Combustion Research Facility – Industry Interactions and Impact

Bob Hwang
Director, Transportation Energy Center
Sandia National Laboratories, Livermore, CA
Sandia Sites

Albuquerque, New Mexico

Livermore, California

Kauai, Hawaii

Pantex Plant, Amarillo, Texas

Waste Isolation Pilot Plant, Carlsbad, New Mexico

Tonopah, Nevada
CRF - Understanding Combustion Processes

* A Clearly Defined Partnership Mission from the Beginning *

- Born out of gasoline crises of 1970’s – created in 1980
- Built to tap into strengths of existing NNSA laboratory
  - Premier optical diagnostics
  - High Performance Computing
  - Flagship experimental facilities
- Teaming at DOE
  - Office of Science unwavering “Do great science” mandate
    - “Basic Energy Sciences (BES) supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security.”
  - Vehicle Technologies partnership: “make an impact”
    - “The U.S. Department of Energy's Vehicle Technologies Office supports research, development (R&D), and deployment of efficient and sustainable highway transportation technologies to improve vehicles’ fuel economy and minimize petroleum use.”
- Strong industrial and academic ties from day #1
Combustion Research Facility

A DOE Collaborative Research Facility dedicated to energy science and technology for the twenty-first century

- Leadership in combustion research since 1980
- 8200-m² office and laboratory facility
- 36 highly specialized labs
  - Laser-based diagnostics
  - Combustible and toxic gas handling
  - Computer-controlled safety system
- New 800-m² computational facility
- 42 Staff, 30 Postdocs, 130 visiting researchers
- Jointly funded by DOE Office of Science and EERE
  - $32M/year
Diesel Combustion Breakthrough

Sandia led the development of the new understanding of diesel combustion

Optical engine platforms & Laser diagnostics

Diesel combustion

Scaling of critical processes
- Liquid fuel penetration
- Flame lift-off

In-cylinder flows
- Non-optimal swirl
- Optimal swirl
A milestone in science-based engineering is achieved

- Cummins designs 2007 diesel engine using computer modeling and analysis.
  - After-the-fact testing only
  - Reduced development time and cost
  - Improved tank mileage
  - Emission compliant (new 2007 regulations)
  - Customer constraints met
  - More robust design
- Larger parameter space explored

The key enabler was the development of a detailed, science-based understanding of diesel combustion.
“In my view, the real power in this relationship is the partnership. It’s truly collaborative work where each of us brings specialized technical knowledge into the partnership, Cummins brings business perspective, DOE brings experimental analytical capabilities well beyond our own, and together we create something new and valuable.

In the case of the Cummins-CRF partnership, we have together not only contributed to the general combustion knowledge base in a significant way, we have literally changed the way Cummins does engine design. We have accelerated the pace of development through Analysis Led Design while at the same time increasing the depth of our design optimization by several orders of magnitude.

And we have similar experiences with collaborations with other national laboratories on engine efficiency and emission control systems. These partnerships have formed a key part of our research portfolio in the past and we look forward to continuing and expanding them in the future.”

— John Wall, Cummins Vice President & Chief Technical Officer
Laser Diagnostics, Optical Engines & Combustion Modeling

Sandia led investments in these areas are high impact solutions

- **Environmental**: Reduced criteria pollutants and CO₂.
- **Energy security**: Reduced dependence on imported oil.
- **Knowledge**:
  - A foundation for advancing more than a dozen high-impact technologies.
  - Substantial patent linkage to later industry patents.

... **benefits that continue to accrue**
Principles for Industry Impact

- Building foundational scientific understanding
- Focus on industry needs, including emerging challenges
- Deliver valuable pre-competitive results
- Synching with industry pace
  - Bi-weekly conference calls
  - Bi-annual scientific/technical meetings
- Share results and challenges – trust
- Spin off of targeted projects
- Post Docs and Student Interns – large numbers, exceptional opportunities, tech transfer
Advanced Engine Combustion MOU

Led/Managed by Sandia with the following partners

Research ⇒ Products

Started in 2003 and recently renewed through 2018

Next AEC Program Review: 8/19-21, 2014 at USCAR
Advanced Engine Combustion MOU

- Bi-annual meetings of over 100 attendees for 1 week
  - Sandia (winter) and Detroit at USCAR (spring)
- Pre-published results and latest discussion of collaborations
- DOE and NSF participation
A Global Collaboration: Industry, Universities & Labs

