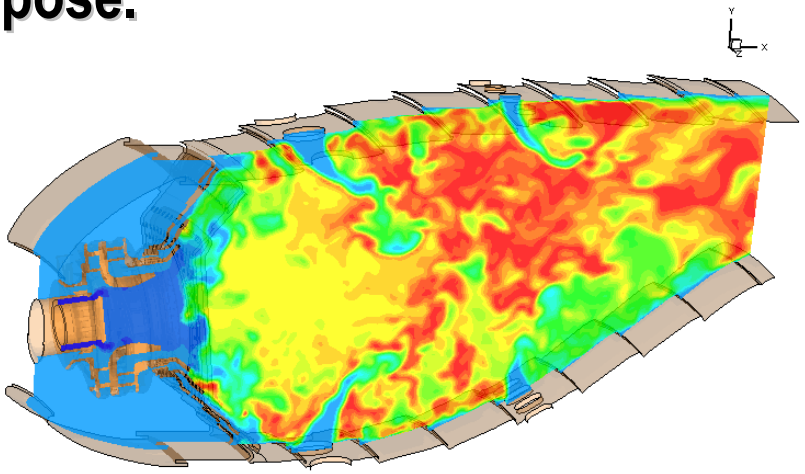




PRD 3: Breakthrough Discovery Tools

Summary

- Alternative fuel use in novel engine and gas turbine designs will require fundamental new understanding of in-cylinder and combustion chamber processes.
- Breakthrough optical (or x-ray) measurement tools will need to be developed for this purpose.

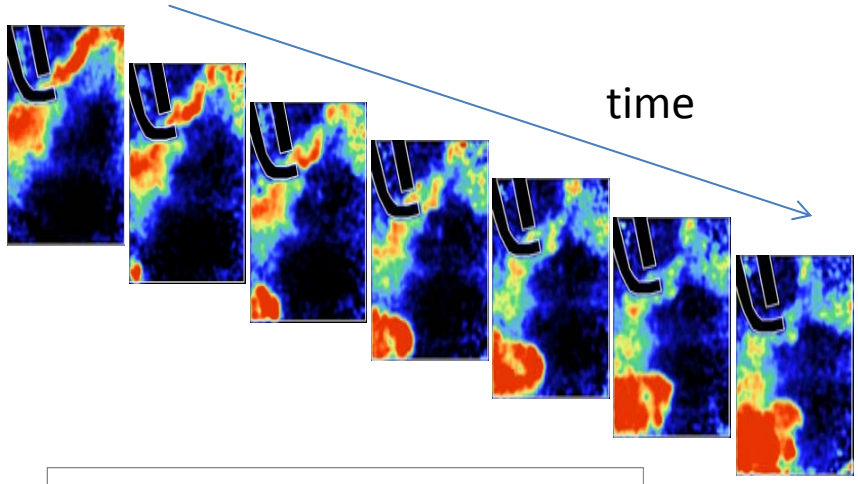


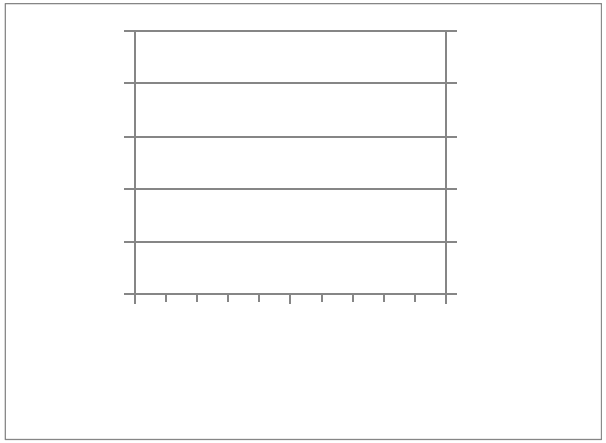
- These tools are vital for providing high-fidelity experimental data for development and validation of combustion simulations.

