CEFRC *news*

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

VOLUME 1 ISSUE 2 JULY—DEC 2010

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CEFRC - FIRST ANNUAL CONFERENCE HELD

The first annual technical conference of the Combustion Energy Frontier Research Center (CEFRC) was held on Thursday and Friday, September 23-24, 2010, at the Wyndham Conference Center near Princeton. The conference was conducted in coordination with the annual meeting of the Multi-Agency Coordination Committee for Combustion Research (MACCCR), which took place Monday through Thursday of the week, hence sharing our Thursday's program. The joint meetings provided an opportunity for increased interaction among the participants and useful sharing of research results, especially those on fuels chemistry. In attendance were representatives from the Department of Energy (DOE), members of the CEFRC's International Advisory Committee, the Center's fifteen principal investigators, Combustion Energy Research Fellows, research associates and students, and members of the combustion community.

The purpose of the Conference was to review the progress made during the Center's first year of operations with regard to research that addresses the over-arching grand challenge identified at an earlier DOE workshop – to develop a "validated, predictive, multi-scale, combustion modeling capability to optimize the design and operation of evolving fuels in advanced engines for transportation application". In year one, butanol was selected as the first fuel for the Center to concentrate on. In part because of its practical application as a possible transportation fuel given its higher energy density than ethanol, miscibility with gasoline, the potential for its synthesis from non-food sources of biomass, and also because its oxidation mechanism is small enough for modeling and computation.

The Book of Abstracts for the conference, containing extended abstracts reporting accomplishments by the principal investigators, can be

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COMBUSTION SUMMER SCHOOL HOST TO 122

During the blisteringly hot days of the last weekend of June 2010, 122 enthusiastic graduate students and researchers representing 36 universities, four national laboratories, corporations including General Motors and ExxonMobil, arrived at Princeton University to attend the inaugural session of the Princeton-CEFRC Combustion Summer School.

Photo: M. Littman

The summer school, which ran from June 27 to July 3, was organized by the CEFRC. Participants began arriving from all parts of the country on Sunday afternoon to attend the orientation and welcome barbeque. The week-long program featured courses that introduced the fundamentals of combustion theory and chemistry. The courses were taught by the eminent combustion scientists

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CEFRC - FIRST ANNUAL CONFERENCE HELD

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accessed at the CEFRC website. The Book also contains a list of challenging problems in combustion research identified by the principal investigators. The presentation slides from the conference may be accessed at the CEFRC website as well. The technical exchange of the conference program was greatly enriched by the attendance and active participation of members of our International Advisory Committee: Dr. Meredith B. Colket of the United Technologies Research Center, Dr. Michael C. Drake of the GM Research Lab, Dr. John T. Farrell of ExxonMobil Research Lab, Professor Katharina Kohse-Höeinghaus of the Bielefeld University, Germany, Professor Norbert Peters of the RWTH Aachen, Germany, Professor Adel F. Sarofim of the University of Utah, and Dr. Wing Tsang of NIST, with Professor Sarofim chairing the committee. The committee has since written a report on their evaluation of the progress of the Center, containing many valuable suggestions.

The Conference afforded the PIs and the international advisors a splendid opportunity for extensive brainstorming on the research needs of combustion energy science in general and the research direction and focus of the Center in particular. We shall report to you our plan of action in the next issue of the Newsletter.

Work-in-progress posters were presented by CEFRC research associates and students. The poster titles and presenters were:

"*Ab initio* multi-reference correlated wavefunction calculations of bond dissociation energies in methyl esters"
V. Oyeyemi, Princeton University

"Autoignition of n-butanol at elevated pressure and low to intermediate temperature"
B. Weber, University of Connecticut

"Kinetic modeling of methyl formate oxidation"
R. West, MIT

"Gas phase reactions of methanol with the hydroperoxyl and methyl radicals: Computational thermochemistry and dynamics"
J. Alecu, University of Minnesota and MIT

"Molecular transport, chemical kinetics, and turbulent flame modeling at high pressures"
P. Zhang, Princeton University

"Experimental and modeling study of the oxidation of isobutane and isobutene"
B. Yang, Sandia National Laboratories and University of Southern California

"MBMS and modeling study of the flames of C_6H_{12} isomers"
B. Yang, Sandia National Laboratories and University of Southern California

"The Reaction of Benzene + $O(^3P)$: A theoretical and experimental study"
E. Dames, University of Southern California

