Recent CEFRC Progress in Theoretical Chemistry for Combustion
By Stephen J. Klippenstein

Chemical mechanisms for combustion of fuels such as butanol consist of thermochemical data for hundreds of species and rate coefficients for thousands of reactions. Historically, these data have largely been obtained from experimental measurements, with theory providing an empirical tool for correlating sets of data and representing and extrapolating the temperature and pressure dependence of the experimental observations. However, recent and continuing advances in theoretical methodologies and software, coupled with ever increasing computational power, have transformed theoretical kinetics from an empirical to a predictive science. For many reactions it is now possible to make a priori theoretical kinetic predictions with an accuracy rivaling that of most experiments.

In recognition of this paradigm shift, a number of theoretical chemists (Carter, Green, Klippenstein and Truhlar) were included as PIs in the CEFRC. These theoreticians have a dual role within the CEFRC. One is to continue to develop and improve methods for accurately predicting thermochemistry and rate coefficients. The other is to apply these methods to reactions of importance to the development of accurate chemical models for combustion. The modeling efforts in other parts of the CEFRC motivate these theoretical efforts and provide the key connection between it and the experimental work.

The accurate treatment of torsional anharmonicity has been a long-standing challenge for a priori theoretical kinetics. These problems become particularly severe for large species with multiple torsional modes and when there are hydrogen bonds formed for some of the geometries. The presence of hydrogen bonds particularly complicates things by coupling some of the other vibrational motions to the torsional motions. In particular, many of the bending frequencies become quite strongly dependent on the torsional geometry. Truhlar has developed a method that treats this difficulty by explicitly considering the contributions from each of the different torsional minima. The implementation of this multi-atoms torsional (MS-T) approach yields improved thermochemical and kinetic estimates as illustrated with sample calculations for a variety of alkanes, alcohols, and corresponding radicals. A computer code for implementing the MS-T method is now available to the community at http://comp.chem.umn.edu/mstor. Truhlar has used this approach to obtain high level kinetic predictions for a number of abstraction reactions involving butanol. These predictions are playing important role in the continuing refinement of the CEFRC mechanism for butanol combustion.

The prediction of the thermochemistry and kinetics for large ester molecules presents considerable difficulties due to the scaling of the computational effort of standard electronic structure methods with molecular size. Carter has proposed a new ab initio composite scheme based on hybrid DFT, for molecular geometries and vibrational frequencies, and on CBS-MRSDCI for refining electronic energies. Validation against bond dissociation energies (BDEs) for hydrogen and for more complex heteroatom containing molecules demonstrated the ability of this approach to achieve chemical accuracy. Carter also found that inclusion of more than 25% exact exchange remedies a failure of commonly used exchange-correlation functionals to predict accurate molecular structures for the specific case of a-alkynyl radicals, which in turn is crucial to predicting accurate BDEs. These methods have now been used to examine the kinetics of H-abstractions and the subsequent β-scission reactions of small methyl esters, namely methyl formate (MF) and methyl acetate (MA), for which reliable experimental data exists. For H-abstraction from MF by H, CH₃, O, OH, and HO₂ radicals, barrier heights are directly predicted to within chemical accuracy (comparing to low... (Continued on page 2)
Recent CEFRC Progress in Theoretical Chemistry for Combustion (continued)

(Continued from page 1)

The ab initio transition state theory based master equation approach provides a procedure for accurately predicting the temperature and pressure dependence of complex multiple well multiple channel reactions. Klippenstein has been using this approach to predict the kinetics of a variety of such reactions including (i) the decomposition of $\text{C}_4\text{H}_9\text{O}$ species, which are key intermediates in butanol combustion, (ii) the reactions of $\text{H}$ with $\text{HO}_2$ and $\text{HCO}$ with $\text{O}_2$, which were determined to be key reactions for our foundational fuels model building efforts, and (iii) the kinetics of $\text{OC}$ fission in esters, as a contribution to our biodiesel modeling efforts. In a joint effort with the Argonne-Sandia consortium on high-pressure combustion chemistry Klippenstein and Green have undertaken a detailed ab initio transition state theory based master equation study of the second oxidation of propyl radical. This reaction provides the simplest prototype for $\text{QOOH}+\text{O}_2$ reactions, which are deemed to be of key significance to the negative temperature coefficient regime in low temperature combustion. The combination of a complete representation of the temperature and pressure dependence for this reaction and the implementation of a simple model scheme for the overall oxidation are helping to delineate the significance of this kinetics.