Sandia’s open forum collaboration to leverage research on fuel sprays

- Provides an open forum for collaboration among experimental and computational researchers ([http://www.ca.sandia.gov/ECN/](http://www.ca.sandia.gov/ECN/))
  - Establish an internet library of well-documented experiments for model validation and advancement of understanding.
  - Provide a framework for collaborative comparisons of measured and modeled results.
- Developed/led by Sandia - close collaboration IFP Energies Nouvelles (France)
- Research being conducted canonical systems
  - fuel injection conditions
- More than 30 participating groups worldwide

Leveraging international fundamental spray combustion research to speed progress
Engine Combustion Network

Industry has identified spray physics as a key enabler for future advancement

- Needle motion
- Argonne
- Nozzle geometry
- Liquid – phase penetration, size, structure
- Sandia
- Cool flame
- Ignition
- Lift-off length
- Soot
- Temperature
- Radiation
- Vapor penetration
- Minor species
- Velocity & Turbulence

**Diesel Spray A**

- 90°C
- 900 K
- 60 bar
- Rate of injection & momentum
- Liquid vol. fraction
- Fuel concentration
- Sandia
- Spray structure
- HS microscopy
- Mie/Schlieren/DBI

**Gasoline Spray G**

- 90°C
- 573 K, 6 bar
- 8-hole, stepped 80° total angle
- Liquid mixture fraction
- Vapor mixture fraction in Engine
- Spray structure
- HS microscopy
- Liq. & vap. penetration

**Notes:**
- CRF Image
- Bosch Logo
- Delphi Logo
Spray Combustion Consortium (SCC)

- Suppliers of vehicles, engines, injection equipment and software

- Initial partners include:
  - Cummins
  - Renault
  - Scania/VW
  - Caterpillar
  - Convergent Science
  - CD-ADAPCO
  - Isuzu
  - Hino Motors
  - Bosch

- July 1 kickoff
Advanced Technology Consultants

- Southern California start-up that partnered w/ Sandia to advance their technology commercialization
- Prepared proof of concept DOE SBIR proposal
  - Light activated single-wall carbon nanotubes (SWCNT) ignition
- Could improve engine efficiency by 30 – 50%

Transient Plasma Systems, Inc.

- USC spinoff that partnered w/ Sandia to evaluate their plasma ignition systems for advanced engine combustion
- **Action**: Ongoing evaluation plasma ignition systems
  - Engine tests demonstrated a 17% improvement in fuel economy
- Plasma ignition systems augment ignition chemistry and improves combustion efficiency
  - Sandia partnership has accelerated technology commercial readiness
  - TPS has developed a prototype system
LDRD Investments essential for new capabilities

Laboratory Directed Research and Development enables capability development
$13M in last 10 years

- New High-Speed Imaging
- First high-speed tomographic particle image velocimetry measurements in flames reveal 3-D structure and dynamics of flow field in turbulent jet flames.

10 kHz Tomo-PIV and OH-LIF Imaging of Turbulent Jet Flame (blue = strain-rate isosurfaces)
Cyclopentanone is a potential fuel molecule produced by fungal decomposition of cellulose has strong potential as “high octane” fuel or blend component for boosted SI engines ⇒ to prevent knock
A Comparison of Combustion Dynamics

Fundamentally different combustion dynamics require different fuel properties

- Spark ignition (gasoline)
- Kinetically controlled combustion
- Compression ignition (diesel)
Current Fuels Constrain Engine Design

Engine: Ford Ecoboost 1.6L 4-cylinder, turbocharged, direct-injection, 10.1 CR
Source: C.S. Sluder, ORNL
Accelerating the Path to Economic and Sustainable Fuels and Vehicles (Optima)
Stakeholder Group
Open Collaboration - Livermore Valley Open Campus

A joint initiative of Lawrence Livermore National Lab and Sandia National Labs

Open Campus Attributes

- Campus-like environment with collaborative space
- Ready access for all partners, including foreign nationals
- Expansion of academic programs
- Access to world-renown facilities and resources
- Synergistic with 4th Bay Area innovation node
Questions?
In 2003 GM signed an MOU with Caterpillar, Cummins, Chrysler (then DaimlerChrysler), Detroit Diesel, Ford, GE Global Research, International, John Deere, Mack Trucks, and ANL, LLNL, LANL, ORNL, and SNL. This formed the basis for the Advanced Engine Combustion MOU working group that continues to this day.