COMBUSTION SUMMER SCHOOL HOST TO 122 ATTENDEES

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Professor Norbert Peters of the RWTH Aachen in Germany, **Dr. Charles K. Westbrook** of the Lawrence Livermore National Laboratory and **Dr. Stephen J. Klippenstein** of the Argonne National Laboratory. The academic program was conducted at an accelerated pace, with daily three-hour lectures in the morning and afternoon. This intense pace of learning was supported by comfortable living arrangement in single occupancy, air-conditioned dormitory rooms. Throughout the week, the participants also fully utilized the networking opportunities beyond the lecture hall by sharing their meals in the dining hall of the dormitory. Many continued their social bonding over impromptu sporting and social activities in the evenings. A highlight of the week was the combustion lab tour, capped off with spectacular Fourth of July fireworks at dusk, viewed from the University Sports Fields.

Photo: R. West

The summer school was a great success, as judged from the enthusiastic feedback from the attendees. **Brandon Rotavera**, a graduate student from Texas A&M University wrote, "…I had very high expectations for the program and it far exceeded all of them, namely in the technical content provided by the lecturers… The instructors and the conveyance of their knowledge and experience were, to no surprise, top quality. The opportunity to engage in an academic-style setting with Prof. Peters, Dr. Westbrook, and Dr. Klippenstein, who have been and continue to be such leaders, was truly memorable." **Swetaprovo Chaudhuri**, a graduate student from the University of Connecticut and now a post-doctoral fellow at Princeton said it provided an important opportunity not only to dig deep into the fundamental concepts behind combustion science, but also to network with other researchers in the field. "The courses kept in mind future directions of combustion science, its possible and necessary impact on clean energy, and also ensured that we developed firm foundations in the theory" he wrote.

"Rarely do schools offer in-depth courses that combine these two fairly disparate branches of science of combustion theory and chemistry," said **Chung K. Law**, the director of the CEFRC. "But if you want to address the immensely challenging problems of energy sustainability and climate change, you need scientists who know both. Currently, over 80 percent of the global energy consumption comes from burning fossil fuels. Even a small improvement in the combustion efficiency will lead to a huge saving in the overall energy expenditure and the simultaneous reduction in the emission of greenhouse gases."

With the success of the inaugural session and based on the enthusiastic participant feedback, the CEFRC plans to continue offering the combustion summer school annually, with an expanded syllabus in future sessions. Plans are already underway for the 2011 Session of the Combustion Summer School. Interested participants should check the CEFRC website. We will make information on the 2011 Session along with the online application form available in the January/February 2011 timeframe.

"With the Center focused on advancing the science of combustion, we feel we have a huge responsibility to not only conduct the science now, but to prepare the next generation of scientists in this field. That's why we organized this summer school. The impact will be tremendous 10 to 15 years down the road."

C.K. Law

Combustion Chemistry of Small Hydrocarbon Compounds

By Hai Wang

Hai Wang
Northrop Professor in Engineering
Dept. of Aerospace and Mechanical Engineering
University of Southern California

Do you ever wonder why flames look bright and can be blue, yellow, or sometimes even green? These colors are the result of light emission from species or materials produced in a combustion process. These species are often intermediate to the final combustion products, namely carbon dioxide and water. Many of them are short-lived, but persist long enough to give flames bright and interesting colors.

There are many forms of hydrocarbon fuels used for different purposes. We use natural gas (mostly methane, CH_4) in our home stoves and water heaters. Gasoline, diesel, jet fuels and now, bio-derived fuels (e.g., butanol) are used to power cars, trucks, airplanes, and other transportation vehicles. A candle flame burns evaporated wax, and coal or wood are still used for heating and electricity production.

Interestingly, the light emitting species or compounds are always the same regardless what hydrocarbon fuels we burn. For example, the blue color (and sometimes a deep purple) comes from electronically excited CH. The green color is the result of light emission from an excited C_2 species. Of course, thermal radiation of soot (smoke) manifests as the color yellow. The distinctive colors and the fact that there are just a few of them tell us, to an extent, that the different flames share similar chemistry as the parent fuel is oxidized to carbon dioxide and water. The process releases heat as an energy carrier for converting the chemical energy in the fuel into power.

Over the last several decades, researchers learned that the rate of fuel combustion and pollutant formation is governed by several dozen chemical reactions. These reactions are critical to combustion processes of all hydrocarbon fuels. Most of these reactions involve relatively small chemical species. Examples include: carbon monoxide (CO), hydrogen (H_2), methane (CH_4), ethylene (C_2H_4), acetylene (C_2H_2), propene (C_3H_6), and butadiene (C_4H_6).

