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

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

Multi-Scale Modeling
- Quantum chemistry
- Reaction dynamics
- Nanoscale transport
- DNS/LES/PDF of turbulent combustion
- Automatic mechanism generation, reduction, Exascale Computing
The Team: PIs & Expertise

C.-K. Law
F. N. Egolfopoulos
J. A. Miller
F. L. Dryer
W. H. Green
H. Wang
N. Hansen
S. J. Klippenstein
D. G. Truhlar
E. A. Carter
J. H. Chen
S. Pope
Y. Ju

Theoretical Reaction Kinetics

Flame Chemistry and Modeling

HC chemistry/Soot
Flame speeds, extinction and ignition
Turbulent combustion

Small HC chemistry
Reaction rate coefficients

Mechanisms of methyl butanoate
Small HC chemistry

Mechanisms of butanols
Automatic mechanism generation

Soot from biofuels
Butene submechanism
Transport properties
High pressure theories

Flame species by Synchrotron MS
Structure of butanol flames

Shock tube/Laser diagnostics
Ignition delay/species
Rate coefficients

Rapid compression machine
High-pressure ignition

The Teamwork!

DNS modeling of HCCI
High fidelity parallel computing and database
Turbulence/chemistry

LES/PDF/DNS Turbulent combustion modeling
Turbulence/chemistry

Ab initio methods
Potential energy surfaces
Ester thermochemistry

Potential energy surfaces
Rate constants for butanol intermediates, w/tunneling

Flame speeds, extinction and ignition

Turbulent combustion

Model reduction & Multiscale modeling

Transport properties

HC chemistry

The Team:

PIs & Expertise:

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E. A. Carter
J. H. Chen
S. Pope
Y. Ju
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

Inside this issue:
- DOE
- Industry
- Combustion Research
- Energy Frontier Research Centers (EFRCs)
- CEFRC
- Technical Innovations
- CEFRC News
- From Fundamentals to Multiscale Predictive Models for 21st Century Transportation Fuels

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 effort to spur discoveries that lay the groundwork for an economy based on clean replacements for fossil fuels.

The CEFRC is led by three of the nation's leading combustion scientists from three disciplines:
- Stephen J. Kaye of the Argonne National Laboratory
- Stephen R. R gold of Tel-Aviv University, Israel
- William W. Green of METU, Turkey

The Center's goal is to create the fundamental understanding needed to design combustion systems that produce clean energy efficiently.

CEFRC News

From Fundamentals to Multiscale Predictive Models for 21st Century Transportation Fuels

Volume 1, Issue 1

JAN-JUN 2010

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 bimonthly, reporting on the activities of the Center as well as news on combustion energy research that is of interest to you.

It is almost a year ago that the Department of Energy announced the establishment of 10 Energy Frontier Research Centers. This initiative, led by the Office of Science and sponsored by the Office of Basic Energy Sciences, is designed to bring together scientists and engineers from academia, industry, and government to address fundamental challenges in key areas of energy research.

The CEFRC is one of these centers, and its mission is to develop a fundamental understanding of the science and technology of combustion processes that can enable the design of more efficient and environmentally friendly energy systems.

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Upcoming Events

JUNE 2010
- 2010 Princeton-CEFRC Summer Program on Combustion
  June 27 - July 5, 2010, Princeton, New Jersey

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

Programs and events are subject to change. Check the website for the latest information.

Cheng K. Law
Director, CEFRC
Princeton University

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Cheng K. Law
Director, CEFRC
Princeton University
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

• 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)