Computer modeling is playing an increasing role in engineering design, including the design of combustion devices, such as internal combustion (IC) engines and gas turbine combustors. If a model can reliably and accurately predict the performance of a proposed design, then the expensive and time-consuming testing of prototypes can be greatly reduced. Such models are possible only when the underlying physics and chemistry are adequately understood, and the resulting modeled equations can be tractably solved on current computers.

Turbulent combustion, which occurs in practical combustion devices, poses formidable modeling and computational challenges. Among these are (1) the large number of chemical species (2) the large range of length and time scales, and (3) the combination of highly non-linear chemical kinetics and large turbulent fluctuations of temperature and species concentrations. As now described, in the CEFRC we have developed a modeling approach which goes a long way to meeting these challenges.

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Models for the chemistry of hydrocarbon fuels can involve over 7,000 different chemical species. However, a variety of dimension-reduction techniques have been developed which allow several hydrocarbon fuels to be accurately represented by between 20 and 180 species; and computationally-efficient tabulation procedures have been developed to make feasible the use of models with up to 40 species. This is an active area of research within the CEFRC, and we expect to close the gap between the 40 species now tractable and the 180 species needed for the accurate representation of the combustion of some fuels.

The length scales involved range from the size of the combustion device (e.g., 5 cm for an IC engine) down to the smallest scales of the turbulence (e.g., 20 microns) or to the possibly smaller scales of chemical reaction zones. This large range of scales (a dynamic range of 2,500 in the example given) poses a huge challenge to the approach of “direct numerical simulation” (DNS), since all length and time scales have to be resolved within the three-dimensional, unsteady, turbulent flow field. While DNS is an extremely important research tool of increasing value, the range of scales that are currently computationally tractable are significantly less, and it will be several decades before computer power will allow the direct application of DNS to IC engines.

Currently, the usual approach to circumvent the problem of the large range of scales is to use “large-eddy simulations” (LES) in which only the large-scale, unsteady, turbulent motions are explicitly represented. As a consequence, processes occurring at smaller, unresolved scales must be modeled. For turbulent combustion this modeling is crucial, since the important processes of molecular diffusion coupled with chemical reactions occur below the resolved scales.

To model these processes we use a “probability density function” (PDF) method, in which the turbulent fluctuations are fully represented in terms of the joint PDF of the species. The combined LES/PDF method is implemented computationally as a particle/mesh method.

(Continued on page 2)
Computational Modeling (continued)

This is illustrated in Fig.1, which shows the mesh and a small subset of the particles used in the simulation of a non-premixed, piloted turbulent jet flame.

Within the CEFRC there has been a collaboration between Jacqueline Chen’s group at Sandia and the Cornell group. At Sandia, DNS have been performed of a temporally-evolving syngas jet flame. At Cornell, the same flame has been simulated using LES/PDF. Figure 2 shows the conditional mean temperature (conditional on mixture fraction) obtained from the LES/PDF compared to the DNS. The lower conditional temperatures at the non-dimensional time of 20 are indicative of local extinction – an important phenomenon and a challenge to models of turbulent combustion. As may be seen from the figure, there is excellent agreement between the LES/PDF and the DNS. While DNS is currently restricted to relatively simple flames, LES/PDF can be used – and indeed is being used – to model combustion devices.

The challenges of modeling turbulent combustion are formidable, but we are well on the path to developing accurate, reliable, predictive models for the design of clean and efficient combustion devices.

Fig.1: The grid and particles (color coded by temperature) in an LES/PDF simulation of a piloted, non-premixed jet flame.

Fig.2: Conditional mean temperature in a temporally evolving syngas jet flame at three times. From the DNS of Hawkes et al. (2007) and the LES/PDF of Yang et al. (2012).

