



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

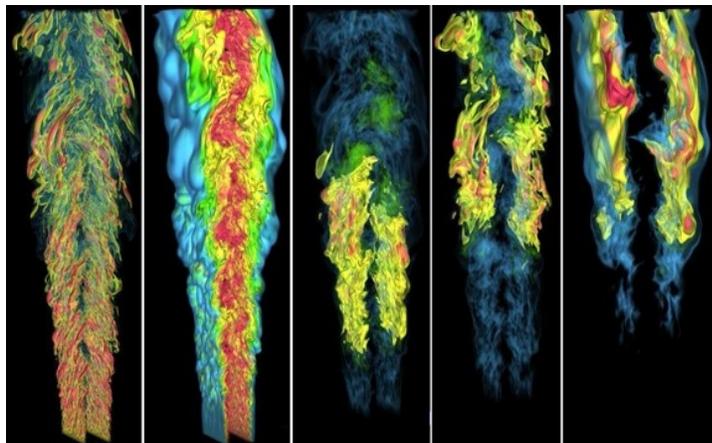
combustion experts needed to address the major challenges facing our nation.

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.

(Continued on page 2)



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)

Combustion Energy Frontier Research Center

(Continued from page 1)

Oversight of the Center is provided by a high-level International Advisory Committee, consisting of twelve members who provide critique and guidance to the CEFRC's research program. These members are:

David Clary (Oxford, UK), Med Colket (United Technologies), Michael Drake (GM Research), John Farrell (ExxonMobil), Katharina Kohse-Hoinghaus (Universität

Bielefeld, Germany), Marsha I. Lester (University of Pennsylvania), Norbert Peters (RWTH Aachen, Germany), Michael Pilling (University of Leeds, UK), Adel Sarofim (University of Utah), Wing Tsang (NIST), Luc Vervisch (INSA-Ruen, France), and Charles K. Westbrook (Lawrence Livermore National Laboratory and President of the Combustion Institute).



Chung K. Law
Director



Emily A. Carter
Co-Director



Jacqueline H. Chen



Fredrick L. Dryer



Fokion N. Egolfopoulos



William H. Green



Nils Hansen



Ronald K. Hanson



Yiguang Ju



Stephen J. Klippenstein



James A. Miller



Stephen B. Pope



Chih-Jen Sung



Donald G. Truhlar



Hai Wang

CEFRC Graduate Students Win Best Presentation Awards



*The 2nd International Forum on
Multidisciplinary Education and Research for Energy Science*

December 12-16, 2009, Okinawa, Japan

CEFRC Principal Investigator **Professor Yiguang Ju** of Princeton University, along with five of the University's graduate students, were invited to speak at the "2nd International Forum on Multidisciplinary Education and

Research for Energy Science". This forum, which is sponsored by the Global COE program "Multidisciplinary Education and Research Center for Energy Science" at the Tokyo Institute of Technology, was conducted in Okinawa, Japan on December 12-16, 2009.

Professor Ju discussed "The Challenges and Advances of Combustion Research for Renewable Transportation Fuels". Congratulations to graduate students Michael Burke and Yuan Xu for "Best Presentation Awards".



Three CEFRC Principal Investigators to Deliver Plenary Lectures at the 33rd International Symposium on Combustion

The 33rd International Symposium on Combustion, organized by the Combustion Institute, will be hosted by Tsinghua University in Beijing, China on August 1-6, 2010.

At this widely-attended biennial symposium, three of the five plenary lectures will be delivered by principal investiga-

tors from the CEFRC. In the opening "Hottel Lecture", **Professor Ronald K. Hanson** of Stanford University will present modern techniques for studying chemical kinetics.

Dr. Jacqueline H. Chen of Sandia National Laboratories will discuss turbulent combustion modeling, and **Professor Hai Wang** of the University of

Southern California will address combustion-generated particulates: soot and material synthesis.

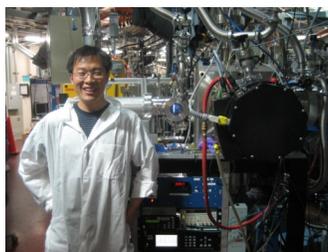
The other two plenary lectures will be delivered by Dr. Marcus Alden of the Lund Institute of Technology and Professor Kaoru Maruta of Tohoku University.