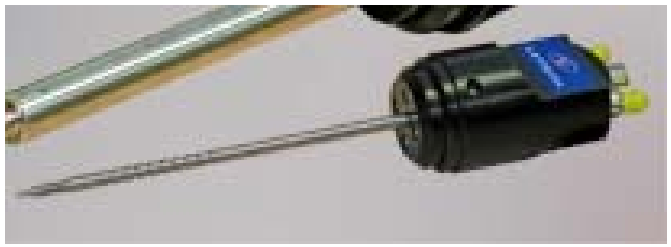
PRD 3: Breakthrough Discovery Tools

Scientific Challenges

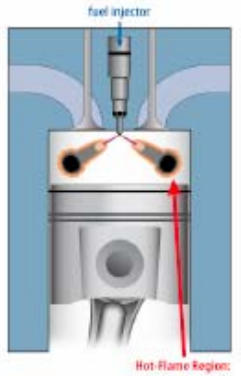
- Four-dimensional measurement capabilities at high repetition rates
- Photophysics at high pressure and temperature
- Detecting currently inaccessible molecules
- Diagnostics for real engines





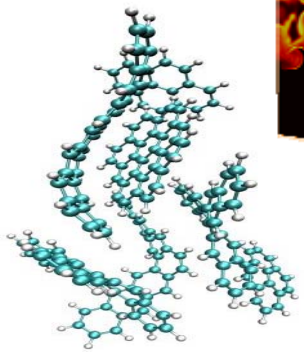


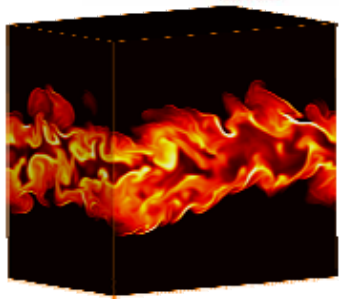
PRD 4: Multi-scale Modeling



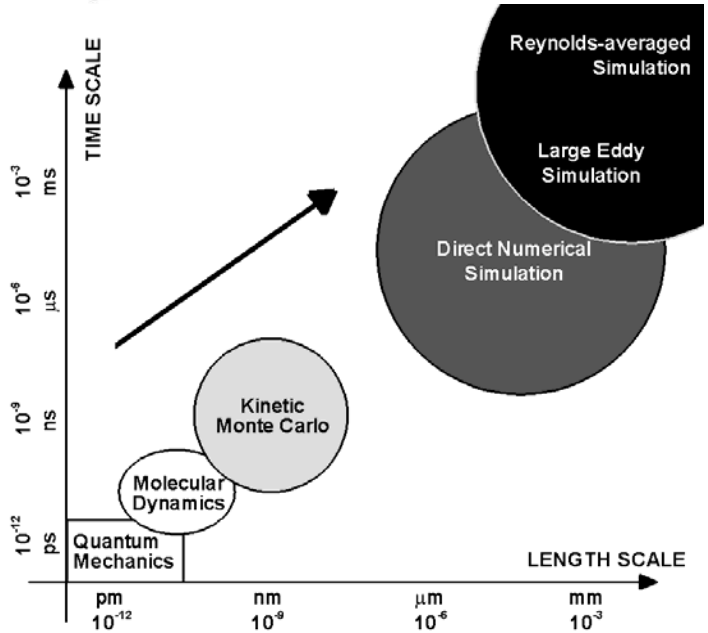
Summary

- IC engine combustion is a complex, multi-physics, multi-scale problem
  - Nanometer (molecular; soot inception)
  - Micrometer (fuel droplets)
  - Millimeter (small-scale mixing & flame dynamics)
  - Centimeter (in-cylinder diagnostics)
  - Meter (intake/engine/exhaust dynamics)





- Multi-scale modeling describes IC engine processes, from quantum scales up to device-level, continuum scales