Upcoming Events

September 2012
MACCCR Fifth Annual Fuels Summit
September 17-20, Livermore, CA

November 2012
Third Annual Conference, CEFRC
November 14-16, Sandia National Laboratories, Livermore, CA

April 2013
Symposium on Combustion Chemistry
Spring National Meeting of the American Chemical Society
April 7-8, New Orleans, LA

May 2013
8th U.S. National Combustion Meeting
May 19-23, Park City, UT
Laminar Flames and Combustion Chemistry

The extraordinary developments in computing, optical diagnostics and combustion science of the past few decades have generated notable hope that eventually practical combustors could be designed based on a first-principles approach. While this is a rather ambitious projection with today’s capabilities, many expect that within the next 10-20 years further advances in computing and model development will allow scientists and engineers to approach that ultimate goal.

The conversion of chemical to thermal energy in practical combustors is controlled largely by the processes of chemical kinetics and turbulence as well as the unavoidable two-way interactions. Given the immense complexities associated with both processes, achieving the attendant fundamental understanding requires that studies of reacting flows are carried out first in geometrically simple and well-controlled environments, granted not realistic.

The importance of chemistry on the combustion process has been recognized at least since the early parts of last century. In his Nobel Lecture of December 11, 1956, Nikolai Semenov, whose work initiated in the 1920’s, emphasized that considering “mechanisms of chemical reactions and in particular chain reactions,” is essential towards the understanding of “combustion and explosion processes.”

Subsequently, Karlovitz (4th Combustion Symposium, 1953) introduced the concept of flame stretch, which established a clear connection between fluid dynamics and the nonequilibrium physical and chemical processes encountered within a flame. In the late 1960’s, Dixon-Lewis introduced the idea of modeling laminar flames by solving the Navier-Stokes equations as well as the species conservation equations for H₂/air one-dimensional flames, and by including chemical source terms that account for contributions from all possible reaction pathways. The work by Dixon-Lewis was the catalyst that changed the landscape of combustion research as it was realized that such simulations could be extended to more complex fuels and/ or flow fields. Indeed, statistical data show that the majority of current research efforts focus on the interactions of fluid dynamics and chemistry at various levels of complexity.

Past experience and current practices dictate that detailed kinetic models should be developed hierarchically both in terms of fuel molecular complexity and the dimensionality of the experimental approach. Regarding the fuel molecular complexity, the chemistry of the lower molecular weight (MW) species needs to be developed first and then build on it the chemistry of the more complex, higher MW molecules. For example, it has been established that the C₂-C₄ kinetics constitute the “foundation” of higher MW species reaction models. Regarding the dimensionality of the experimental approach, the first step is to carry out studies in homogeneous systems, e.g. shock tubes, flow reactors, jet stirred reactors etc., in which molecular diffusion is absent so that rate constants can be characterized at various temperatures and pressures in kinetically controlled environments. As a second step, the kinetic models need to be tested in flames, which on one hand constitute a more realistic environment due to the presence of temperature and species concentration gradients, but on the other makes the validation process far more challenging. Relying only on kinetic models developed in homogeneous systems could be a questionable proposition, as it is not uncommon that such models fail to predict satisfactorily flame properties for various reasons. For example, rate constants may not extrapolate well at the lower temperatures encountered in a flame. Furthermore, certain reaction pathways could be important only in a flame environment due to species diffusion, and the eventual fate of the products (especially radicals) of certain reactions may differ compared to homogeneous systems. Finally, it must be emphasized that mass diffusion plays an important role in flames and thus the validation of kinetic models against flame data could result in errone-

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rather low pressures, i.e. ~30 Torr, and involve typically the use of McKenna-type burners that result in one-dimensional flames, and the use of flame-sampling molecular-beam mass spectrometry and single-photon ionization by synchrotron generated vacuum-ultraviolet photons. The results of such studies have major implications on kinetic model development, as predicting species profiles in flames constitutes a rather stringent validation criterion.