Automated mechanism generators, such as the reaction mechanism generator (RMG) code of Green, provide an approach whose accuracy can be reliably improved with increased knowledge and testing. As such they provide an important path forward. Green has incorporated improved models for H-abstractions within RMG, and pressure dependent rate coefficients were evaluated for numerous additional reactions. Green has ported the CPU intensive part of the RMG code to run on graphical processing units (GPU), which provides an important step forward in its efficiency, thereby facilitating its use in a wider variety of more complex situations. Green has also automated the computation of solvent effects on fuel chemistry, so that the reactions occurring in fuel injectors and fuel droplets can be modeled.

KAUST Clean Combustion Research Center
By Suk Ho Chung

The Clean Combustion Research Center is one of nine Centers at the King Abdullah University of Science and Technology (KAUST). KAUST is an international, graduate research university dedicated to inspiring a new age of scientific achievement in Saudi Arabia, the region and the world. KAUST is located at Thuwal city, on the Red Sea and 75 km north of Jeddah, and opened on September 5, 2009. KAUST was designed from the outset to pursue its research agenda through four strategic thrusts: Energy, Environment, Food, and Water (http://www.kaust.edu.sa/).

The Clean Combustion Research Center seeks solutions to the global challenges that arise from the combustion of fossil fuels, particularly those of clean and efficient combustion, global warming, and petroleum depletion. Both fundamental and application-oriented research in combustion is being carried out based on the multi-disciplinary nature of combustion science and technology. World-class experimental, computational, and theoretical approaches are being employed.

The following areas of research are actively being pursued:
- Technology-driven combustion fundamentals including clean and energy-efficient combustion, combustion characteristics of low-grade and alternative fuels, chemical kinetics of real fuels and soot formation/oxidation, carbon capture and storage processes, innovative combustion technology and combustion safety.
- Application areas including advanced internal combustion engines, gas turbines, utility and industrial boilers, alternative power generation

(Continued on page 3)
KAUST Clean Combustion Research Center (continued)

(Continued from page 2)

systems, emission monitoring and reduction technologies, hybrid energy and cogeneration for industrial systems, gasification and fuel reforming.

The Center has two lab areas (totaling 1800 m²) equipped with state-of-the-art facilities and tools to investigate combustion, flows, and chemical kinetics including laser-based optical diagnostics, flow field, spray and emission measurement facilities, multiple shock tubes, engine test cells including optical access engines, rapid compression machine, ignition quality tester, high-pressure (40 bar) gas turbine combustor test facility, and a high pressure combustion duct. The research centers at KAUST are supported by a combination of core laboratories including Imaging/Characterization, Advanced Nano-

Fabrication, Biosciences and Bioengineering, and Supercomputing Laboratories. Researchers at the Center routinely use the Shaheen Blue Gene/P supercomputer to simulate turbulent reacting and non-reacting flows.

The director of the Clean Combustion Research Center is Professor Suk Ho Chung. The Center currently has five dedicated faculty members, which will grow to nine, four research scientists, 10 post-doctoral fellows and more than 20 graduate students. The Center is looking for faculty, students and post-docs interested in turbulent combustion, chemical kinetics and modeling, IC engines, gas turbines and alternative power generation systems, carbon capture and storage processes, measurement techniques/laser diagnostics, and energy bio-science (http://ccrc.kaust.edu.sa/Pages/Home.aspx).

Announcing the 2012 Princeton-CEFRC Summer School on Combustion

What:
Students and researchers may apply to the 2012 Princeton-CEFRC Summer School on Combustion, an annual one-week program sponsored by the U.S. Department of Energy and hosted by Princeton University. Additional funding for the 2012 session was also received from Army Research Office (ARO), National Science Foundation (NSF), National Aeronautics and Space Administration (NASA) and ExxonMobil Corporation.