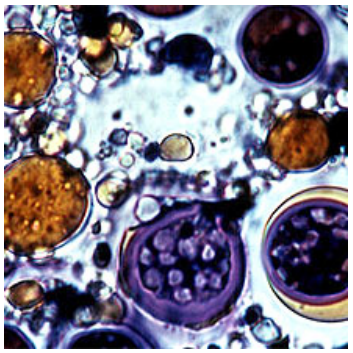


- Needs:
  - Develop a general theoretical framework for transfer of information from one scale to the next
  - Use petascale computing power to bridge the current gap between coarse-grained atomistic approaches and fine-grained continuum approaches

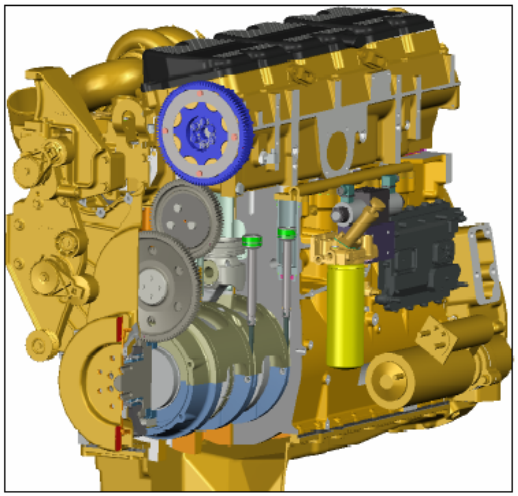
PRD 5: Smart Engines

Summary

- **Problem**
  - Changing fuel feedstocks
  - Advanced, efficient, clean engine combustions strategies are becoming more sensitive to fuel properties
  - Keeping fuel properties tightly controlled while feedstocks change is expensive
- **Impact**
  - Engines and fuels are becoming more complex and expensive
  - Efficiency and emissions may suffer
- **General approach:**
  - Create an engine that can dynamically alter its configuration and fuel composition for optimal performance