CRADA with GM to investigate flow and mixing processes. The working group associated with this CRADA merged into the Cummins NOx CRADA working group in 1996.


GM and Sandia collaborated in 2008 to produce a joint Biomass Deployment Study, which concluded that 90 billion gallons of fuel ethanol could be reproduced annually with enduring government and technical progress.

Continued with significant GM input into the development of a 2-stroke engine facility and research program in the late 1980’s.

Collaborative & WFO work with GM has led to multiple joint publications, and 1 SAE award.

WFO has been renewed annually through 2014, although the focus changed with GM interests and priorities.

The CRF relationship with GM since the 1970’s, beginning with the DISC (Direct Injection Stratified Charge).

Impact: Identification of sources of HC and CO allow GM to design mitigation strategies.

Sandia – GM Partnership Timeline

1970’s
Continued with significant GM input into the development of a 2-stroke engine facility and research program in the late 1980’s.

1980’s
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1990’s
GM and Sandia collaborated in 2008 to produce a joint Biomass Deployment Study, which concluded that 90 billion gallons of fuel ethanol could be reproduced annually with enduring government and technical progress.

2000’s

2010’s
Collaborative & WFO work with GM has led to multiple joint publications, and 1 SAE award.

WFO has been renewed annually through 2014, although the focus changed with GM interests and priorities.
Consistent partnerships and support

Visiting researchers contribute to intellectual vitality of BES Programs

Technology Partners focused on industry challenges

Approximately $32M Annually
ECN Data is Widely Utilized by Industry

Active voluntary experimental and modeling participation worldwide

Top Ten
United States
Germany
Italy
India
China
Japan
France
United Kingdom
Spain
Australia
Sandia’s History

Exceptional service in the national interest

- July 1945: Los Alamos creates Z Division
- Nonnuclear component engineering
- November 1, 1949: Sandia Laboratory established

In my opinion you have here an opportunity to render an exceptional service in the national interest.
Product Development Timing Must Be Accelerated to Meet Energy Goals
Research Approach

Closely coupled in-cylinder experiments and high fidelity-simulation

- Laser-based optical diagnostics.
- Optically accessible, real engine conditions:
  - Pistons
  - Cylinder liner / spacer plates
  - Exhaust ports
- Simulation
  - CFD collaboration with partners
  - Developing next-generation simulation tools for engines (Large Eddy Simulation – LES)
- Research has impacted engine design by providing:
  - Accurate understanding for engine designers
  - Computational design tools
CRF Awards

Lyle Pickett named Fellow of Society of Automotive Engineers

David Osborn received Lockheed Martin NOVA Award

Magnus Sjoberg receives SAE Oral Presentation Award

Hope Michelsen inducted into Alameda County Women’s Hall of Fame

Dave Chandler elected as Chair of the American Physical Society Division of Chemical Physics

Craig Taatjes wins Polanyi Medal

CRF Article chosen by The Journal of Chemical Physics to Commemorate 80th Anniversary

Two CRF papers named Distinguished for 34th International Symposium on Combustion

CRF researchers awarded the David A. Shirley Award for Outstanding Scientific Achievement
Formation of the Spray Combustion Consortium (SCC)

Delivering Experimentally-Validated, Predictive Nozzle Flow Models and Understanding

Injector nozzle flow → Spray formation, Vaporization, Fuel-air mixing → Fuel-air mixing → Combustion: Spark or compression ignited
Back-up
CRF Publication & Citation Chart

Citations

Publications
Cross-cutting

Potential

EERE
Science
Fossil
ARPA-E

USDA
Industry Alliances

• 116 partnership agreements with industry partners over lifetime of CRF (1980-present)
  – 52 Cooperative Research and Development Agreements
  – 64 Strategic Partnership Projects (formerly Work For Others), netting ~$16 million to support further research

