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
Technology, Energy, and Society are Inextricably Intertwined
Today's Energy Technologies and Infrastructures are Firmly Rooted in the 20th Century

U.S. Energy Consumption by Source

Quadrillion Btu

1650 1700 1750 1800 1850 1900 1950 2000

Wind, water, wood, animals, (Mayflower, 1620)

Intercontinental Rail System, mid 1800s

Rural Electrification Act, 1935

Eisenhower Highway System, 1956

Technology, Energy, and Society are Inextricably Intertwined
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What Will the 21st Century Bring?
21st Century Science and Technology Will Exert Control at the Atomic, Molecular, and Nanoscale Levels

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

Quadrillion Btu

DOE Formed, 1977

Designer molecules

High Tc superconductors

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.

Photosystem II

2H₂O 4H⁺ + 4e⁻
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.

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…..
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

Research for a Secure Energy Future
Supply, Carbon Management, Distribution, Consumption

Decision Science and Complex Systems Science

Carbon Energy Sources
- Coal
- Petroleum
- Natural Gas
- Oil shale, tar sands, hydrates, ...

Carbon Management
- CO₂ Sequestration
  - Geologic
    - Terrestrial
    - Oceanic
- Carbon Recycle
- Global Climate Change Science

No-net-carbon Energy Sources
- Nuclear Fission
  - Nuclear Fusion
  - Renewables
    - Hydropower
    - Biomass
    - Geothermal
    - Wind
    - Solar
    - Ocean

Distribution/Storage
- Electricity Production & Grid
- Electric Storage
- Hydrogen
- Alternate Fuels

Energy Consumption
- Transportation
- Buildings
- Industry

Crosscutting – catalysis
Crosscutting – materials under extreme conditions

BRN Workshops
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 Economy**  

- **Nanoscience Research for Energy Needs**  
  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 Superconductivity**  
  BES Workshop, May 8-10, 2006

- **Basic Research Needs for Solid-state Lighting**  
  BES Workshop, May 22-24, 2006

- **Basic Research Needs for Advanced Nuclear Energy Systems**  
  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

  BES Workshop, February 21-23, 2007

- **Basic Research Needs for Electrical Energy Storage**  
  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 Energy**  
  BES Workshop, August 5-10, 2007

- **Basic Research Needs – Final Wrap-up Workshop**  
  BESAC, TBD
### The Continuum of Research, Development, and Deployment

**Grand Challenge Research**
- 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.

**Discovery Research**
- Basic research for fundamental new understanding on materials or systems that may revolutionize or transform today’s energy technologies.

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

**Applied Research**
- 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

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

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**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
(BES) Basic Research Needs Workshops
(BES, BESAC, …) Tools and Facilities in Support of Research
Technology Office/Industry Roadmaps
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
- Printed copies and CDs now available.
Workshop Details

**Novel Combustion**

**Fuel Utilization**

**Crosscut Science**

12% Government

7% Industry

42% University

39% Lab

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
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**
**Grand Challenge**

**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
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.
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
**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
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
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.
Scientific Challenges

• Four-dimensional measurement capabilities at high repetition rates
• Photophysics at high pressure and temperature
• Detecting currently inaccessible molecules
• Diagnostics for real engines
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
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
**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
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
**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**
  - Compilation of large sets of data
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
**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

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

BES

**Applied Energy Offices**

EERE
A Great Plan – Now What?

Research for a Secure Energy Future

Carbon Energy Sources
- Coal
- Petroleum
- Natural Gas
- Oil shale, tar sands, hydrates, ...

Crosscutting – catalysis
Crosscutting – materials under extreme conditions

Energy Management

Energy Consumption
- Transportation
- Buildings
- Industry

Workshops

BRN Workshops
- Crosscutting – catalysis
- Crosscutting – materials under extreme conditions

Solar
Ocean

No-net-carbon Energy Sources
Carbon Distribution/Supply, Carbon Management, Distribution, Consumption

Energy Conservation, Energy Efficiency, and Environmental Stewardship

Global Climate Change Science

CO2 Sequestration
Carbon Recycling
Geologic Terrestrial Oceanic

Decision Science and Complex Systems Science