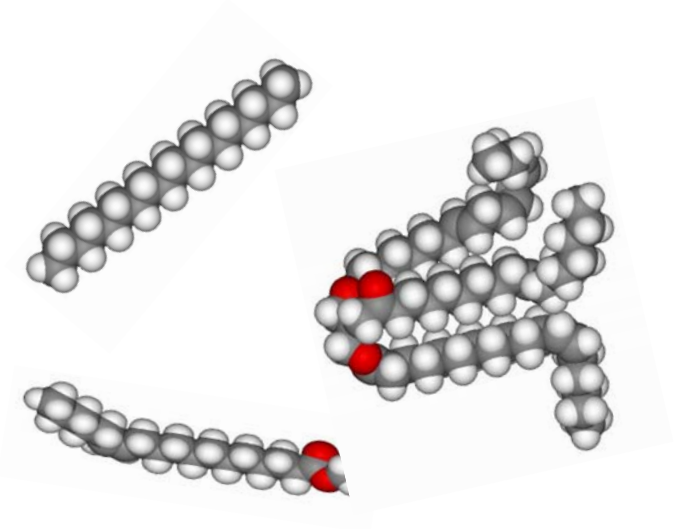


Chronicle / Brant Ward

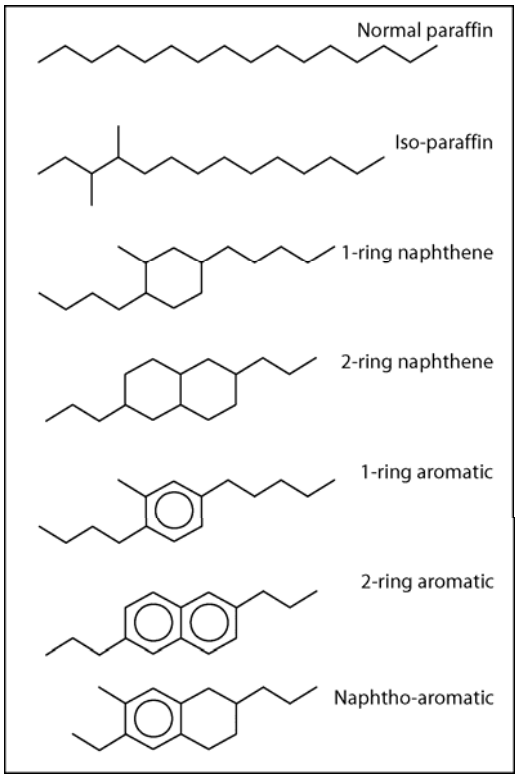


PRD 5: Smart Engines

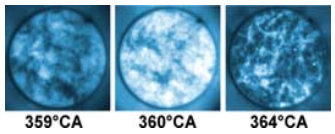
Scientific Challenges



- **Real-time spectroscopic and/or analytical techniques for detection of:**
  - **Fuel composition/properties**
  - **Combustion characteristics**
  - **Engine emissions**



- **Materials and methodologies for on-board fuel:**
  - **Separations**
  - **Chemical transformations**

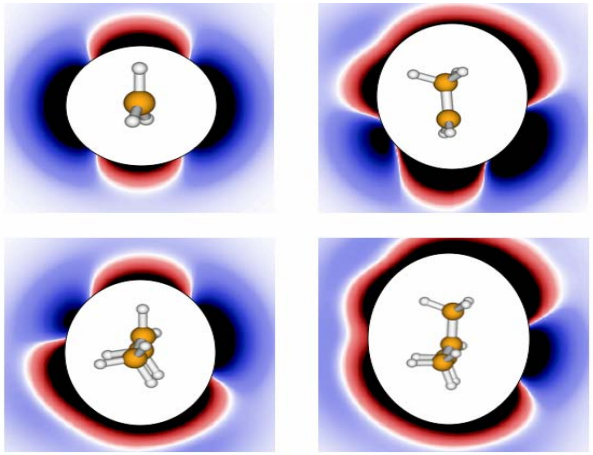


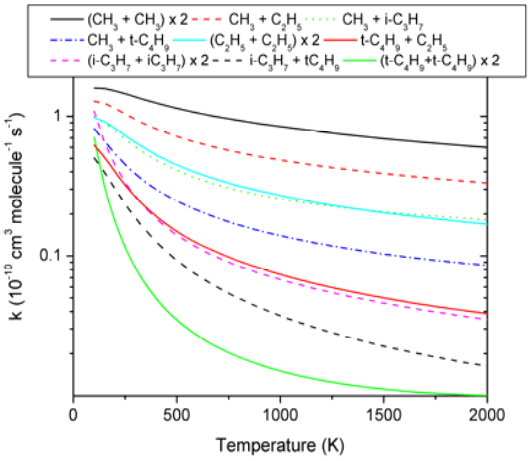
- **Fundamental understanding of fuel-property and engine-configuration effects on combustion characteristics in novel combustion regimes**

PRD 7: Automated Discovery of Fuel Chemistry Kinetics

Summary

- **Increased need to understand fuel chemistry**
  - Alternative fuels – larger, more complex molecules
  - Novel engine designs – lower T, higher P
- **Solution – automated kinetics**
  - Mechanism generators
  - Elementary reaction kinetics and theory
  - Mechanism reduction
  - Mechanism validation
- **Efficiently evaluate impact of novel fuels and engines**
  - Increased efficiency
  - Reduced pollution