The 2012 session will be the third time that the Combustion Summer School is offered. The 2012 session will again offer the foundation courses of Combustion Theory and Combustion Chemistry. Additionally, new to the program is a course on Internal Combustion Engines (Gas Turbines and Reciprocating Engines) and also a five-day lecture series on Frontiers in Combustion which will comprise of five half-day lectures on topics covering: Combustion in a Global Environment Context; New Developments in Combustion Technology; Alternative Fuels Including Biofuels; Cyber-Combustion; and Nano-engineered Reactive Materials and their Combustion and Synthesis.
Announcing the 2012 Princeton-CEFRC Combustion Summer School (continued)

(Continued from page 3)

All participants will enroll in Frontiers in Combustion, the five-day lecture series. Furthermore, first-time participants will select either Combustion Theory or Combustion Chemistry, while returning students have the additional choice of Internal Combustion Engines.

When: June 24 - 29, 2012
Where: Princeton University, Princeton, New Jersey

Important Dates:
- Online application February 17 - March 16, 2012
- Acceptance announcement: March 30, 2012
- Registration deadline: April 15, 2012

Course Descriptions:

Combustion Theory
Lecturer: Prof. Heinz G. Pitsch, RWTH Aachen
Objective: The aim of this fifteen-hour course is to provide graduate students involved in combustion research with the required fundamental knowledge in laminar and turbulent combustion. The nine lectures in laminar combustion will mainly be on flame theory, including premixed and diffusion flame structure as well as flammability limits. The six lectures in turbulent combustion will cover the different regimes in premixed combustion including a common expression for the turbulent burning velocity, as well as the flamelet concept and its applications for non-premixed turbulent combustion.

Combustion Chemistry
Lecturer: Prof. Hai Wang, University of Southern California
Objective: A discussion of the fundamental and application of combustion chemistry with topics ranging from a review of thermodynamics, thermochemical properties, group additivity, basic quantum and statistical mechanics, reaction mechanisms and modeling, transition state theory, Rice-Ramsperger-Kassel-Markus theory, to solution of the master equation of collision energy transfer. Topics of transport theory and properties include the Chapman-Enskog theory and its applications. Concepts and application of detailed kinetic modeling of laminar reacting flows will be discussed.

Internal Combustion Engines

Part I: Gas Turbines (Monday – Tuesday)
Lecturer: Prof. Timothy C. Lieuwen, Georgia Institute Of Technology
Objective: This course will discuss fundamental combustion problems arising from gas turbine combustion or, more generally, from combustion in steady flowing, premixed systems. We will briefly overview key metrics defining a “good combustor” - operability, emissions, turndown, and durability. We will then focus on fundamental issues arising out of operability metrics - namely flame stabilization and flashback, and combustion instabilities. Topics will include flame stabilization in high shear regions, thermoacoustic instabilities, and response of flames to harmonic perturbations.

Part II: Reciprocating Engines (Wednesday – Friday)
Lecturer: Prof. Rolf D. Reitz, University of Wisconsin-Madison
Objective: The goal of any engine is to convert the energy contained in a fuel into useful work, as efficiently and cost-effectively as possible. Engines can be classified into various families based on how this conversion is accomplished. The reciprocating internal combustion engine is one such family that will be discussed in this series of lectures. We begin the first day by motivating the importance of engines and engine research to our world. A brief review of engine fundamentals and a discussion of some of the basic metrics used to define engine performance will follow. Fuel property effects will also be reviewed. The second day reviews computer modeling tools that are increasingly being used by the engine industry for engine design. Successful modeling requires an in-depth understanding of fundamental engine processes, and modeling helps reveal where information about important processes is missing or incomplete. Finally, on day 3 future directions in engine research will be reviewed. The role of computer modeling and detailed experiments in engine design optimization will also be discussed.
Announcing the 2012 Princeton-CEFRC Combustion Summer School (continued)

(Continued from page 4)

Frontiers in Combustion

*Combustion in a Global Environmental Context (Monday)*
Lecturer: Prof. Robert H. Socolow, Princeton University
Objective: Human civilization is confronting global environmental limits. The assignment of “fitting on the earth” is unfamiliar and unwelcome, and it presents daunting challenges for technology. Today, combustion is by far the dominant energy conversion process driving the global economy, dwarfing the contributions from fission-based heating of steam, the channeling of falling water, the slowing of wind, and the absorption of solar photons in semiconductors. What transformations of the global energy system are in view for the next half century, and how will environmental objectives and necessities shape this transformation?

