State of Combustion Energy Frontier Research Center (CEFRC): An Annual Report to the Combustion and Fuels Community

Chung K. Law, Center Director

Fuels Summit, September 23, 2010

The Overarching Goal

The development of a validated, predictive, multi-scale, combustion modeling capability to optimize the design and operation of evolving fuels in advanced engines for transportation applications

Scientific Objectives (1/2)

- *To advance* fundamental understanding and practice of combustion and fuel science
- *To create* experimental validation platforms and databases for kinetics, thermochemistry, transport processes, and flame structure
- *To enable* automated kinetic model generation and reduction
- *To implement* validated, multi-scale, quantitative prediction methods

Scientific Objectives (2/2)

- *To establish* a knowledge highway connecting the CEFRC (Combustion Energy Frontier Research Center), academic and research institutions, and the transportation and fuel industries
- *To train* the next generation of combustion scientists

Research Strategies

1. Clearly-defined and focused scope
2. Technically-strong and balanced team
3. Tight coordination
4. Agility to exploit new opportunities
5. Identify and tackle (grand) challenge problems

Scope of the CEFRC

Combustion and Fuels Science

- High-pressure kinetics and thermochemistry
- Nonequilibrium transport
- High-pressure near-limit flames
- Turbulence-chemistry interactions
- Nanoparticle growth & oxidation

Advanced Diagnostics & Experimental Validation

- Advanced light source
- Laser diagnostics
- High-pressure reactors
- Kinetic, flame, transport data
- Emission measurements

Validated Multi-scale Predictions of Alternative Fuels

Foundation fuels (C_0-C_{16})
Synthetic fuels
Fuels from biomass

Multi-Scale Modeling

- Quantum chemistry
- Reaction dynamics
- Nanoscale transport
- DNS/LES/PDF of turbulent combustion
- Automatic mechanism generation, reduction,
- Exascale Computing