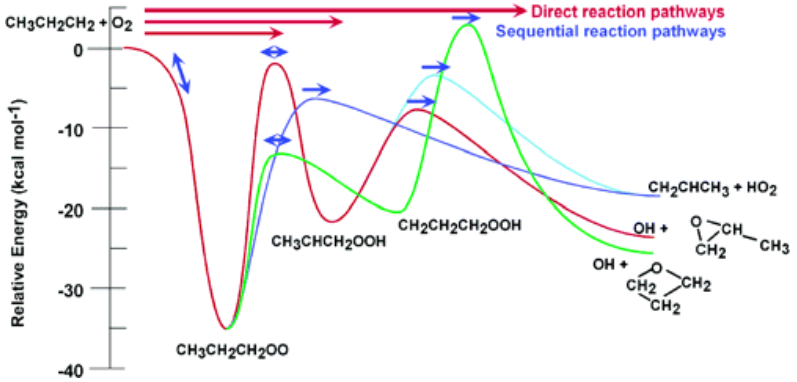


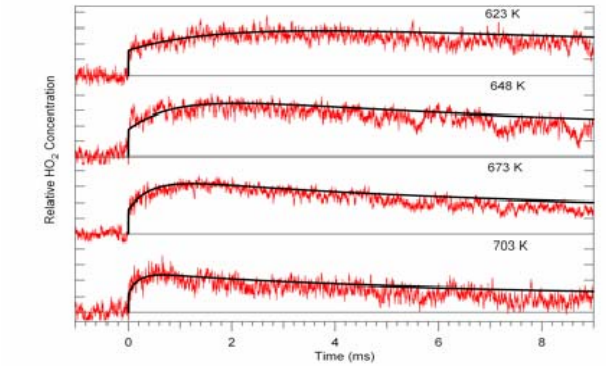


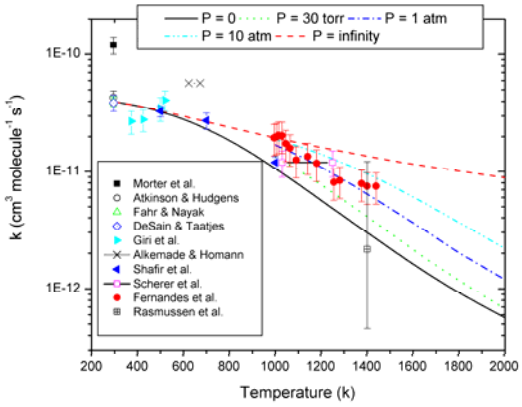
PRD 7: Automated Discovery of Fuel Chemistry Kinetics

Scientific Challenges

- How to automate?
- Rate constants
  - Transition state searching
  - Potential energy surface(s)
  - RRKM theory + master equation
  - To get rate constants
- Mechanism reduction
  - Graph methods
  - Dimension reduction
  - Quasi-steady state
  - Storage/retrieval
- Validation
  - Compiliation of large sets of data