*New Developments in Combustion Technology (Tuesday)*
Lecturer: Dr. George Richards, NETL, DOE
Objective: Combustion is the workhorse of today’s energy and propulsion technologies, and powers much of our modern world. While concern over carbon dioxide emission has fostered many debates over the role of combustion in the decades ahead, it is important to emphasize that combustion research can provide an important answer to this debate. New combustion technologies hold the promise of addressing carbon dioxide management, efficient power production, and effective use of both fossil and renewable fuels. This course will describe how emerging technologies, all related to traditional combustion disciplines, can play a role in boosting energy efficiency, and providing cost-effective methods to manage carbon dioxide. Topics covered will include chemical looping combustion, oxy-fuel combustion, magnetohydrodynamics, pressure-gain combustion, and others.

*Alternative Fuels including Biofuels (Wednesday)*
Lecturer: Prof. William H. Green, Massachusetts Institute of Technology
Objective: An overview of the field of alternative and biofuels, focusing on the requirements for a new fuel to be successful: production issues; marketing, distribution, & business issues; fuel performance issues; environmental issues. Methods used for assessing whether a proposed fuel could be a significant contribution to solving the energy problem will be discussed. Alternative fuels now being considered will be used as case studies.

*Cyber-Combustion (Thursday)*
Lecturer: Dr. Jacqueline H. Chen, Sandia National Laboratories
Objective: The aim of this course is to provide graduate students in combustion with an overview of the role of high performance computation in combustion as a third pillar to experimentation and theory in discovery combustion science. The three hour lecture will cover topics including opportunities and challenges for petascale direct numerical simulation of turbulent combustion of alternative fuels, co-design of combustion simulation and exascale computer architectures, and the cyberinfrastructure required to share large simulation data with a global modeling community.

*Nanoengineered Reactive Materials and their Combustion and Synthesis (Friday)*
Lecturer: Prof. Richard A. Yetter, Pennsylvania State University
Objective: In the nanotechnology community, there has been tremendous progress in the molecular sciences toward the total command of chemistry at all length scales. This progress has been inspired by advances in the structural determination of biological systems. Similar advancements in assembly of molecular and nanoscale elements have been made in the pharmaceutical and microelectronics fields as well. These developments make it clear that in the foreseeable future it will be possible to synthesize any desired macroscopic structure with precise location of every atom. This course examines how nanotechnology methodologies are currently being applied to develop multifunctional smart reactive materials for combustion applications and the combustion methods for materials synthesis.
A signature component of the CEFRC, unique among the DOE’s Energy Frontier Research Centers (EFRCs), is the Combustion Energy Research Fellows program, also known as the Roving Post-doc program. In this program each fellow is sponsored by two or more of the Center PIs, splits his/her time approximately equally at the sites of the PIs, and works on new problems that arise since formation of the Center and that are inherently collaborative in nature between the sponsoring PIs. This structure therefore promotes synergy, ensuring the outcome of the Center’s research is greater than the sum of the parts of the individual PIs, and provides the Center with nimbleness in responding to new developments. The program is strictly merit based, with each fellow and the proposed study competitively selected, and is highly demanding on the fellows as it requires either frequently commuting or relocation between the sites of the sponsoring PIs. It is therefore particularly gratifying that the program has attracted some of the brightest and most dedicated young combustion researchers, who rose to the challenge and in turn were richly benefitted through this unique research experience. We are therefore proud to present to you these Fellows, their research projects, the sponsoring PIs, and the appointment dates. The recent appointees are also separately introduced in this Newsletter.