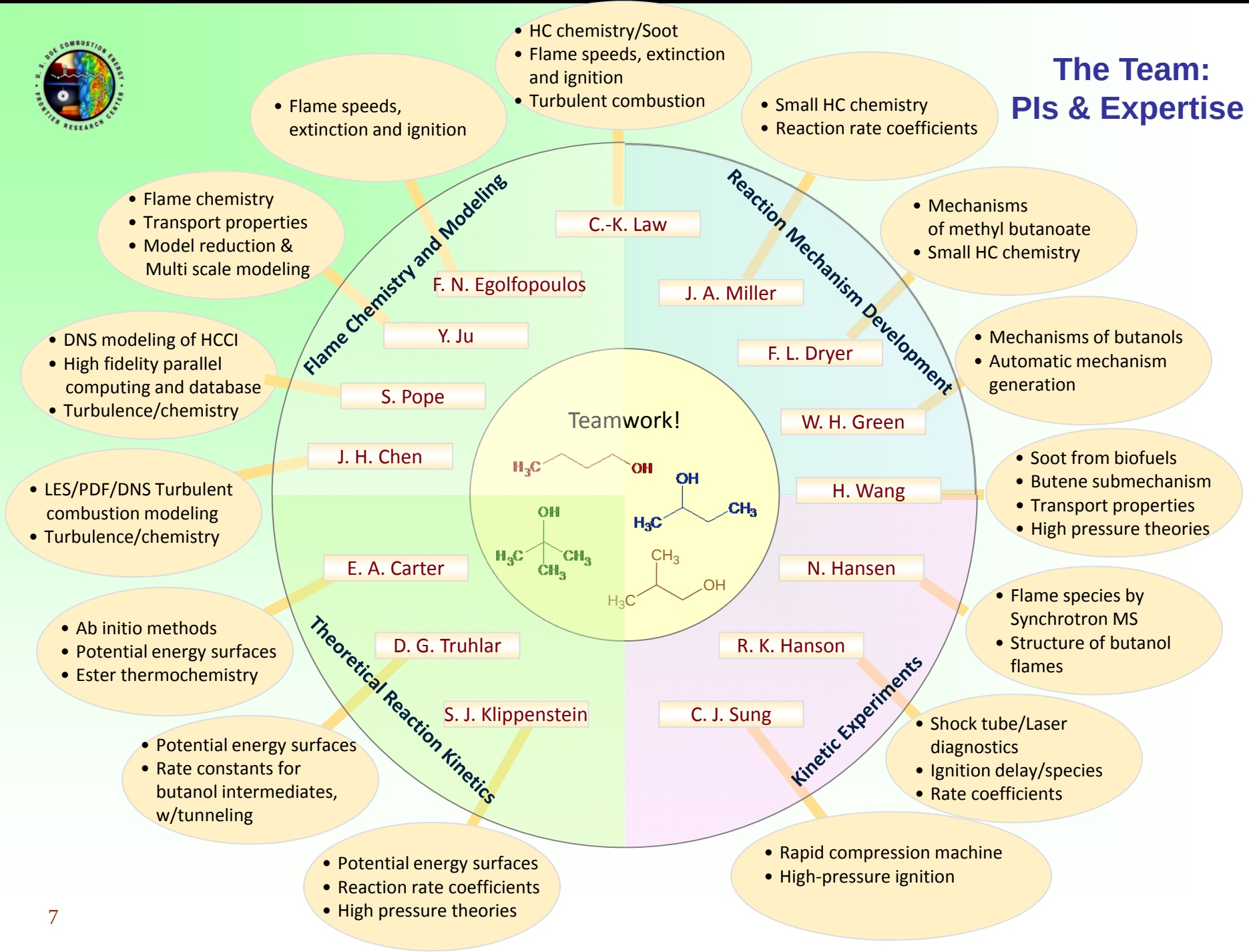
Emissions & Efficiency

- New combustion regimes
- Emissions reductions
- Science-based innovation

Knowledge Highway

- EFRC webpage (PRIME-linked)
- Seminars, workshop, conferences
- International advisory committee
- Summer school & visiting scholars
- Roving postdoctoral fellows
- Seed program for innovation

The Team: PIs & Expertise



Coordinated Approach: Common Research Thread Ties the Team Together

- The thread: Team-wide investigation based on an agreed-upon class of fuels, yielding validated reaction mechanisms that can be used in simulations of combustion in complex flows
  - Fuel selected should be relevant: practical interest, potential societal impact
  - Fuel should facilitate advances in scientific knowledge applicable to other fuels and combustion problems

First Target: Butanol as the Thread (Practical Considerations)

- Higher energy density (as compared to ethanol)
- Non-corrosive
- Same range of volatility as gasoline (b.p.: 82 – 117°C)
- High miscibility with gasoline
- Knock resistance (octane number) similar to gasoline.
- Can be made from many different types of biomass.
- n-Butanol & iso-butanol from fermentation are expected to be commercialized by BP/Dupont by 2013 through their Butamax joint venture. Several other companies also developing processes for producing butanol.

Butanol as the Thread: Scientific Considerations

- Butanol is the smallest alcohol with all three (primary, secondary, tertiary) isomeric structures.
- C4 chain long enough to display intramolecular isomerization chemistry important in larger fuels.
- Small enough that high accuracy quantum chemistry and rate calculations are feasible.
- Volatility allows experiments and detailed analytical chemistry techniques which are impossible for heavy biofuels.

Technical Accomplishments

- Progress to be reported by the 15 Principal Investigators in three disciplinary working groups (DWGs)
  - Chemistry: Theory
  - Chemistry: Experiment and Mechanisms
  - Transport and chemistry
- Journal publications (Inaugural year)
  - 7 appeared
  - 30 in press

Outreach Programs

1. Combustion Energy Research Fellows
2. Summer School
3. Newsletter
4. Website

1. Combustion Energy Research Fellows

- The Program
  - Four to five appointments per year for two-year appointment, co-sponsored by two (or more) PIs
  - Roving assignment on-site of sponsoring PIs, working on joint projects
  - 25% of total research budget