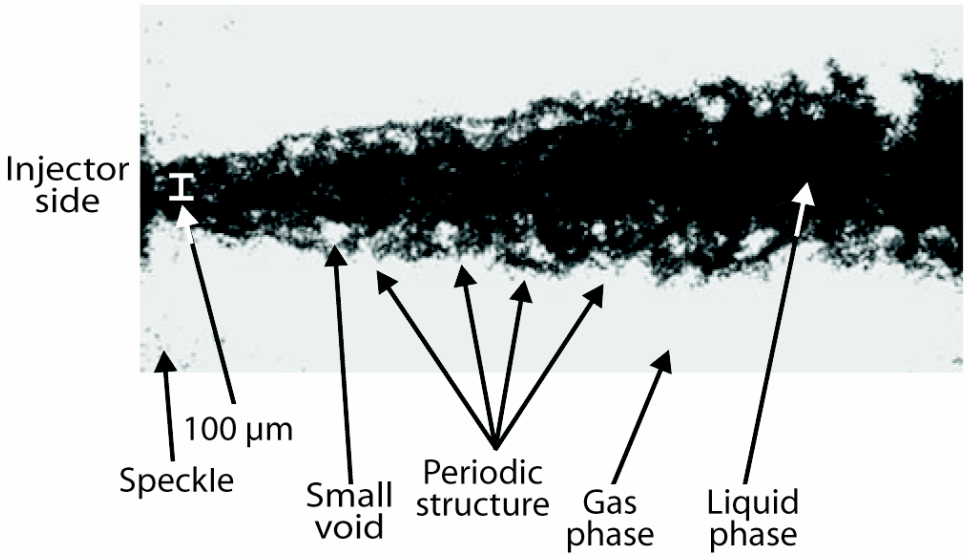


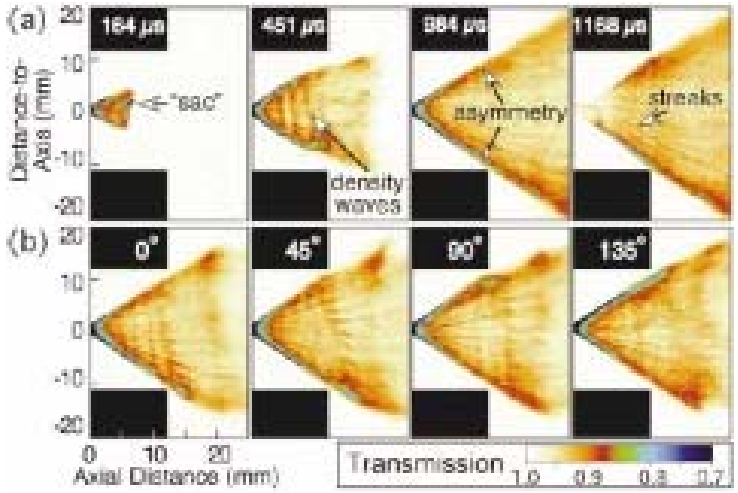


PRD 8: Spray Dynamics and Chemistry for New Fuels

Summary

- **Problem: Poor understanding of fuel spray behavior**
- **Impact: Predictions of alternative fuel injection/mixing**
- **Approach:**
  - **Development of new multi-phase spray-imaging techniques**
  - **Development of first-principles models of spray breakup**
  - **Strong coupling between experiment and modeling**