• Continued and repeated partnerships with leading industry corporations
  – General Motors, Ford, GE, Whirlpool, Cummins, Caterpillar, Boeing

• Sustained impact on U.S. based small businesses through SBIR grants and research collaborations
Strategic Partnership Projects

- 64 SPPs with industry partners since 1997
- SPPs brought in ~$16 million to support further research at the CRF
- Notable projects currently funding bleeding edge combustion research:
  - $1.8 million from Caterpillar to evaluate advanced combustion technology in an optical engine
  - $1.2 million from GM to improve the emissions and efficiency of light-duty diesel engines
  - $1.8 million from Chevron to extend HCCI operating range using advanced petroleum-base fuels
CRF Granted Patents

- 58 total patents since 1989
- Patents in last 10 years:

<table>
<thead>
<tr>
<th>Invention Title</th>
<th>Issue Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat Exchanger Device and Method for Heat Removal or Transfer</td>
<td>3/24/2015</td>
</tr>
<tr>
<td>Bulk Synthesis of Nanoporous Palladium and Platinum Powders</td>
<td>4/15/2014</td>
</tr>
<tr>
<td>Dual-Etalon Cavity Ring-Down Frequency-Comb Spectroscopy</td>
<td>4/8/2014</td>
</tr>
<tr>
<td>Rotary Electrical Contact Device and Method for Providing Current to and/or from a Rotating Member</td>
<td>11/19/2013</td>
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<tr>
<td>Heat Exchanger Device and Method For Heat Removal or Transfer</td>
<td>9/20/2013</td>
</tr>
<tr>
<td>Improved Multidimensional Bioseparation with Modular Microfluidics</td>
<td>8/27/2013</td>
</tr>
<tr>
<td>MOBILE LIGHTING APPARATUS</td>
<td>5/14/2013</td>
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<tr>
<td>Complex Admixtures of Clathrate Hydrates in a Water Desalination Metho</td>
<td>7/14/2009</td>
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<tr>
<td>Mid-Based Sensors with Hydrogen Selectivity</td>
<td>3/11/2008</td>
</tr>
<tr>
<td>Fast Time-Correlated Multi-Element Photon Detector and Method</td>
<td>12/18/2007</td>
</tr>
<tr>
<td>Method for Control of NOx Emissions from Combustors Using Fuel Dilution</td>
<td>1/16/2007</td>
</tr>
<tr>
<td>Fuel Mixture Stratification as a Method for Improving Homogeneous Charge Compression Ignition Engine Operation</td>
<td>10/31/2006</td>
</tr>
<tr>
<td>Apparatus for Measuring the Concentration of a Species at a Distance</td>
<td>4/11/2006</td>
</tr>
<tr>
<td>Axially Tapered and Bilayer Microchannels for Evaporative Cooling Devices</td>
<td>10/4/2005</td>
</tr>
<tr>
<td>Method for Measuring the Rate of Cell Reproduction by Analysis of Nanoliter Cell Samples</td>
<td>4/26/2005</td>
</tr>
</tbody>
</table>
Cooperative Research & Development Agreements

- 52 CRADAs since 1992
- CRADAs in last 10 years:

<table>
<thead>
<tr>
<th>Partner</th>
<th>Title</th>
<th>Actual Funds-In LTD</th>
<th>Execution Date</th>
<th>Expiration Date</th>
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<tbody>
<tr>
<td>General Electric Company</td>
<td>Gas Turbine Diagnostics</td>
<td>$50,000</td>
<td>8/31/2013</td>
<td>11/30/2013</td>
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<tr>
<td>General Motors</td>
<td>Sandia/General Motors Liaison Exchange</td>
<td>$0</td>
<td>10/11/2010</td>
<td>10/11/2012</td>
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<tr>
<td>The Boeing Company</td>
<td>Advanced Materials</td>
<td>$103,000</td>
<td>8/17/2010</td>
<td>12/17/2010</td>
</tr>
</tbody>
</table>
Next Generation Engines for Future Fuels

A collaboration with industry, national labs and universities to move engine development forward

• Advanced lean/dilute combustion strategies for enabling high-efficiency, low-emission engines.
  – SI, Diesel, and Low-Temperature Combustion (HCCI, PCCI, ...)