On the other hand, global flame properties can be determined at both low and high pressures as resolving the flame is not required and (flow velocity) measurements are made in the hydrodynamic zone that can be arbitrarily large. While global flame data do not contain the same level of kinetic information compared to speciation data, still they exhibit notable sensitivity to a large number of reactions that can vary with the reactants’ initial thermodynamic condition; laminar flame speeds exhibit a square root dependence on kinetics as well as on diffusion, while that dependence is directly proportional for the flame ignition and extinction limits. At the same time it should be realized that global flame properties is the only means to validate flame kinetics at conditions that approach or resemble those encountered in practical combustors. The use of stagnation flames allows for the determination of laminar flame speeds and ignition/extinction limits by measuring flow velocities and temperatures, and the configuration can be modeled directly as quasi-one-dimensional with well-defined boundary conditions. This approach is applicable for pressures ranging from about 0.25 to about 10 atm, with the lower limit being imposed by flame stability and the higher limit by Reynolds number considerations. Uncertainties can be introduced by non-uniformities at the burner exits resulting from radial pressure gradients and/or momentum and thermal boundary layers, and special care is required to either minimize them or account for them. Additional uncertainties can be introduced by extrapolations to zero stretch that are required for the determination of laminar flame speeds. The use of spherical expanding flames (SEFs) in constant volume/pressure environments allows for the determination of laminar flame speeds and ignition/extinction limits by measuring flow velocities and temperatures, and the configuration can be modeled directly as quasi-one-dimensional with well-defined boundary conditions. This approach is applicable for pressures ranging from about 0.25 to about 10 atm, with the lower limit being imposed by flame stability and the higher limit by Reynolds number considerations. Uncertainties can be introduced by non-uniformities at the burner exits resulting from radial pressure gradients and/or momentum and thermal boundary layers, and special care is required to either minimize them or account for them. Additional uncertainties can be introduced by extrapolations to zero stretch that are required for the determination of laminar flame speeds. 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Laminar Flames and Combustion Chemistry (continued)

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pressure chambers is mostly meritorious in deriving flame data at pressures exceeding 5-10 atm. Traditionally, the measurements involve the monitoring of the flame surface either by Schlieren and Shadowgraph and the determination of the laminar flame speeds by invoking certain assumptions related to the thermodynamic states of burned and unburned gases and the fluid motion within the chamber. Recently though, direct measurements of flow velocities have been made and with the use of kHz lasers it is expected that this approach will provide further insight into the phenomenon of flame propagation at high pressures and will allow for the validation of the commonly used assumptions. Limitations of SEF’s stem from buoyancy, thermo-diffusional instabilities for sub-unity Lewis number mixtures, and hydrodynamic instabilities that can be aggravated at high pressures even for thermo-diffusional stable flames. Uncertainties in SEF experiments are associated with the assumptions involved during the data processing stage, with the determination of gradients from the raw data, and with the extrapolations to zero stretch especially when a narrow range of data is available.

Several members of the CEFRC team are involved in all aforementioned approaches related to flame kinetics. While much has been learned so far, it is expected that even more exciting contributions will be made by the team in the near and foreseeable future, as a result of recent and ongoing advances in diagnostic capabilities, theoretical/computational approaches, and in the basic understanding of combustion science.

34th International Symposium on Combustion

The biennial international Symposium on Combustion was held in Warsaw, Poland on July 29 to August 3, 2012. There were about 1,300 participants, including many of the CEFRC PIs, post-docs and students. 395 podium papers were presented, with 44 having CEFRC authorship. When compared to the 41 CEFRC podium papers presented at the 33rd Symposium, it demonstrates the continuing active representation of the CEFRC at this important combustion conference.

At the symposium, Principal Investigator Stephen B. Pope of Cornell University delivered the Hottel Lecture entitled “Small Scales, Many Species and the Manifold Challenges of Turbulent Combustion”. This is the fourth Hottel Lecture given by a CEFRC member in the past four consecutive symposia, with PIs Ron K. Hanson and C.K. Law presenting at the 33rd and 31st symposia and advisor Norbert Peters at the 32nd symposium. We are justifiably proud of the recognition of technical leadership of our PIs and advisors.

A highlight event of the symposium is the announcement of the gold medal winners at the symposium banquet. The CEFRC again claimed a share in this recognition, with PI Frederick L. Dryer awarded the Egerton Gold Medal for “distinguished, continuing and encouraging contributions to the field of combustion”. He joins PIs Ron K. Hanson, C.K. Law and Stephen B. Pope in this honorific recognition as the Institute’s Gold Medalist. The CEFRC also congratulates Mitchell D. Smooke of Yale University and Brian S. Haynes of the University of Sydney, who respectively received the Zel’dovich and Lewis Gold Medals.