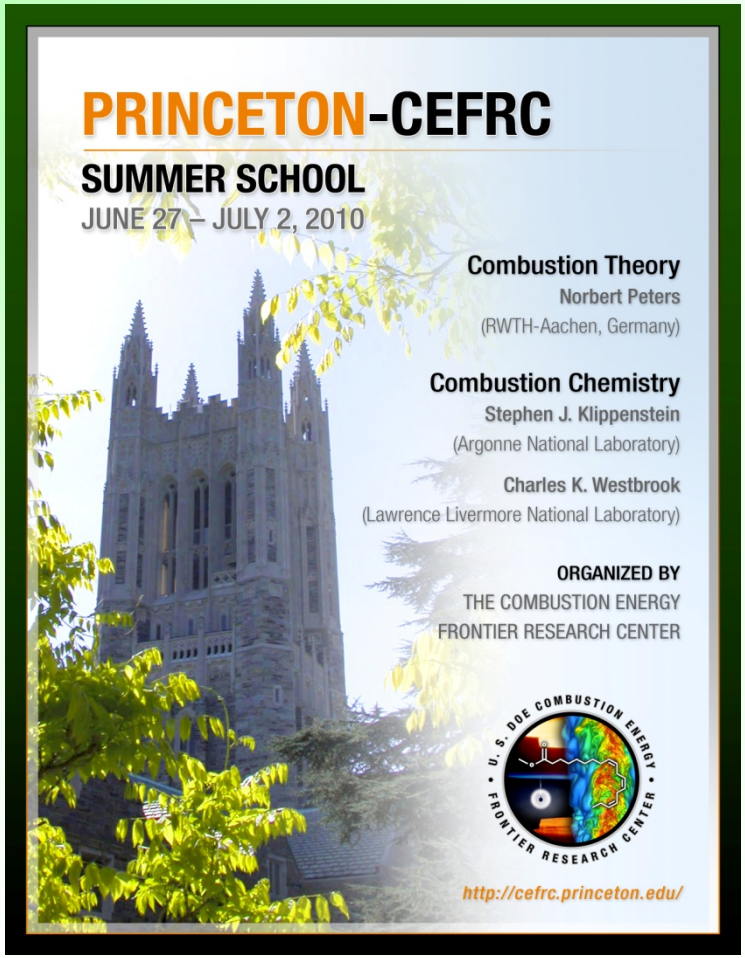
Merits of the Fellows Program

- Ensures a robust program
  - Facilitates collaboration between sponsoring PIs
  - Responding to new developments to ensure nimbleness
  - High-risk, high-payoff projects
  - Competition for slots ensures robust program
- Attraction to candidates
  - Benefited from cross-disciplinary collaboration
  - Benefits career development
  - Moderately attractive compensation

2. Summer School Program

- Motivation:
  - A modern combustion researcher must be expert in either fluid mechanics or chemical kinetics, and reasonably conversant in the other discipline. Breakthrough research could require knowledge in both disciplines
  - It is quite difficult, and rare, for an institution to be able to offer advanced courses in both disciplines
  - Intense instruction by world-class researchers who are excellent lecturers can greatly enhance comprehensiveness in knowledge

Summer School Announcement Flyer



Program Overview

- Two 15-hour courses, on combustion physics and combustion chemistry, are offered over five days: two three-hour lectures in the morning and afternoon each day
- Students live in single, air-conditioned dormitory rooms and have their meals together in the cafeteria
- Room & board covered for students
- Non-students have the option of living and eating off campus

2010 Academic Program

- Combustion Theory (15 hours)
  - Instructor: Norbert Peters (RWTH Aachen, Germany)
- Combustion Chemistry: Chemical kinetics and kinetic modeling (6 hours)
  - Instructor: Charles K. Westbrook (Lawrence Livermore Lab)
- Combustion Chemistry: *Ab Initio* theoretical chemical kinetics (9 hours)
  - Instructor: Stephen J. Klippenstein (Argonne National Lab)

Industrial Sponsorship

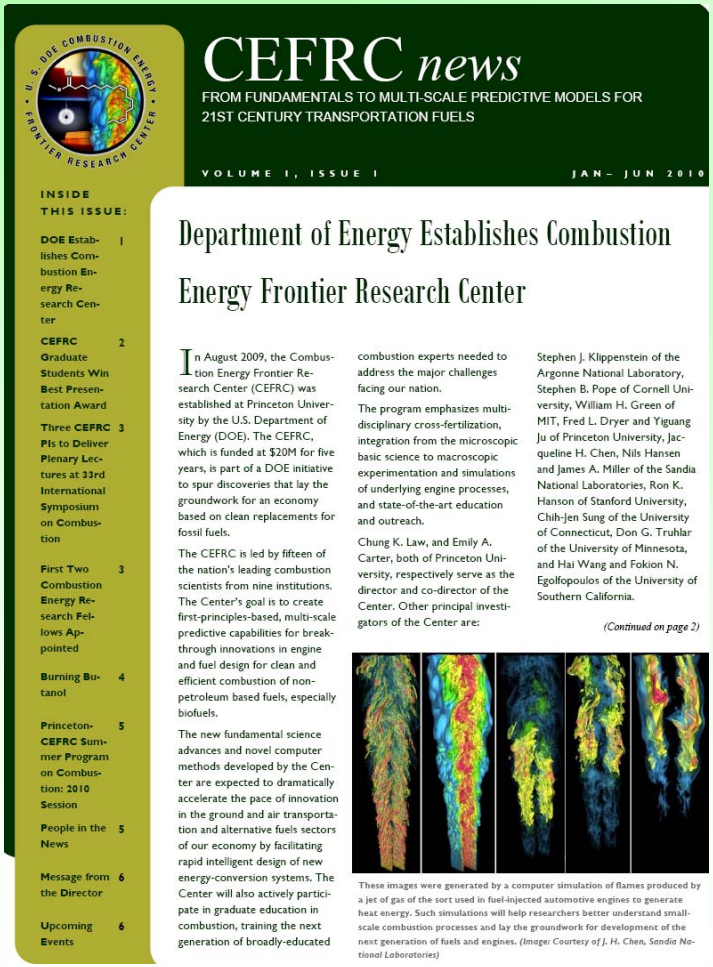
- Funding from an industrial donor allowed purchase of commemorative items for participants