**Ionut Alecu**: 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. (Green/Truhlar; 07/10)

**Enoch Dames**: The work concerns the active design of multispecies time-history experiment in shock tubes using the method of uncertainty quantification. The study is expected to deliver much-needed computational tools and methodologies that can integrate the various center research activities in reaction model development. The research also proposes to combine the method with Processor Green’s reaction mechanism generator code as a critical center deliverable for advanced computational tool development. (Green/Hanson/Wang; 06/12)

**Yury Suleymanov**: Generate the accurate theoretical estimates of the rate coefficients using state-of-art techniques of quantum chemistry and rate theory for reactions controlling concentrations of the HO$_2$ radical. (Green/Klippenstein; 12/11)

**Gbenga Oyedepo**: Systematic utilization of ab initio quantum mechanical and density functional methodologies as predictive tools in the determination of thermodynamic properties, reaction rates and mechanisms of innovative non-petroleum based resources for optimum integration of energy conversion and new fuel compositions. (Carter/Truhlar; 09/11)

**Mruthunjaya Uddi**: Study of low temperature (500-600K) oxidation mechanisms of fuels such as ethane, methane in nanosecond discharge plasma under various conditions of temperature and pressure. (Ju/Sung; 05/10)

**Damir Valiev**: Investigation of various aspects of high-pressure combustion, both laminar and turbulent, by means of direct numerical simulation (DNS). The goal is to perform DNS and extend theory and modeling of premixed flames at high pressure with or without turbulence and including intrinsic flame instabilities (hydrodynamic, diffusive-thermal, and pulsating), depending upon the Lewis number of the fuel. (Chen/Law; 09/11)

**Bret Windom**: Experimental modeling studies of high pressure flames. The goal of this research is to characterize flames by measuring temperatures, flow velocities, and stable and radical species concentrations for flames under pressures typically experienced in practical applications. (Egolfopoulos/Ju; 05/11)

**Bin Yang**: MBMS study of low-pressure burner stabilized flames, ab initio calculation and Master Equation
Status Update: The Combustion Energy Research Fellows Program (continued)

modeling for thermal decomposition and detailed kinetic modeling for small oxygenates and related hydrocarbons. (Hansen/Wang; 02/10)

**Yue Yang**: Advanced simulations of turbulent combustion. The goal of his research is to assess and to improve the capabilities of LES/FDF by making detailed comparisons with DNS of the same flames and developing advanced SGS models. (Chen/Pope; 03/11)

**Peng Zhang**: Modeling of turbulent flames at high pressures and the re-examination of the extent of validity of the various “laws” governing the transport and reaction of reactive flows at exceedingly high pressures. (Klippenstein/Law/Pope/Wang; 08/10)

**CEFRC People in the News**

**Prof. Emily A. Carter** was awarded the August Wilhelm von Hofmann Lecture by the German Chemical Society in September 2011 and gave the plenary lecture at the opening ceremonies. The award is given once every two years to one foreign scientist worldwide. Prof. Carter’s lecture was entitled “How Quantum Mechanics Can Help Solve the World’s Energy Problems.”

**Prof. Yiguang Ju** received an Alexander von Humboldt Foundation award to perform research on combustion model development for prototypical fuel components with Prof. K. Kohse-Höinghaus of Bielefeld University, who is a member of the CEFRC’s International Advisory Committee. In October 2011, Prof. Ju was elected as a Fellow of the American Society of Mechanical Engineers (ASME).

**Dr. Nils Hansen** also received an award from the Alexander von Humboldt Foundation to perform research with Prof. K. Kohse-Höinghaus. The work will focus on experimental studies on the molecular-growth chemistry of soot precursors in combustion environments. He also delivered a plenary talk at the 7th International Seminar on Flame Structure in Novosibirsk, Russia.

**Prof. Ronald K. Hanson** delivered the Crocco Lecture at Princeton University in October, 2011. His lecture was entitled “Advance Diagnostics for combustion and propulsion system”. In November 2011, Prof. Hanson delivered a plenary lecture entitled “Diode Laser Absorption Diagnostics of Combustion Processes” at the annual Chinese National Combustion Symposium, in Hangzhou, China.

**Prof. Chung K. Law** delivered the Hawkins Memorial Lecture in Heat Transfer at Purdue University in October, 2011. The title of the lecture was “Challenges and Frontiers in Combustion”. He also delivered a plenary Lecture entitled “In Pursuit of Beauty and Unification in Combustion Theory” at the annual Chinese National Combustion Symposium, in Hangzhou, China. In November 2011, he was appointed an Honorary Professor of the Shanghai Jiao Tong University.

**Prof. Stephen B. Pope** will deliver the Hottel lecture on “Turbulent Combustion Modeling” at the 34th Combustion Symposium at Warsaw University, Poland.