The PIs attending the symposium also held a meeting to review the state of the CEFRC research and plan for activities ahead. There was considerable discussion on identifying the grand challenge problems in combustion – problems that could transform the landscape of combustion science and technology.
First International Workshop on Flame Chemistry

The First International Workshop on Flame Chemistry was held on July 28-29, 2012 at Warsaw University of Technology as a satellite meeting of the 34th Combustion Symposium. Attended by 120 participants, the goal of the Workshop was to assemble experts in combustion chemistry, flames, kinetic modeling, and diagnostics to identify the gap in knowledge and pathways for development of predictive high-pressure flame chemistry and to establish a framework for collaborative research. The Workshop was co-organized by PIs Yiguang Ju and Hai Wang, with CEFRC being a co-sponsor.

The two-day workshop consisted of four invited lecture sessions, a poster session, and two discussion panels, focusing on identifying the roadmap, challenges and collaborations in the areas of mechanism, elementary kinetics, and flame chemistry.

There was extensive participation by the Center PIs and advisors. Summaries of the panel discussion and presentations of the invited lectures are available on the Flame Chemistry Workshop website at http://www.princeton.edu/~yju/1st_flame_chemistry_workshop.

Feedback received for this initial Workshop was highly positive, with encouragement to organize a future session in 2014, in tandem with the 35th Combustion Symposium.

DOE/BES Mid-Program Review

In the third year of the five-year award period, the DOE-BES conducted science reviews on all 46 Energy Frontier Research Centers (EFRCs) established in 2009. This mid-term review was intended to provide a critical assessment of the individual EFRC’s strategic vision, scientific plans and progress, technical accomplishments, management, synergy, collaborative research, and communication mechanisms. A specific aspect for each EFRC to demonstrate is how the EFRC effort is “greater than the sum of its parts”.

The CEFRC administration and the PIs recognized the serious nature of this review, and devoted considerable effort to provide our sponsor and an independent, external review panel with an accurate portfolio of our Center for their assessment. Preparation for a substantial and comprehensive review document required by mid-January, 2012 started in early October, 2011, culminating in the formal review which took place in Baltimore on March 8. In order to present the diverse range of our activities and the participants, the CEFRC fielded a team consisting of ten PIs (Carter, Chen, Green, Hansen, Ju, Klippenstein, Law, Pope, Sung, Wang), five roving post-docs (John Alecu, Swe-taprovo Chaudhuri, Enoch Dames, Peter Veloo, and Bin Yang) and three doctoral students (Victor Oyeyemi, Bryan Weber, and Joseph Lefkowitz), with Center administrator Lilian Tsang providing overall coordination. The team converged at the review venue a day early to prepare for the actual presentation.

The formal review was kicked off with the Director’s overview of the Center, followed by technical presentations of the butanol thrust, theoretical chemistry developments, foundation fuels thrust, biodiesel diesel thrust, and turbulent combustion, respectively by PIs Green, Klippenstein, Wang, Ju and Chen. There was also a poster presentation, prepared and manned with the participation of several roving postdocs and doctoral students, demonstrating accomplishments as well as synergistic activities of the Center’s core research program, the Combustion Energy Research Fellows Program and other significant outreach activities such as the Summer School on Combustion. The review was closed by a round-robin small-group discussion between three CEFRC and three review teams.

We are pleased to report that our DOE-BES sponsor commended the CEFRC for the clarity of its vision and the good synergy between all the Center participants,

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DOE/BES Mid-Program Review

(Continued from page 6)

from PIs to postdoctoral researchers and graduate students. It also applauded that all CERFC members are working together well and freely share prepublication information at a level not typically seen in this specific community. Specifically, the evaluation states that: “Overall, the CERC was viewed as well integrated with a good choice of research topics and flexibility of direction.” We are pleased with this encouraging assessment; especially the fact that we have collectively and effectively communicated what we have accomplished technically to our sponsor and the independent reviewers.