Also, many of the intermediate species are free radicals with at least one unpaired electron, making them extremely reactive. The radical species are the chain carriers for a radical branching process that can lead to fuel explosion and a flame resistant to extinction. To name a few, the hydrogen and oxygen atoms (H• and O•), hydroxyl (OH•), methyl (CH_3•), propargyl (C_3H_3•) radicals, and those blue- and green-light emitting species belong to this class of reactive species.

Along with molecular oxygen, the chemical reactions among these species play the most critical role in the combustion of any hydrocarbon fuels. Larger hydrocarbon fuels, for example, gasoline fuel, must crack into these small fragments before they are oxidized. The bottleneck of this entire rate process is usually in the oxidation of the smaller frag-

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Combustion Chemistry of Small Hydrocarbon Compounds

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ments. These are CO, H_2 and the C_1-C_4 compounds listed above.

Researchers understood for many years that the reaction chemistry of CO, H_2 and C_1-C_4 compounds are the foundation for reliable predictions of the combustion behavior and pollutant emission for all hydrocarbon fuels. Collectively, the chemistry of these compounds is dubbed the C0-C4 chemistry.

For many years, scientists around the world have tried to advance predictive, physics-based C0-C4 models. Much progress has been made. There exist many varieties and versions of similar models today; some of which are already quite predictive, while others can be better justified from physics considerations. Yet, not a single model is accepted as a universal model all researchers can agree on. This situation leads to many fundamental and practical problems in our pursue of predictive combustion chemistry as design tools for energy-efficient combustion engines.

This year, the center researchers started an endeavor to collectively develop a unified C0-C4 reaction model. They believe that this effort will not only ensure the consistency and coherence among the different research efforts of the center in the years to come, but that it will also have a broad impact on combustion research. The resulting C0-C4 model is expected to serve as the industry standard for combustion research worldwide.

CEFRC PRINCIPAL INVESTIGATORS DELIVERED PLENARY AND TECHNICAL LECTURES AT 33rd INTERNATIONAL SYMPOSIUM ON COMBUSTION

The CEFRC was well represented by the principal investigators and their research associates and students at the 33rd International Symposium on Combustion, held at Tsinghua University in Beijing, China from August 1-6, 2010. It was a great honor that CEFRC principal investigators **Dr. Jacqueline H. Chen, Professor Ronald K. Hanson, and Professor Hai Wang** delivered three of the five plenary lectures of the symposium, with Professor **Hanson's** lecture being the opening Hottel Lecture. These plenary lectures were:

Jacqueline H. Chen, "Petascale direct numerical simulations of turbulent combustion: Opportunities and challenges."

Ronald K. Hanson "Applications of quantitative laser sensors to kinetics, propulsion and practical energy systems."

Hai Wang, "Formation of nascent soot and other condensed-phase materials in flames."

In addition, the Center PIs and their associates delivered a large number of contributed papers at the Symposium through both podium and poster presentations, and 38 papers authored by the Center PIs, in addition to the three plenary papers, will be published in the Symposium Proceedings, which is ISI-indexed.

COMBUSTION WORKSHOP HELD AT TSINGHUA CCE

Background of stage at opening ceremony of Tsinghua Center for Combustion Energy

In coordination with the 33rd International Combustion Symposium, on August 1, 2010, Tsinghua University in Beijing, China, established a Center for Combustion Energy (CCE). The goal of the Center is to perform combustion research in the broadest sense, with focuses on energy science, foundation science, and interdisciplinary science.

As part of the opening ceremony, a workshop on *"Combustion Research in an Energy-Constrained World"* was held on the Tsinghua campus on July 31, 2010, the day before the start of the Combustion Symposium. The one-day workshop consisted of three sessions, covering a wide range of topics that are of both fundamental and practical importance to combustion science and energy. The state of the art and the research needs of each topic were reviewed by a leading expert in that area, with input from other colleagues. There was extensive participation by the Center PIs and advisors. These sessions, the specific topics and their respective participants and presenters (indicated by asterisks) are listed in the following:

Session on Foundation Science

Combustion Chemistry
C.K. Westbrook*

Combustion Theory
M. Matalon*

Turbulent Combustion
J.H. Chen*, J.H. Frank, S.B. Pope

Advanced Diagnostic Techniques
K. Kohse-Höeinghaus*

Cybercombustion
J.H. Chen*, M.D. Smooke

Session on Energy Science

Clean Engine Combustion
S.H. Chung, C.F. Lee*, L.M. Pickett

Clean Coal Combustion
Q. Yao*

Fuel Chemistry and Surrogate Modeling
W.H. Green, Y. Ju*, C.J. Sung

Session on Interdisciplinary Science

Functional Nanomaterials
Y. Ju*, S.D. Tse, X.L. Zheng

Combustion and Beyond
H. Wang*

CAREER OPPORTUNITIES

CEFRC COMBUSTION ENERGY POST-DOCTORAL RESEARCH FELLOWSHIP

Two-year positions as Combustion Energy Postdoctoral Research Fellows are available for co-sponsored postdoctoral or senior research associates to perform joint, high-risk/high-payoff research projects with at least two principal investigators of the CEFRC at their respective locations, providing synergy and continuous rejuvenation of research directions. These are highly competitive appointments which provide rigorous training for the next generation of leaders in combustion science and technology. Starting salary for a fresh Ph.D. is $48,000/year plus benefits.

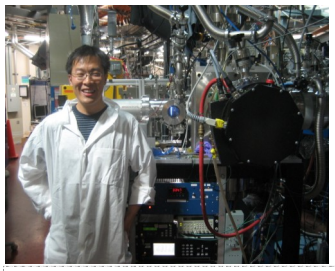
Applications for the Combustion Energy Research Fellows program are considered on a rolling basis, with three annual deadlines for application submission: April 30, August 31, and December 31. Visit http://cefrc.princeton.edu/programs/combustion-research-fellowships.aspx for additional information and application instructions.

RECENT CEFRC RESEARCH

In each issue of the CEFRC News, we will highlight the research being conducted by some of the Center's students and research associates including the Combustion Energy Postdoctoral Research Fellows. In this issue, we spotlight the research of **Dr. Bin Yang** and **Dr. John Alecu.**

EXPERIMENTAL AND MODELING STUDY OF THE OXIDATION OF ISOBUTANE AND ISOBUTENE

By Dr. Bin Yang



Dr. Yang is conducting joint research at the Advanced Light Source (ALS) at LBNL, the Sandia National Labs, and the University of Southern California, under the joint sponsorship of CEFRC principal investigators Dr. Nils Hansen and Professor Hai Wang.

Kinetic modeling of isobutanol combustion requires a reliable chemical kinetic submodel for the pyrolysis and oxidation of isobutene. To establish the validity of a base model for isobutanol combustion, validation tests need to be performed for the oxidation of isobutane and isobutene against a wide range of experimental observations.

Low-pressure isobutane and isobutene burner-stabilized flame experiments were performed at the Advanced Light Source Facility at the Lawrence Berkeley National Laboratory. The apparatus consists of a low-pressure flame chamber, a differentially pumped flame-sampling system, and a time-of-flight mass spectrometer. In these experiments, premixed, flat flames are probed by a quartz nozzle and the sampled gases expand into the ionization chamber of a mass spectrometer, where the molecular beam is intersected by monochromated VUV synchrotron light. Photo-ions are then separated using time-of-flight mass spectrometry. Mole fraction profiles were measured for most flame species, which were identified by the photoionization efficiency.

Flame chemistry modeling results from USC Mech II are compared to the data for premixed low-pressure isobutane and isobutene flames, as well as the laminar flame speeds of isobutane/air and isobutene/air over an extensive range of the equivalence ratio (0.7-1.8) at room temperature and atmospheric pressure (Davis and Law). The model is also tested against over 45 sets of ignition delay data from literatures. For isobutane-oxygen-argon and isobutane-oxygen-nitrogen mixtures, the model predicts fairly well the ignition delay times throughout the entire temperature range. For isobutene-oxygen-argon mixture, the predicted ignition delay times are higher than the experimental data at lower temperatures (1300-1500K).

The results suggest that USC Mech II provides a reasonably good starting point for the development of an isobutanol combustion chemistry model. Nevertheless, minor

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RECENT CEFRC RESEARCH

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revisions and updates are required for the reaction chemistry of isobutene pyrolysis and oxidation. Future work will be focused on completing an isobutanol reaction kinetic model with its base model well validated.