Very Satisfactory Outcome

- Extremely enthusiastic response
  - Planned: 25 – 50 students
  - Applicants: > 130
  - Admitted:120 (about 90 students & 30 post-docs and research staff from government & industrial labs), limited by size of lecture facility
- Students enjoyed the lectures as well as the networking opportunities with their peers
- A CEFRC Facebook Group "2010 Princeton-CEFRC Summer School" with 91 active members

120+ Smiling Faces

3. CEFRC (Biannual) Newsletter



CEFRC *news*

FROM FUNDAMENTALS TO MULTI-SCALE PREDICTIVE MODELS FOR 21ST CENTURY TRANSPORTATION FUELS

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Department of Energy Establishes Combustion Energy Frontier Research Center

In August 2009, the Combustion Energy Frontier Research Center (CEFRC) was established at Princeton University by the U.S. Department of Energy (DOE). The CEFRC, which is funded at $20M for five years, is part of a DOE initiative to spur discoveries that lay the groundwork for an economy based on clean replacements for fossil fuels.

The CEFRC is led by fifteen of the nation's leading combustion scientists from nine institutions. The Center's goal is to create first-principles-based, multi-scale predictive capabilities for breakthrough innovations in engine and fuel design for clean and efficient combustion of non-petroleum based fuels, especially biofuels.

The new fundamental science advances and novel computer methods developed by the Center are expected to dramatically accelerate the pace of innovation in the ground and air transportation and alternative fuels sectors of our economy by facilitating rapid intelligent design of new energy-conversion systems. The Center will also actively participate in graduate education in combustion, training the next generation of broadly-educated combustion experts needed to address the major challenges facing our nation.

The program emphasizes multidisciplinary cross-fertilization, integration from the microscopic basic science to macroscopic experimentation and simulations of underlying engine processes, and state-of-the-art education and outreach.

Chung K. Law, and Emily A. Carter, both of Princeton University, respectively serve as the director and co-director of the Center. Other principal investigators of the Center are: Stephen J. Klippenstein of the Argonne National Laboratory, Stephen B. Pope of Cornell University, William H. Green of MIT, Fred L. Dryer and Yiguang Ju of Princeton University, Jacqueline H. Chen, Nils Hansen and James A. Miller of the Sandia National Laboratories, Ron K. Hanson of Stanford University, Chih-Jen Sung of the University of Connecticut, Don G. Truhlar of the University of Minnesota, and Hai Wang and Fokion N. Egolfopoulos of the University of Southern California.

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These images were generated by a computer simulation of flames produced by a jet of gas of the sort used in fuel-injected automotive engines to generate heat energy. Such simulations will help researchers better understand small-scale combustion processes and lay the groundwork for development of the next generation of fuels and engines. *(Image: Courtesy of J. H. Chen, Sandia National Laboratories)*

Message from the Director

Dear Colleagues:

With this issue we launch the Newsletter of the Combustion Energy Frontier Research Center (CEFRC). This Newsletter will be issued biannually, reporting on the activities of the Center as well as other news on combustion energy research that are of interest to you.

It was almost a year ago that the Department of Energy announced the establishment of 46 Energy Frontier Research Centers. This substantive move by the Obama administration to tackle the twin issues of energy sustainability and climate change was enthusiastically received by the scientific community at large. The fifteen principal investigators of the Center, while similarly joyous with given the opportunity to participate in such a major and concerted effort, also felt the burden of responsibility, especially in recognizing that our Center is the only one on combustion selected for funding.