A specific recommendation of the review assessment is; “Consider approaches to stay abreast of relevant trends and developments in industry and ways to encourage industry awareness of scientific results from the CEFRC.” In response to this recommendation, the Center has since added a PI, Prof. Rolf D. Reitz of the University of Wisconsin at Madison, in order to promote industry awareness of the scientific results from the CEFRC and proactively establish collaborative activities with industry. Prof. Reitz is a leading expert in engine combustion research, including the development and application of computational combustion. His participation in the CEFRC PI team extends the scope of our research activities from *ab initio* quantum chemistry analysis to the modeling of engine processes, thereby completes the spectrum of coverage to ensure the success of our mission.

In summary, the CEFRC Science Review has been a useful and enlightening experience. The CEFRC appreciates the thoroughness with which our DOE-BES sponsor planned the review and guided us through it, recognizes and treasures this unique opportunity to address and contribute to the solution of clean and sustainable combustion energy, and shall continue to deliver and meet our overarching goal of: “Developing a validated, predictive, multi-scale, combustion modeling capability to optimize the design and operation of evolving fuels in advanced engines for transportation applications” as we approach the final review in 2014.

Spotlight on CEFRC Students and Research Fellows

In each issue of the CEFRC News, we 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. Bret Windom.

**An Investigation on the Propagation of Spherically Expanding Flames**

By Dr. Bret Windom

There is a high priority to develop accurate kinetic models to aid in the design and development of more efficient and superior performing engines. To accomplish this, it is necessary to have experimental observations that are capable of validating the effectiveness of such models under a wide range of conditions. The laminar flame speed is a fundamental property of a reacting mixture and offers a unique capability to judge/validate kinetic models at a wide range of temperatures, pressures, and fuel types. Despite the already common use of laminar flame speeds, there is still a need for accurate high pressure flame validation targets. This has led to interest by the CEFRC in developing new strategies to improve the characterization of flames, in particular flame propagation, at pressures of relevance to engines.

The spherically expanding flame (SEF) is one of the flame configurations capable of producing stable propagating flames from which flame speed measurements can be obtained. SEF is an outwardly propagating flame initiated at the center of a chamber that is filled with the desired premixed fuel/oxidizer/inert composition. In traditional approaches, the radial expansion rate of the flame is measured (often via high speed Schlieren/shadowgraph imaging techniques) and used to extrapolate the laminar flame speed. However, despite the common use of this measurement, there are some basic assumptions associated with the experimental procedures and the post processing of the data that need to be tested and understood more completely. For these reasons, recent efforts have focused on investigating the fundamental concepts associated with SEFs and developing novel measurement techniques with the goal of stretching the boundaries of flame speed measurements while providing a more accurate description and determination of SEF flame propagation.

At the University of Southern California, under the supervision of Professor Egolfopoulos, a relatively new technique, which uses particle image velocimetry (PIV), is being implemented to investi-
Spotlight on CEFRC Research (continued)

(Continued from page 7) gate the propagation of SEFs. This technique provides a direct measurement of the flame speed by simultaneously measuring the flame displacement and the unburned gas velocity ahead of the propagating flame. Implementing this direct measurement removes the need for using certain assumptions that are applied to traditional techniques when attempting to determine the flame speed from the experimental data. By performing the PIV technique in concert with the aforementioned traditional approaches the validity of these assumptions are being tested. The new approach provides also an advantage in its ability to measure flame speeds locally, allowing thus for the detailed investigation of the flow field of the unburned and burned gas. Furthermore, it can provide meaningful insight into possible couplings between flame propagation and fluid mechanics, which can contribute to the development of instabilities and eventually to turbulence. The work is expected to advance the measurements of laminar flame speeds at elevated pressures by providing a better understanding of SEFs ultimately assisting in the development of highly accurate and effective kinetic models.