MECHANISTIC REFINEMENT: SYSTEMATICALLY IMPROVING THE *N*-BUTANOL COMBUSTION MECHANISM

By Dr. John Alecu

One of the aims of the interdisciplinary collaborative effort between the research groups of Professors Truhlar and Green is to improve on the existing *n*-butanol combustion mechanism by refining the rate coefficients of several critical reactions. The initial mechanism for *n*-butanol combustion was developed recently at MIT using the Reaction Mechanism Generator (RMG). The RMG simulations indicated that the overall *n*-butanol combustion mechanism is highly sensitive to the rates of several elementary reactions involving radicals and the intermediates generated; consequently, our initial research has been directed toward computing high-quality thermochemical and kinetic information for these important radical reactions. Future research will be aimed at measuring several of the rate coefficients to which the overall combustion mechanism is the most sensitive using the laser-photolysis experimental technique coupled with the laser-absorption and/or time-of-flight mass spectrometry detection methods.

Many of the key species implicated in the radical processes of interest are cyclic or possess multiple torsions that can couple to yield numerous structural conformers, and one of the main challenges in our research thus far has been to devise a systematic approach for accurately and efficiently treating these complex reaction systems. We've focused our attention on improving on the accuracy with which electronic energies, zero-point energies, and partition functions can be predicted from computations. To find practical electronic model chemistries (i.e., combinations of levels of theory and one-electron basis sets) that are well-suited for computing the electronic energies of species in these kinds of reactions, we have first explored the analogous prototypical reactions of the simplest alcohol, methanol, with the important hydroperoxyl and methyl radicals. Accounting for the anharmonicity present in high-frequency modes is crucial to improving on the accuracy with which energies and rates can be predicted from computations, and to this end, we have optimized scale factors for important properties such as zero-point energies, that can be applied to systematically correct the harmonic vibrational frequencies computed from a host of important electronic model chemistries for anharmonicity. Finally, we have developed a set of practical methods capable of reliably treating torsional anharmonicity even in systems with multiple torsions, called the multi-structural (MS) torsional methods, through which the effects of torsions coupling to one another and to external rotation are included in the partition function, and the problem of associating certain normal modes with specific torsions is circumvented by using internal coordinates. Therefore, our research objective of improving the existing *n*-butanol combustion mechanism is currently in the process of being realized, as the rate coefficients of several radical reactions identified as important by the RMG are being refined through the employment of the electronic model chemistries recently found to give good performance for prototypical reaction systems (and scaling the ensuing computed vibrational frequencies by the newly optimized scale factors) in direct dynamics calculations based on variational transition state theory with a curvilinear dividing surface, a multi-structural treatment of torsions, and a multidimensional treatment of tunneling. Crossing interdisciplinary boundaries continues to be central to the success of this endeavor, as it is for much of the research being conducted at the CEFRC.

Dr. Alecu is co-sponsored by Prof. William H. Green and Prof. Donald G. Truhlar. His research focuses on accurately computing and directly measuring the thermochemistry and rate coefficients over a wide temperature range for important reactions in the combustion of new and potential biofuels.

CEFRC PEOPLE IN THE NEWS

In September 2010, **Professor Emily A. Carter**, the Arthur W. Marks '19 Professor of Mechanical and Aerospace Engineering and Applied and Computational Mathematics was appointed the founding director of Princeton University's Andlinger Center for Energy and the Environment. The Andlinger Center was created in 2008 with the support of a $100 million gift from international business leader Gerhard Andlinger, a member of Princeton's class of 1952. The mission of the center is to build on Princeton's strengths in environmental science, materials science and policy to develop sustainable sources of energy that satisfy the world's energy demand in a way that preserves natural resources and the health of the environment for future generations. **Carter** was also named Chair, Energy Subdivision of the PHYS Division of the ACS, 2010-2011; Chair, DOE-BES Council on Chemical and Biochemical Sciences, 2011-2013; and Member, Board on Chemical Sciences and Technology, National Research Council, National Academy of Sciences, 2010-2012.

Professor Frederick L. Dryer of Princeton University and **Professor Fokion N. Egolfopoulos** of the University of Southern California were elected Associate Fellows of the American Institute of Aeronautics and Astronautics (AIAA).

In July 2010, **Dr. Stephen J. Klippenstein**, Senior Chemist at the Chemical Sciences and Engineering Division of Argonne National Laboratory, was presented with a Distinguished Performance Award by the Argonne Board of Governors in recognition for his outstanding scientific achievements.