The Center was officially established on August 1, 2009. During the past eight months we have met formally as a group and informally at conferences as opportunities arose. We have also conducted monthly telecons. In addition to reporting by individual PIs on their research progress, the discussions have also emphasized on three issues: (1) how we can coordinate and "glue" our research efforts leading to a unified outcome; (2) identify and then tackle the grand challenges in combustion research; and (3) how to maximize the impact of our various outreach programs.

Regarding a unified research effort, we have decided to initially use butanol as a target biofuel, based on which each PI would conduct his/her research. In this issue you will find a report by Professor Bill Green on our efforts towards developing reaction mechanisms for butanol oxidation.

Regarding the grand challenges, we have come up with a number of candidates, and are still weighing their relative scientific and technological importance. We shall present the list to the community when it is fully compiled. In the meantime, we invite you to suggest such grand challenge problems that could revolutionize combustion science and technology.

Progress on the outreach programs has been very satisfying. For the CEFRC Energy Fellows program, we have already finished two rounds of selection; you will find a write-up on the two appointees from the first round here. You will also find a write-up on the Summer Program, which has attracted a large number of applicants, way beyond our initial expectation. Being limited by facility, eventually we were able to accept 120 participants that consist of 90 graduate students and 30 researchers. We look forward to welcoming them to Princeton in late June, and have every reason to expect that it will be a stimulating and rewarding experience for them.

We have also included news items on some of our PIs and students. We hope you find them informative.

Finally, I am pleased to report that preparation for the local program of the 33rd Combustion Symposium is shaping up nicely. Following the official site visit by President Charles Westbrook of the Combustion Institute and the Technical Program Chairs Professors Philippe Dagaut and Paul Ronney, I was in Beijing last month to provide some additional coordination. After discussing with Professor Qiang Yao, Chair of the Local Program Committee, and his colleagues, I was very much impressed with the care and thoroughness with which various tasks and events are planned.

I wish you all the best in your research, and look forward to seeing you in Beijing in August.

Chung K. Law

Upcoming Events

JUNE 2010

2010 Princeton-CEFRC Summer Program on Combustion
June 27— July 3, 2010, Princeton, New Jersey

AUGUST 2010

33rd International Symposium on Combustion
August 1— August 6, 2010, Beijing, China

SEPTEMBER 2010

Multi-Agency Coordinating Committee for Combustion Research (MACCCR) Fuels Research Review
September 20 — September 23, 2010, Princeton, New Jersey

2nd Annual Meeting of the Combustion Energy Frontier Research Center
September 23—September 24, 2010, Princeton, New Jersey

4. CEFRC Website
http://cefrc.princeton.edu

Web Lectures

- All Summer School lectures were professionally taped and are publicly available through our website at http://cefrc.princeton.edu/news--publications/news-articles/2010-princeton-cefrc-summer-school-lecture-videos.aspx and soon to be available to all with unrestricted access via iTunes University

Some CEFRC Recognitions

- At 33rd International Combustion Symposium in Beijing:
  - 18 CEFRC-supported papers were presented and will be published in the Proceedings
  - CEFRC PIs (Chen, Hanson, Wang) delivered 3 of the 5 plenary lectures, including the opening Hottel Lecture by Hanson
- Election to national academies
  - Law: American Academy of Arts and Sciences (2010)
  - Pope: National Academy of Engineering (2010)
  - Truhlar: National Academy of Sciences (2009)
- Major energy-related appointments
  - Carter: Founding Director, Andlinger Center for Energy and the Environment, Princeton University
  - Law: Founding Director, Center for Combustion Energy, Tsinghua University

Schedule of Technical Program

Fuels-Summit Conference

- Thursday Day Session
  - Progress Report by DWGs
    - Chemistry – Theory
      - Carter, Truhlar, Miller, Klippenstein, Green
    - Chemistry – Experiment and mechanisms
      - Hanson, Dryer, Sung, Hansen, Wang
    - Chemistry and transport
      - Law, Egolfopoulos, Ju, Chen, Pope
  - Poster session during lunch hour
  - Open Discussion: Role of CEFRC in fuels research

CEFRC Conference

- Thursday Evening Session
  - Discussing challenging problems
- Friday Session
  - Future plans by disciplinary working groups (DWGs)
  - Informal intra- and inter-DWG discussions
  - Report from the International Advisory Committee (Sarofim)