Students and Researchers Attend 3rd Annual Princeton-CEFRC Summer School on Combustion

Close to 200 graduate students and researchers attended a week of lecturing at the third annual Princeton-CEFRC Summer School on Combustion, held on the Princeton campus from June 24 – 29, 2012. The summer school’s mission is to provide the next generation of combustion researchers with comprehensive knowledge in the technical areas of combustion theory, experimentation, computation and application.

This year’s group was even greater in number than the previous two years of 120 and 140 participants. The participants came from 24 states of the U.S. and 16 foreign countries, representing 36 U.S. and 16 international academic institutions, three U.S. government labs, six foreign research labs and six U.S. corporations. Refer to the graphics (Tables 1-3) in this article for some demographics of this year’s participant pool.

Participants began arriving Saturday afternoon and all day Sunday to check into the air-conditioned dormitory reserved for the Combustion Summer School. The many reunion-like greetings amongst returning students were truly heart-warming. On Sunday, the program kicked off with a welcome BBQ at the Cloister Inn, one of Princeton University’s eating clubs. The participants also attended a tour of the research labs of CEFRC PIs Professors Frederick L. Dryer, Yiguang Ju and Chung K. Law.

For the academic program, the foundational courses of Combustion Theory and Combustion Chemistry were offered again, as in previous years. This year, they were taught by Professors Heinz G. Pitsch of RWTH-Aachen and Hai Wang of USC, respectively. A new course on Internal Combustion Engines was jointly given by Professors Timothy C. Lieuwen of Georgia Tech (on gas turbines) and Rolf D. Reitz of Wisconsin (on reciprocating engines). Also new this year, in response to pre-

(Continued on page 9)
Students and Researchers Attend 3rd Annual Princeton-CEFRC

Summer School on Combustion (continued)

Table 1: 2012 summer school participants came from 16 international academic institutions.

- Cardiff University, UK
- Ecole Central Paris
- Graz University of Technology
- Ilie Murgulescu Institute of Physical Chemistry
- KAUST
- KTH, Royal Inst of Technology
- Kyoto University
- McGill University
- National Univ. of Ireland
- Peking University
- RWTH Aachen University
- Tsinghua University
- University of Maribor
- University of Miskolc
- University of Tsukuba

Table 2: 2012 summer school participants came from 16 foreign countries and the U.S.

- Austria
- Brazil
- Canada
- China
- France
- Germany
- Hungary
- Ireland
- Italy
- Japan
- Mexico
- Romania
- Saudi Arabia
- Slovenia
- Sweden
- Case Western Reserve
- Clemson University
- Colorado State University
- Cornell University
- Drexel University
- Georgia Institute of Technology
- Massachusetts Institute of Technology
- North Carolina State University
- Northeastern University
- Penn State University
- Princeton University
- Purdue University
- Rensselaer Polytechnic Institute
- Rutgers University
- Stanford University
- Syracuse University
- Texas A&M University
- University of Alabama
- University of Iowa
- UC San Diego
- UC Irvine
- University of Colorado
- University of Connecticut
- University of Dayton
- University of Illinois-Urbana
- University of Maryland
- University of Michigan
- University of Nebraska
- University of Southern California
- University of Texas-Austin
- University of Utah
- University of Wisconsin-Madison

Table 3: 2012 summer school participants came from 36 U.S academic institutions representing 24 states.

Also in response to suggestions from previous year’s participant feedback requesting greater exposure to current topics of combustion research, was a five-day lecture series on “Frontiers of Combustion” offered to all participants. Intended to be an end-to-end broad overview, the topics covered were Combustion in a Global Environment Context, given by Professor Robert H. Socolow of Princeton; New Developments in Combustion Technology, given by Dr. George A. Richards of DOE-NETL; Alternative Fuels Including Biofuels, given by Professor William H. Green of MIT; Cyber-Combustion, given by Dr. Jacqueline H. Chen of Sandia; and Nano-engineered Reactive Materials and Their Combustion and Synthesis, given by Professor Richard A. Yetter of Penn State.

