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
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

PRINCETON-CEFRC
SUMMER SCHOOL
JUNE 27 – JULY 2, 2010

Combustion Theory
Norbert Peters
(RWTH-Aachen, Germany)

Combustion Chemistry
Stephen J. Klippenstein
(Argonne National Laboratory)
Charles K. Westbrook
(Lawrence Livermore National Laboratory)

ORGANIZED BY
THE COMBUSTION ENERGY FRONTIER RESEARCH CENTER

http://cefrc.princeton.edu/
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

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 $30M for five years, is part of a DOE initiative to spur discoveries that bolster the technology and science needed for a sustainable transportation sector.

CEFRC is led by fifteen of the nation’s leading combustion scientists from nine institutions. The Center’s goal is to create a unified, cross-disciplinary research program in advanced combustion technologies, focusing on the development of new fuels and energy conversion systems. The Center, led by Professor Stephen J. Kippelen of Argonne National Laboratory, currently has over 100 researchers working on projects in areas such as coal combustion, biomass conversion, and catalysis.

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 the Combustion Energy Frontier Research Centers. This initiative was a major step forward in the field of combustion energy research, and it was one of the major factors in attracting the support of the DOE.

The Center is working on a range of projects, from the development of new fuels to the optimization of existing engines. I am confident that we will continue to make significant progress in these areas, and I look forward to sharing this progress with you in future issues of the newsletter.

Best regards,

[Director's Name]

Upcoming Events

**JUNE 2010**
- **Princeton/CEFRC Summer Program on Combustion**

**AUGUST 2010**
- **3rd International Symposium on Combustion**
  - August 9–August 14, 2010, Beijing, China
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-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

• 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)