**Professor Chih-Jen (Jackie) Sung** was appointed Associate Director of the CEFRC effective November 16, 2011, replacing outgoing Dr. Andrey Starikovskiy. Prof. Sung has been a Center PI since the CEFRC’s founding in August, 2009, and a member of the Center’s Experiment and Mechanism Disciplinary Working Group.

**Prof. Hai Wang** received the 2011 Senior Research Award from the Viterbi School of Engineering at USC. He also gave several plenary talks, including the Second Annual Meeting of Detailed Chemical Models for Cleaner Combustion, held in Zaragoza, Spain and the 7th International Seminar on Flame Structure in Novosibirsk, Russia on topics range from soot formation, alternative energy and combustion chemistry.

Due to the untimely death of Professor Adel F. Sarofim (see In Memoriam), Dr. Charles K. Westbrook has accepted the invitation of the CEFRC PIs to serve as chair of the CEFRC’s International Advisory Committee (IAC). Dr. Westbrook has been a member of the IAC since it’s founding in 2009, and will continue to bring his considerable organizational and managerial experience, his personal interest and tremendous accomplishments in mechanism development, and his stature in the combustion and scientific community especially as president of the Combustion Institute, to this important role in the CEFRC.
Combustion Energy Research Fellows News

Four new appointments to the CEFRC’s Combustion Energy Research Fellows Program (otherwise known as the “roving postdoc program”) were made: Enoch Dames, Gbenga Oyedepo, Damir Valiev, and Yury Suleymanov. Each will begin two-year research positions, co-sponsored by two of the Center’s principal investigators.

Enoch Dames will receive his Ph.D. from USC in May, 2012. He is co-sponsored by Prof. William H. Green of MIT, Prof. Ronald K. Hanson of Stanford University and Prof. Hai Wang of USC. His area of research will focus on the active design of multispecies time-history experiments in shock tubes using the method of uncertainty quantification.

Gbenga Oyedepo obtained his Ph.D. from the University of North Texas in 2011, and joined the CEFRC in September of the same year. Dr. Oyedepo is co-sponsored by Prof. Emily A. Carter of Princeton University and Prof. Donald G. Truhlar of the University of Minnesota. Dr. Oyedepo’s research is in the systematic utilization of ab initio quantum mechanical and density functional methodologies as predictive tools in the determination of thermodynamic properties, reaction rates and mechanisms of innovative non-petroleum based resources for optimum integration of energy conversion and new fuel compositions.

Yury Suleymanov obtained his Ph.D. from Lomonosov Moscow State University in 2008, and joined the CEFRC in September, 2011. Dr. Suleymanov is co-sponsored by Prof. William H. Green of MIT and Dr. Stephen J. Klippenstein of Argonne National Laboratory. The focus of Dr. Suleymanov’s research is to generate accurate theoretical estimates of the rate coefficients using state-of-art techniques of quantum chemistry and rate theory for reactions controlling concentrations of the HO₂ radical.

Damir Valiev obtained his Ph.D. from the Royal Institute of Technology (KTH), Stockholm, Sweden in 2008, and joined the CEFRC in September 2011. Dr. Valiev is co-sponsored by Dr. Jacqueline Chen of Sandia National Laboratories and Prof. Chung K. Law of Princeton University. Dr. Valiev is investigating various aspects of high-pressure combustion, both laminar and turbulent, by means of direct numerical simulation (DNS). The goal is to perform DNS and extend theory and modeling of premixed flames at high pressure with or without turbulence and including intrinsic flame-front instabilities of either hydrodynamic or diffusive-thermal in nature.

Congratulations to Bin Yang, the Center’s first Combustion Energy Research Fellow, on his selection into China’s 1000 Young Talents Program under the sponsorship of Tsinghua University. The Chinese government launched the 1000 Young Talents program to recruit young researchers from around the world to work in China. Dr. Yang, soon to complete his two-year appointment as CEFRC roving post doc, has been co-sponsored by Dr. Nils Hansen of Sandia National Laboratories and Prof. Hai Wang of the University of Southern California modeling for thermal decomposition and detail. His research includes MBMS study of low-pressure burner stabilized flames, ab initio calculation and Master equation in kinetic modeling for small oxygenates and related hydrocarbons.