Also in response to suggestions from previous year participants, the program was updated to include more “special events”. Last year, we initiated a career panel for the participants during lunch time. It was conducted as an informal panel discussion with each speaker making remarks on career prospects and market needs followed by questions from the participants. The feedback was hugely positive so that this year, with more lecturers scheduled for the week, two separate career panels were offered, with a good mix of academic, government and industry research staff represented in each. We were fortunate to have Professors Chung K. Law, Timothy A. Lieuwen, Heinz Pitsch, and Dr. Geo A. Richards for the first session, and Dr. Jacqueline H. Chen, Professor Rolf Reitz, Dr. John Farrell, and Professor Hai Wang for the second session. On both days, the participants hurried back early from their lunch break to attend the career panels. Based on the very positive feedback, we plan to offer this component of the summer school next year.

Another special event was an evening lecture given by Professor Tianfeng Lu of the University of Connecticut. His talk was entitled “Computational Tools for Diagnostics and Reduction of Detailed Chemical Kinetics” which provided a good segue into Dr. Chen’s lecture on Cyber-Combustion the following day.

(Continued on page 10)
The Summer School concluded Friday evening with a farewell dinner at the Frist Chemistry Building. Judging by the enthusiastic feedback from the participants, the summer school was again a great success. The CEFRC plans to continue offering the combustion summer school next year. Interested participants should check the CEFRC website. Information on the 2013 Session will be available in January.
Combustion Summer School Goes Global

The success of the 2010 and 2011 sessions of the Princeton-CEFRC Summer School, and the increasing participation of international students, demonstrated the need for such intense, high-level instructions on the key areas needed to advance combustion science and technology. Consequently, it has stimulated discussions of holding summer schools in other major geographical areas in the world, adopting similar goals and arrangements as those of the CEFRC Summer School. Tsinghua University in Beijing, China took the initiative and organized the first session of the Tsinghua-Princeton Summer School on Combustion through her Center for Combustion Energy, of which CEFRC PI C.K. Law is the founding director. This inaugural session, held on May 13-19, 2012, attracted over 300 participants, with 93 percent from mainland China and the rest from Korea, Japan and Taiwan. Eighty percent of the participants were graduate students with the remaining 20 percent made up of postdoctoral researchers and professional research staff from academic institutions and corporations.

The week-long program featured the two foundational courses of combustion theory and chemistry, which were respectively taught by PI C.K. Law and CEFRC advisor Michael J. Pilling of Leeds University. This pan-Asian summer school was also a huge success, as judged by the participants’ feedbacks, and will certainly be offered again in 2013.

CEFRC People in the News

Members of the CEFRC are proud to be the recipients of numerous awards and recognitions. Listed in the following are those announced recently.

Combustion and Flame, the official journal of the Combustion Institute, recently identified authors with the most publications in that journal from 2008 to 2012, showing PI Chung K. Law topping the list, at 22, followed by CEFRC advisor Katharina Kohse-Hoinghaus (at 17) and PIs Fokion N. Egolfopoulos (16), Chih-Jen Sung (13), Jacqueline H. Chen and Yiguang Ju (at 11 each). Fred Dryer, Ron Hanson and Hai Wang (at 10 each), occupying the 2nd, 3rd, 6th, 10th (tied) and 15th (tied) rankings respectively. Congratulations to all! It is of course also note that all the CEFRC PIs are prolific authors of high-quality papers, and Combustion and Flame is only one of the many prestigious publication outlets for the wide-range of our PIs’ research specialties. For example, other equally favored, high-level outlets include Journal of Physical Chemistry, International Journal of Chemical Kinetics, Journal of Fluid Mechanics, Physics of Fluids, and the various Physical Review journals.

Prof. Emily Carter delivered a National Science Foundation Mathematical and Physical Sciences Distinguished Lecture on February 24th at the NSF headquarters in Arlington, VA. The title of the lecture was: “The Role of Science in Moving the Planet to Green Energy and a Sustainable Future”. Prof. Carter was also inducted as a 2012 American Chemical Society Fellow in August, 2012.

Dr. Jacqueline H. Chen’s work on exascale computing systems was featured in the National Geographic’s Daily News section. Entitled: “Supercomputing Power Could Pave the Way to Energy-Efficient Engines,” the news article focuses on how the world’s most powerful supercomputers provide critical knowledge to spur the design of...