Professor Chung K. Law, Director of the CEFRC and Robert H. Goddard Professor at Princeton University, was elected a Fellow of the American Academy of Arts and Sciences (http://www.amacad.org/news/new2010.aspx). THE AAAS is one of the nation's oldest and most prestigious honorary societies.

Professor Donald G. Truhlar was elected to a three-year term as officer of the Division of Chemical Physics of the American Physical Society. Additionally, he was awarded Doctor Honoris Causa of Technical University of Lodz, Poland, 2010, "for his contributions to the development of quantum chemistry and vivid collaboration with our and other Polish universities." Furthermore, he was inducted into the National Academy of Sciences in April, 2010. Members are elected in recognition of their distinguished and continuing achievements in original research.

Dr. James A. Miller, Distinguished Member of the Technical Staff at the Combustion Research Facility at Sandia National Laboratories, has transferred to the Argonne National Laboratory where he continues his research.

Professor Chih-Jen Sung joined the Mechanical Engineering Department of the University of Connecticut as a School of Engineering Professor in Sustainable Energy. He was previously a faculty member at Case Western Reserve University from 1999 to 2009.

Professor Hai Wang was appointed Northrop Chair in Engineering at University of Southern California, as well as a Chang Jiang Scholar of Shanghai Jiaotung University in Shanghai, China.

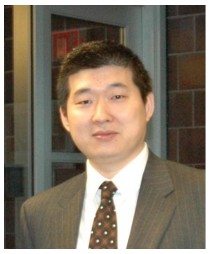
NEW ADDITIONS TO THE CEFRC

Dr. Andrey Starikovskiy was appointed Associate Director of the Center on September 1, 2010. Dr. Starikovskiy was formerly a member of the Scientific-Technical Committee of the Moscow Institute of Physics and Technology (MIPT), and Head of its Scientific Research Center. Before joining the Princeton CEFRC, he was a Research Professor at Drexel University, and the Associate Director of the Drexel Plasma Institute. Dr. Starikovskiy is an eminent scientist in reacting and plasma flows, and brings considerable experience in large center administration.

Three new appointments to the CEFRC's Combustion Energy Research Fellows Program (otherwise known as the "roving postdoc program") were made. Dr. John Alecu, Dr. Mruthunjaya Uddi, and Dr. Peng Zhang joined the Center, each to begin two-year research positions, co-sponsored by two or more of the Center's principal investigators:

Dr. John Alecu obtained his Ph.D. from the University of North Texas in 2009, and joined the CEFRC in July, 2010. Dr. Alecu is co-sponsored by Professor William H. Green of MIT, and Professor Donald G. Truhlar of the University of Minnesota. The goal of the joint research is to accurately compute and/or directly measure the thermochemistry and rate coefficients over a wide temperature range for important reactions in the combustion of new and potential biofuels. The initial focus is to improve on the existing n-butanol combustion mechanism by refining the rate coefficients of several critical reactions through high-level quantum-chemistry-based direct dynamics calculations using variational transition state theory with a curvilinear dividing surface, a multi-structural treatment of torsions (MS-T), and a multidimensional treatment of tunneling.

Dr. Mruthunjaya Uddi obtained his Ph.D. from the Ohio State University in 2008, and joined the CEFRC in May 2010. Dr. Uddi is co-sponsored by Professor Yiguang Ju of Princeton University and Professor Chih-Jen Sung of the University of Connecticut. He is studying low temperature (500-600K) oxidation mechanisms of fuels such as ethane and methane in nanosecond discharge plasma under various conditions of temperature and pressure. Dr. Uddi is using advanced laser diagnostics such as Mid-IR absorption and TALIF to measure important radical species' temporal densities. He is also doing similar studies for biofuels (methyl esters and butanols) in a rapid compression machine.



Dr. Peng Zhang obtained his Ph.D. from Princeton University in June 2010, and joined the CEFRC in August 2010. He is sponsored by four principal investi-

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NEW ADDITIONS TO THE CEFRC

(Continued from page 10)

gators on two major collaborative efforts which share the element of high pressure combustion. The first involves the collaboration between Professor Chung K. Law of Princeton University and Professor Stephen B. Pope of Cornell University on the modeling of turbulent flames at high pressures. The second involves the collaboration with Professor Law, Dr. Stephen J. Klippenstein of Argonne National Laboratory and Professor Hai Wang of the University of Southern California on a re-examination of the various "laws" governing the transport and reaction of flows as the system pressure becomes exceedingly high. Dr. Zhang's research topic is one of the grand challenge problems identified by the CEFRC, requiring both theoretical and numerical studies in diverse areas of fluid flows and chemical kinetics.