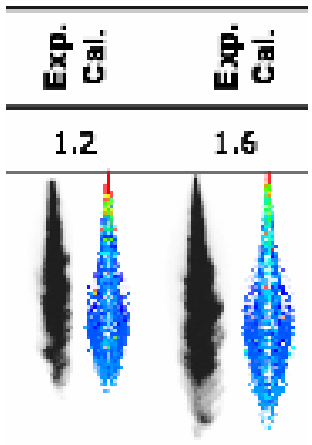


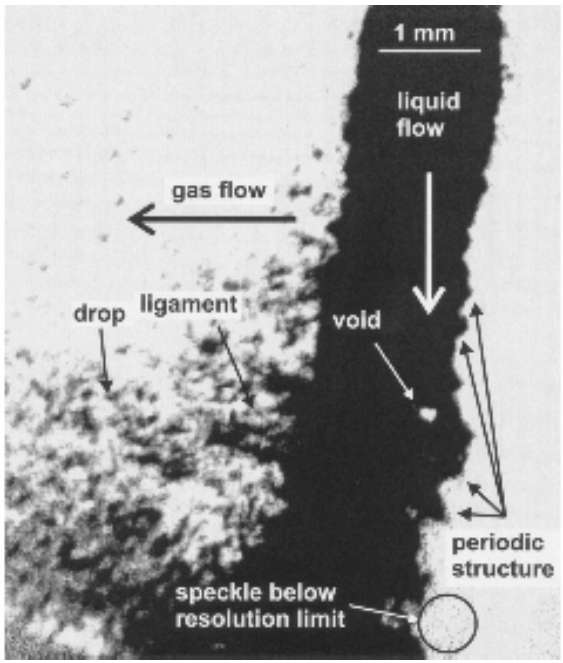


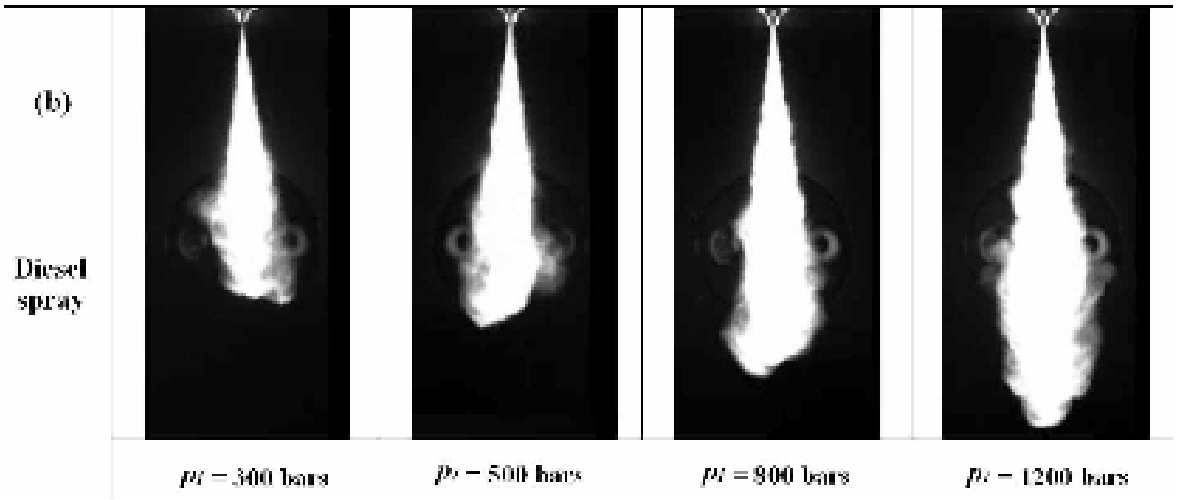
PRD 8: Spray Dynamics and Chemistry for New Fuels

Scientific Challenges

- Dense liquid-jet sprays difficult to probe experimentally
- Complex systems of high-pressure/high-speed fuel sprays are difficult to model
- Model development/validation will require:
  - Efficient, high-order numerical methods
  - Detailed measurements under extreme conditions







Combustion Science for 21st Century Fuels and Engines

Discovery Research	Use-inspired Basic Research	Applied Research	Technology Maturation & Deployment
•Reaction chemistry of large molecules at high pressure •Heterogeneous combustion and soot chemistry •Turbulent reacting flows with a large range of chemical time scales •Liquid fuel spray chemistry and dynamics •Multi-scale modeling: from quantum to continuum •High-fidelity computational approaches (DNS, LES) •4-D diagnostics at high pressure and under multi-phase conditions	•Automatic generation & reduction of chemical kinetics models of 21st Century Fuels •Soot formation, composition, morphology, oxidation and atmospheric evolution •High-fidelity CFD for complex and deformable engine geometries •Elucidating combustion dynamics for control strategies •Uncertainty quantification in multi-scale modeling •Development of novel diagnostics for molecular characterization at high pressure •Data and simulation framework built upon collaboratory and cyber-infrastructure tools •Modeling of turbulent sprays and turbulent multi-mode combustion	•High-fidelity CFD for device scale research: Virtual Engine Simulators (VES) •Application of VES to engine design, optimization, and real-time control •High-resolution optical diagnostics for device scale research •Device scale research on the impact of alternative fuel properties on novel combustion and emission processes •Exploration of high pressure engine combustion •Joint optimization of alternative fuel formulation and engine design •Smart vehicle strategies and sensor development	•New generation of vehicles with alternative fuels: achieving high efficiencies with emission compliance •Enable realization of next-generation efficiency and emissions standards •Smart vehicles with VES-based control systems

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A Great Plan – Now What?