• Future fuels
  – adv. petroleum
  – bio-fuel,
  – gas-to-liquid,
  – oil sand and shale
  – natural gas & H2

• Next generation computational tools
  – massively parallel machines

Time varying, 3 million cell grids
Licensing CHEMKIN to Reaction Design

A Small Business Success Story

• CHEMKIN, the gold standard for modeling gas-phase and surface chemistry, created and copyrighted at Sandia in 1980
  – Enabled significant strides in the modeling of a variety of complex chemical processes
  – Used in the microelectronics, combustion, and chemical processing industries

• Reaction Design, a small business based in San Diego, founded as the exclusive developer and licensing partner for CHEMKIN in 1997
  – Sandia tech transfer, technical line, and licensee collaborated over 15+ years to ensure continued success

• Sandia’s longest continuous license enabled a small start up to become a multi-million dollar company
  – Royalties brought in to Sandia: over $1.7 million and growing
  – Reaction Design total sales: over $40 million, 1/3 of sales directly from licensed Sandia IP
  – Reaction Design sold to ANSYS for $19.25 Million in January of 2014
    • ANSYS to continue licensing from Sandia
A Pathway to Efficiency

Our DOE research focuses on lean/dilute combustion strategies

- Stratified Direct-Injection Spark Ignition (DISI)
  - Stochastic processes (misfire, super-knock)
- Advanced Diesel Combustion
  - Exhaust Gas Recirculation (EGR), high pressure and multi-pulse injection, soot-free combustion,…
- Low Temperature Combustion (LTC)
  - Diesel LTC (PCCI, PPCi, PCI, MK,…)
  - Gasoline LTC (LTGC, HCCI)
  - Challenges
    - Combustion timing
    - Load range
    - Heat release rate
    - Transient control
    - HC and CO emissions
BES and VT Programs Developing & Applying First Principles Large Eddy Simulation Capabilities

- Goal ... use “high-fidelity” LES and “first-principles” models to complement key experiments, bridge gap between basic/applied research
  - Detailed simulations that match geometry, operating conditions (i.e., high Re)
  - Retain full system coupling and incorporate detailed physics
  - Validation using available data, then joint analysis ...
    - Fundamental insights not available from experiments alone
    - Data reduction aimed at affordable models for engineering

- Use high-performance computing as enabler (both local and DOE platforms)
Visitor Stats

CRF Visitor Stats

Domestic & International Visitors

- Academy
- Industry
- Other Research Institutes
The Future of Fuels

Sandia is developing the science base for the next generation of engines and fuels

- Advanced combustion strategies for enabling high-efficiency, low-emission engines (with potential for 4 MBD reduction in oil use).
  - Low temperature combustion (HCCI, PCCI, ...)

- Future fuels
  - bio-fuel,
  - gas-to-liquid,
  - oil sand and shale
  - ...

- Next generation computational tools
  - Massively parallel machines

Time varying, 3 million cell grids
Methods of Delivering Impact

• Licensing, Patents, & Copyrights
  – 58 issued patents

• Publications & Conference Presentations
  – Primary approach to broad dissemination of our work
  – Outstanding recognition, awards, citations
    • 54 publications in *Combustion and Flame* (419 cites)
    • 47 publications in *Proceedings of the Combustion Institute* (778 cites)

• Collaborative Networks – Open collaboration

• Industrial Alliances
  – Funded Research – Projects with GM, Caterpillar, Ford, Toyota, Chevron, Aramco, TACOM, GE
  – Strategic Alliances – GM and GE— influence LDRD’s

• Visitors – Two-way short (weeks) and longer term (months) R&D

• Post Docs and Student Interns – large numbers, exceptional opportunities
Engine Combustion Research Program

- Mission: Provide the combustion and emission knowledge-base needed by industry to develop high-efficiency, clean engines for future fuels.
- Primary sponsor is DOE Office of Vehicle Technologies (VT) ($7M)
- Industry and other sponsors – Leveraging research: GM, Ford, Caterpillar, Toyota, Chevron, U.S. Army, and LDRDs. ($1.5M).
- Research directions are aligned with DOE/industry USDRIVE and 21st Century Truck roadmaps.
- Strong collaboration with industry, universities, and national labs (since the start).
- >30 PIs, technologists, post docs, and visiting researchers
  - Staff deeply engaged in leadership roles in the field.
  - 6 SAE Fellows and 1 ASME Fellow
Diagnostic development for next-generation gas turbine combustion

- **Motivation**: GE Power & Water solicited Sandia’s advice on *in situ* diagnostics that could detect CO sources within their ground-based gas turbine combustors.