First Two Combustion Energy Research Fellows Appointed

Two-year positions as Combustion Energy Research Fellows are available for co-sponsored post-doctoral or more senior research associates to perform joint, high-risk, high-payoff research projects with at least two principal investigators of the Center in their respective locations. These "roving post doctoral" positions are designed to provide synergy and continuous rejuvenation of research directions. They are highly competitive appointments and offer rigorous training for the next generation of leaders in combustion science and technology. We anticipate four to five appointments being offered each year, each for a two-year tenure.

In January 2010, the CEFRC announced the appointment of the Center's first Combustion Energy Research Fellows, Dr. Bin Yang and Dr. Andrew Garmory.

Dr. Bin Yang, formerly a post doctoral fellow at Cornell University, joined the team in January 2010 to conduct joint research at the Ad-



Bin Yang

vanced Light Source (ALS) at Lawrence Berkeley National Laboratory (LBNL) and Sandia National Laboratories with Dr. Nils Hansen and at the University of Southern California (USC) with Professor Hai Wang. The goal of his research is to establish a fundamental and predictive reaction model for isobutanol and furan combustion.

Dr. Andrew Garmory, formerly a post doctoral research associate at Cambridge University, joined the CEFRC on Feb. 1, 2010. He will conduct research on using data from direct numerical simulations (DNS) to validate and improve large-eddy simulation/filtered density function (LES/FDF) computations. Dr. Garmory will be working



Andrew Garmory

with Professor Stephen Pope of Cornell University, and Dr. Jacqueline Chen of Sandia National Laboratories.

Interested applicants are invited to submit their curriculum vitae including publications, contact information for three references, and identification of potential sponsors among the fifteen principal investigators. Candidates to be given serious consideration will be contacted for further information. Visit the Combustion Research Fellowships page at the CEFRC website <http://cefr.princeton.edu/programs/combustion-research-fellowships.aspx> for additional information or contact Lilian Tsang at cefr@princeton.edu.



William H. Green, Jr.
Professor, Dept. of Chemical
Engineering
MIT

Burning Butanol: Fundamentals of Alternative Fuel Chemistry

By William H. Green, Jr.

Researchers around the world are hard at work developing new biofuels, to take advantage of the large underutilized biomass resource, and the capability of micro-organisms to create specific fuel molecules. However, many of these proposed new fuels have never been tested in engines, and it is not clear how they should best be deployed. An accurate understanding of the fuel chemistry would allow engineers to simulate the performance of the proposed fuels in a variety of engines, to identify the best opportunities.

One of the new biofuels that is closest to commercialization is butanol (either *n*-butanol or *iso*-butanol). It is being produced by BUTAMAX, a joint venture between BP and DuPont, and is expected to be commercialized within the next three years. Butanol has a high energy content and is more compatible with conventional fuels and engines than ethanol, which currently dominates the biofuel market in the United States.

To facilitate a rapid and accurate determination of how the new biofuel could be most effectively used, the CEFRC team decided to work together to rapidly construct a kinetic model for *n*-butanol combustion chemistry, and to

validate this model against a variety of experiments probing different reaction conditions. The initial kinetic model, which was developed at the Massachusetts Institute of Technology in the Fall of 2009 by graduate student Michael Harper, visiting postdoc Kevin Van Geem of Gent University, and Professor William Green, was compared with existing data (mostly literature data, plus new pyrolysis data measured in Gent and new butanol ignition delays measured in CEFRC member Professor Ron Hanson's lab at Stanford). The model agrees very well with all this data.

While this model was being developed, several other members of the CEFRC team were working in parallel, making new measurements and calculations on butanol chemistry. The flame speed of butanol under various conditions was measured by Professor Egolfopoulos' group at University of Southern California and Professor Law's group at Princeton University. Professor Law's group also measured the ignition behavior of liquid butanol. Professor Truhlar's group at the University of Minnesota computed the rates of several isomerization reactions of the butoxyl radical, a key intermediate. And Professor Dryer's group at Princeton University began a series of measurements on the dehydra-

tion reactions of butanols which convert the alcohols into olefins, significantly changing their ignition chemistry.

In January, Professor Chih-Jen Sung at the University of Connecticut directly measured butanol ignition delays at high pressure conditions important in many engines, and observed that both the new CEFRC model and all previous models for butanol ignition seriously overestimate the ignition delay. Professor Hanson's group is now confirming and extending these ignition measurements to higher temperatures, and directly measuring the key OH + butanol reaction rate.