Peng Zhang, a roving post-doc who has been conducting research with Dr. Stephen J. Klippenstein, Prof. Chung K. Law and Prof. Stephen B. Pope, has accepted an assistant professor appointment at the Hong Kong Polytechnic University, effective July 1, 2012. Dr. Zhang’s research program at the CEFRC is diverse in its nature, ranging from quantum chemistry calculations to turbulent flame modeling. We wish him all the best as he embarks the next phase of his scientific career.

CEFRC Introduces An Alternate Logo

One of our PIs has recently come up with a figure which neatly encapsulates the Center’s scientific research activities and the deliverables — comprehensive reaction mechanisms for foundation fuels, alcohols, and biodiesels. The three disciplinary working groups and the deliverables, which have been selected around target fuel chemistry, serve as a unifying theme for the CEFRC, demonstrating our multi-scale integration from the scale of the atom to the scale of turbulent processes. We feel that this figure is so representative of who we are and what we aspire to do that we have recently been using it as an alternative logo of the Center, when the occasion allows a larger image so that the letters are legible. We hope you like the design.
In Memoriam

ADEL F. SAROFIM

October 21, 1934 – December 4, 2011

It was with great sorrow that we received the news of the passing of Professor Adel Fares Sarofim in Virginia on December 4, 2011. Professor Sarofim had been the Chair of the International Advisory Committee of the Combustion Energy Frontier Research Center since its founding in August, 2009.

Professor Sarofim was born on October 21, 1934 in Cairo, Egypt. He received a B.A. in chemistry from Oxford University in 1955, an S.M. in chemical engineering practice in 1957 from MIT, and a ScD. in chemical engineering in 1965, also from MIT. He joined the faculty of MIT after graduation, becoming the Lammot DuPont Professor of Chemical Engineering at 1989. In 1996 he moved to the University of Utah as the Presidential Professor and Co-Director of the Utah Clean Coal Program. Professor Sarofim was an extraordinary scientist, gentleman, human being, mentor and friend. He authored and co-authored over 200 papers covering the diverse subjects of radioactive heat transfer, furnace design, circulation patterns in glass melts, the freeze process for desalination, nitric oxide formation in combustion systems, combustion generated aerosols, soot and polycyclic aromatic hydrocarbon formation, and the characterization of carbon structure and reactivity. For his research contributions, he received more than a dozen international prizes related to engineering and environmental science, including the Sir Alfred Egerton Gold Medal from the Combustion Institute in 1984; the Kuwait Prize for Petrochemical Engineering in 1983; the Walter Ahlström Environmental Prize of the Finnish Academies of Technology in 1993; the Senior Thermal Engineering and the Towend-BCURA Awards of the Institute of Energy in 1994; the University of Pittsburgh’s 1995 Award for Innovation in Coal Conversion; the U.S. Department of Energy’s 1996 Homer H. Lowry Award in Fossil Energy; the American Society of Mechanical Engineers’ 1996 Percy Nichols Award; the 1998 Lawrence K. Cecil Award of the Environmental Division of the American Institute of Chemical Engineers; and an honorary doctorate in chemical engineering from the University of Naples “Federico II” in 1998. He was the Hoyt C. Hotel Lecturer at the 21st Combustion Symposium in 1986 and the Lacey Lecturer at the California Institute of Technology in 1987. Dr. Sarofim was elected to the U.S. National Academy of Engineering in 2003 “for advancing our understanding of the mechanisms and modeling of processes that control radiation in and pollution emission from combustors.” In addition to his teaching responsibilities, he supervised and mentored over 80 PhD students, many of whom currently hold responsible academic, industrial and governmental positions.

Professor Sarofim played an important role in the development of many combustion researchers, particularly junior faculty, not just at his own institution but across the world. “Although he had already left MIT for Utah, Professor Sarofim helped recruit me to join the MIT chemical engineering faculty,” said William Green, a Principal Investigator of the CEFRC and the Hottel Professor of Chemical Engineering at MIT, “and then at several crucial points he provided advice and important letters of support. It was difficult starting as an assistant professor in the field of combustion during the 1990’s, when there was not much interest in energy, but his support and encouragement helped me succeed. And I know I am not the only one he supported in this way. By doing this, he helped the field of combustion continue to develop talented young faculty through a difficult period.”