Upcoming Events

March 2011

7th U.S. National Combustion Meeting,

Combustion Institute

Georgia Institute of Technology
March 20-23, 2011, Atlanta GA

May 2011

Science for Our Nation's Energy Future

Energy Frontier Research Centers Summit & Forum
May 25-27, 2011, Washington, D.C.

July 2011

The 7th International Conference on Chemical Kinetics

Massachusetts Institute of Technology
July 10-14, 2011, Cambridge, MA

Announcements

- **On January 4, 2011, the CEFRC launched a redesigned website. Visit us at our NEW website—http://www.princeton.edu/cefrc/.**
- **Combustion Summer School lectures are now available for download at http://deimos.apple.com/WebObjects/Core.woa/Browse/princeton.edu.4746982603.04746982605 or if you do not have access to iTunes, http://www.princeton.edu/engineering/video/combustion-2010/ .**

MESSAGE FROM THE DIRECTOR

Dear Colleagues:

I hope this message finds you in the best of spirits for 2011. Much has happened with the CEFRC since the release of the last Newsletter; I will report to you the highlights of three of them.

From June 27 to July 3, the CEFRC held its inaugural session of the Princeton-CEFRC Summer School. As reported in the last Newsletter, the response to the call for applications was overwhelmingly enthusiastic, leading us to have to quickly find alternate lodging and lecturing venues to accommodate the unexpectedly large number of applicants. The session started off with a barbeque reception on Sunday evening, followed by five days of intense lecturing. The lecturers meticulously prepared for the lectures and masterfully delivered them, with extensive handouts distributed beforehand to guide the lecturing. The participants were obviously appreciative of the opportunity to learn from the masters and the efforts that they had put in, and many of them have communicated their appreciation to us as well as the lecturers afterwards. During the week I was equally pleased in witnessing the spirit of camaraderie that the participants developed during lecture breaks, meals, and evenings. These friendships will no doubt last a long time in their respective professional careers.

The Summer School was by all measures a great success, and was a highly gratifying experience for me personally. I came away feeling enthusiastic and assured about the future of combustion research, as I know that it will be in competent hands. I am also pleased to report to you that planning for the 2011 session is well on its way. In response to the interest of many participants of the 2010 session to return for the 2011 session, the two foundational courses of Combustion Theory and Combustion Chemistry will be given by different lecturers so that the returning students can get a different perspective. In future sessions the lecturers will be rotated on alternate years. In addition, we will also offer a third course, on Combustion (Laser) Diagnostics. These courses will be given by three combustion scientists who are in every respect as distinguished as our 2010 lecturers. The program will be posted on our website shortly.

The CERFC held its first conference on September 23-24. We spent half of the time in reporting and synthesizing what was accomplished, with the remaining half brainstorming on what are the important problems in combustion science, how the roadmap identified previously can be further refined, and how the research goals can be achieved individually and collectively. Members of the international advisory committee, led by its Chair, Professor Adel F. Sarofim, actively participated in the discussion. We have since received the report from the advisory committee, and are reviewing our research plan to include their valuable recommendations.

Throughout the conference I was constantly reminded of the distinguished group of investigators that we have assembled at the Center, and the wonderful science that we can do together. This is a rare opportunity and an obligation, and we must deliver.

The Combustion Institute held its 33rd International Symposium at Tsinghua University in Beijing, China on August 1-6. This is the "go-to" conference for combustion researchers and the CEFRC had an impressive presence there. As noted elsewhere in this Newsletter, three of our PIs (Chen, Hanson, Wang) delivered three of the five plenary talks, with Hanson delivering the opening Hottel Lecture. In addition, a large number of papers related to the Center PIs were delivered, and a total of 41 papers authored/co-authored by them will appear in the Proceedings of the Combustion Institute. This represents over 10% of all the papers to be published in the Proceedings. Needless to say we are justifiably pleased with this outcome.

Please also note that our web-site has been re-designed. Do take a look at it. We plan to greatly expand its content in order to serve the energy and combustion community well.

I close this message by wishing you a productive 2011.

Chung K. Law

The CEFRC *news* is published biannually by the Combustion Energy Frontier Research Center
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