- **Action**: Transferred CO laser induced fluorescence diagnostic to GE Global Research
  - *In situ* diagnostic that provides spatially & temporally resolved CO information
  - Low CO detection limits (75 ppm) at relevant conditions
  - GE researcher spent 2-months as a Sandia visitor

- **Impact**: GE leveraged the diagnostic in their gas turbine test rigs to:
  - Validate numerical simulation results
  - Improve their understanding of CO formation & burnout processes
  - Identify CO emission sources
  - *Develop CO reduction strategies that led to cleaner and more efficient gas turbine engines*
Our Unique Core Capabilities and Expertise for the DOE/VT program

Low-temperature gasoline combustion
- fundamentals:
  PI – John Dec

Automotive low-temperature gasoline combustion:
PIs – Dick Steeper and Isaac Ekoto

Diesel/Low-temperature diesel combustion – heavy-duty:
PI – Mark Musculus

Diesel/Low-temperature diesel combustion – light-duty:
PI – Paul Miles

Alternative fuels – heavy-duty:
PI – Chuck Mueller

Alternative fuels – light-duty:
PI – Magnus Sjoberg

Fuel sprays:
PIs – Lyle Pickett and Scott Skeen

Large Eddy Simulation:
PIs – Joe Oefelein and Guilhem Lacaze

BES & VT
**Energy & Fuels: Institutions Ranked by Citations**

<table>
<thead>
<tr>
<th>Rank</th>
<th>Institution</th>
<th>Citations 1998-2008</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>Sandia National Labs</td>
<td>4,147</td>
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<tr>
<td>2</td>
<td>Natl. Renewable Energy Lab</td>
<td>3,773</td>
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<tr>
<td>3</td>
<td>CSIC (Spain)</td>
<td>3,678</td>
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<tr>
<td>4</td>
<td>Chinese Academy of Sciences</td>
<td>3,541</td>
</tr>
<tr>
<td>5</td>
<td>Indian Institutes of Technology</td>
<td>3,166</td>
</tr>
</tbody>
</table>

“...Among institutions ranked by total citations, none surpasses Sandia National Laboratories, with more than 4,100 citations to its 395 papers”

Approximately ½ of these citations are linked to the CRF.

http://sciencewatch.com/ana/fea/08novdecFea/
Sandia’s Advanced Engine Combustion Research Program

1975
- Laser diagnostic development and application in engines begins
- Alternative fuels research begins
- Combustion Research Facility (CRF) opens to researchers

1985
- New understanding of SI engine processes developed (knock and flame propagation)
- Introduction of realistic optical engines

1995
- New conceptual model developed and mixing physics clarified for heavy-duty diesel combustion

2005
- Comprehensive understanding of light-duty diesel combustion developed
- Cummins develops first computationally designed engine
- Pathway to full load range gasoline LTC revealed

2015
- Conceptual model for diesel-LTC developed
- Retrospective study – $70B return on less than $1B
- Engine Combustion Network - Global collaboration and leveraging
- Industry engages CRF in WFOs
- Industry engages CRF in WFOs

Energy crisis of the early 70s
- Congress establishes DOE’s Tech Transfer Initiative. Many CRADAs with industry established over next decade (e.g., GM, Ford, Caterpillar, Cummins, ...)
- DOE ECUT begins engine research.

Light-duty engine working groups with industry/national labs/universities (DISC, DHC, Knock)
- Heavy-duty diesel working group
- Sandia led Advanced Engine Combustion MOU – 21 industry and national lab partners
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1995
- Cummins develops first computationally designed engine
- High-efficiency, clean Low Temperature Combustion (LTC) research initiated

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- 1985
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Knowledge Clarified for Heavy-Duty Diesel Combustion
- New conceptual model developed and mixing physics clarified for heavy-duty diesel combustion
- Conceptual model
- Flame lift-off

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