“Professor Sarofim was a giant in the combustion community,” added C. K. Law, Director of the CEFRC, “his technical contributions to combustion science and technology was singularly important, and he was immensely admired and respected by his colleagues for his warm and encouraging personality. He has provided critical guidance during the formative stage of the CEFRC in the past couple of years. We will miss his leadership.”
A Message from the Director

The CEFRC is now at the mid-point of its operation since it was established by the DOE in August 2009 for a five-year funding period. It is therefore a time to reflect what we have done, and project what lies ahead. The overarching goal of the Center is: “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”. This is a monumentally challenging task recognizing the multi-physics and the associated multiscale nature of the problem, ranging from electronic excitation to turbulent mixing. To achieve this goal, we have assembled a group of combustion researchers (see Newsletter V.1, Issue 1) with theoretical, computational and experimental expertise to cover the entire spectrum of the phenomena. Furthermore, in order to integrate the activities of the individual principal investigators such that the whole is greater than the sum of the parts, and to ensure that results from our basic research would meaningfully impact the landscape of combustion and fuels technology, we have decided to develop the reaction mechanisms for three major classes of fuels, namely the C4 foundation fuels, alcohols especially the butanols, and biodiesel. Subsequently we have developed new theories and methods allowing the predictions of the thermochemical and kinetic properties of key combustion species, and applied them to reactions identified by the modeling efforts of the team. These theoretical and modeling efforts were supplemented by an extensive experimental regimen in the study of combustion chemistry, including synchrotron radiation, shock tube, flow reactor, rapid compression machine and laminar flames, and with the application of error analysis and uncertainty quantification. It is our goal to release functioning mechanisms of these three classes of fuels, with quantified limitations, during the second half of the funding period.

I am also pleased to report that the two signature outreach activities of the Center, namely the Combustion Energy Research Fellows (aka the roving post-docs) program and the Summer School on Combustion, are both progressing well. For the roving post-doc program, we have now reached the steady-state level of ten fellows, with the first two appointees, Bin Yang and Jay Uddi, about to “graduate” soon. For the 2012 Summer School, we have further enriched the academic program by offering a course on internal combustion engines and a lecture series on Frontiers of Combustion. You can find the details of the program elsewhere in this Newsletter.

In the past 50 years combustion research has become progressively more international, as evidenced by presentations at the biennial combustion symposia. This is a welcome development as the problems of energy sustainability and climate change are global. This trend is continuing as major research centers on combustion are now being established overseas. One of them is the Clean Combustion Research Center at the KAUST (King Abdullah University of Science and Technology) in Saudi Arabia, under the direction of Professor Suk-Ho Chung, previously of the Seoul National University. This center is now largely operational, and Professor Chung has sent in a report on its progress. Another noteworthy international development is that the concept of the Summer School is being actively considered for implementation in other geographical regions. In particular, a similar program will be offered at Tsinghua University in Beijing, China on May 13-19, 2012 (www.cce.tsinghua.edu.cn); Professor Mike Pilling of Leeds University and I will lecture on combustion chemistry and combustion theory, respectively.

Submission to the 34th International Combustion Symposium is at an all-time high of 1011, demonstrating that the interest in combustion research is growing. Professor Stephen Pope, a principal investigator of the Center, will deliver the plenary, Hottel lecture. This follows Professor Ron Hanson, another PI of our Center, and Professor Norbert Peters, an advisor to the Center, who delivered the Hottel lectures at the 33rd and 32nd symposia, respectively. Our Center is justifiably proud of this record of accomplishment of our associates.

Enjoy your research and with best wishes,

Chung K. Law

Upcoming Events and Announcements

MARCH 2012
Western States Section Technical Meeting, March 19-20, 2012, Tempe, AZ

APRIL 2012
Central States Combustion Meeting, April 22-24, 2012, Dayton, OH

MAY 2012
Tsinghua-Princeton Summer School on Combustion, May 13-19, 2012, Beijing, China

JUNE 2012
Princeton-CEFRC Summer School on Combustion, June 24-29, 2012, Princeton, NJ

JULY 2012
34th International Symposium on Combustion, July 29-August 3, 2012, Warsaw, Poland