Later this year, the CEFRC team plans to combine all the new information with the literature data to construct a reliably accurate, heavily validated kinetic model for *n*-butanol combustion.

"It is amazing how much progress the team has made on this problem since the Center started six months ago", said Professor Green. "Five years ago almost nothing was known about the combustion chemistry of butanol, but now it looks like we will be able to publish an accurate, detailed, well-validated kinetic model suitable for flame and engine simulations before the end of 2010."

Princeton-CEFRC Summer Program On Combustion: 2010 Session

The CEFRC recognizes that combustion research has reached the stage where there is a strong interplay between theory, experiment, and computation, between fundamentals and applications, and between fluid mechanics and chemistry. Thus, to be equipped to tackle the challenging combustion problems facing us, particularly those on energy sustainability and climate change, a modern combustion researcher must be reasonably familiar with the important technical issues associated with the various disciplines of combustion.

In response to such a need, the Center offers an annual, one-week summer program, held at Princeton University, during which senior graduate students and researchers in combustion and energy will take two courses of 15 hours each. The students will live in a dormitory setting to further foster friendship. Scholarships are available to domestic students to partially defray the expense of attending the program.

The 2010 session, scheduled for June 27 through July 3, comprises the following two courses: (1) **Combustion Theory**, delivered by Professor Norbert Peters of RWTH-Aachen, Germany, and (2) **Combustion Chemistry**, jointly delivered by

Dr. Charles K. Westbrook of the Lawrence Livermore National Laboratory and Dr. Stephen J. Klippenstein of the Argonne National Laboratory, who will respectively lecture on kinetic modeling and ab initio chemical kinetics.

The announcement for the program was released for distribution through the Combustion Institute in late February, as well as through the CEFRC website at <http://cefric.princeton.edu/programs/summer-program.aspx>. The response from students and professionals in the combustion and energy community was immediate and abundantly positive. While the original plan called for 25 to 50 participants, 120 applicants were admitted. Professor Ronald K. Hanson commented "...this opportunity particularly motivates those with lots of drive; they want to avail themselves of all possible opportunities that will give them a chance to be next-generation leaders. In short, this is part of the globalization of research." Participants include 90 graduate students and 30 research and teaching professionals from academic institutions, government laboratories, and corporate research facilities from the United States and abroad.

"We are really excited about this inaugural year of the Program. The applicants are letting us know, with their overwhelmingly positive



response, that there is such a need in the combustion community. These are our next-generation leaders who are seeking to be exposed to teachings from current leaders outside of their own institutions," says Professor Chung K. Law, director of the CEFRC.

For more information about the 2010 Princeton-CEFRC Summer Program on Combustion, visit the CEFRC website at <http://cefric.princeton.edu/>.

People in the News



Fokion Egolfopoulos

Professor Fokion N. Egolfopoulos of the University of Southern California, was elected a Fellow of the American Society of Mechanical Engineers (ASME). Egolfopoulos is currently a co-Editor-in-Chief of *Combustion and Flame*, the official

journal of the Combustion Institute. He has published extensively in journals on heat and mass transfer, energy, fuels, the environment, combustion and propulsion.

Professor Stephen B. Pope of Cornell University, was elected to the National Academy of Engineering. Pope, the Sibley College Professor of Mechanical and Aerospace Engineering, was recognized for his "contributions to the modeling of turbulent flow, including the development of probability distribution

function methodologies for turbulent combustion." Pope conducts research in turbulence as well as computational methods for combustion chemistry. He is a fellow of the Royal Society and was recently awarded the Fluid Dynamics



Stephen B. Pope

Prize from the American Physical Society.

Prize from the American Physical Society.

Prize from the American Physical Society.

Message from the Director



Dear Colleagues:

With this issue we launch the Newsletter of the Combustion Energy Frontier Research Center (CEFRFC). 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 CEFRFC 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.

A handwritten signature in black ink that reads "Chung K. Law". The signature is written in a cursive, flowing style.

Chung K. Law

Upcoming Events

JUNE 2010

2010 Princeton-CEFRFC 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

The CEFRFC news is published biannually by the Combustion Energy Frontier Research Center.
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