Prof. Frederick L. Dryer received the Alfred C. Egerton Gold Medal at the 34th International Symposium on Combustion in Warsaw, Poland. The award honors Dr. Dryer “for elucidating fundamentals of combustion chemistry and rates with distinguished, sustained and significant impact on combustion science and practical applications”.

Prof. Fokion N. Egolfopoulos delivered the keynote lecture entitled “Combustion Science and its Relevance to the Energy Needs of the 21st Century,” at the 22nd National Conference on Combustion Science and Technology at Kao Yuan University, Kaohsiung Science Park, Taiwan, April, 2012.

Prof. Yiguang Ju received the Bessel Research Award from the Alexander von Humboldt Foundation. Ju’s research in Germany will be devoted to combustion diagnostics and model development.


Prof. Rolf D. Reitz of the University of Wisconsin-Madison has joined the CEFRC as Principal Investigator. The addition of Dr. Reitz, who is associated with the Engine Research Center at Wisconsin, will strengthen our activities in turbulent combustion in the engine environment and provide closer liaison with the engine user community.

Prof. Donald G. Truhlar delivered one of the three keynote lectures in the symposium on Theory and Simulation in Energy and Fuel Production and Utilization at the National ACS Meeting in Philadelphia on August 21, 2012. His talk is entitled: “Multistructural and multipath variational transition state theory for predicting rate constants for mechanistic studies of biofuels combustion”.

Prof. Stephen B. Pope delivered the Hottel Lecture at the 34th International Symposium on Combustion in Warsaw, Poland. His talk was entitled: “Small scales, many species and the manifold challenges of turbulent combustion.” Prof. Pope also received the American Institute of Aeronautics and Astronautics (AIAA) Propellants and Combustion Award for in August, 2012. The award is presented for outstanding technical contributions to aeronautical or astronomical combustion engineering. Previous CEFRC PI winners of this award include C. K. Law (1994) and Ron K. Hanson (2005).

Dr. Haifeng Wang, a former CEFRC post doc supervised by Prof. Pope, received a Bernard Lewis Fellowship at the 34th International Combustion Symposium. Dr. Wang is currently an Assistant Professor at Purdue University.

Dr. Greg Smith of SRI, International has joined the CEFRC to work in collaboration with PI Hai Wang and other Center PIs on the foundational H2/CO/C1–4 chemistry model.

Dr. Jeffrey Sutton of Ohio State University has joined the CEFRC to experimentally investigate the turbulent flame structure in coordination with the modeling efforts of PIs Jacqueline Chen and Stephen Pope.

Dr. John Alecu, a roving post doc who had been conducting research with Prof. Donald G. Truhlar and Prof. William H. Green, has accepted a position with Hydrotex Partners Ltd. as Manager of Research and Development. We wish Dr. Alecu all the best in the next phase of his career.
Message from the Director

As the CEFRC enters its fourth year of operation, our sponsor DOE/BES has also just completed its mid-term review of our Center (see article on DOE/BES Mid-Program Review), with a largely complimentary evaluation of our operations and accomplishments. The PIs were understandably encouraged and gratified with the outcome, as we had indeed intensely and thoroughly prepared for the review, over a period of almost six months. The preparation was made even more challenging as this period overlapped with that for the paper preparation and submission to the 34th Combustion Symposium, with the deadlines for the submission of the review document and symposium manuscripts almost coincident. Hard choices had to be made and the Center is most grateful to those primary organizing PIs who had steered their time to the preparation of this mid-term review. Indeed, it is this sense of mission and dedication of the PIs, together with our fabulous team of junior associates, which has made my job as director such a rewarding one.

While being researchers we are by nature perpetually self-critical, it is nevertheless also useful and motivating to reflect on what we have done right so far in getting to where we are. Without any question the overriding factor is the technical excellence of our PIs, who in addition are dedicated to our mission and are collegial and collaborative in their technical interactions. Furthermore, in order to assure that we work as a single organism instead of 15 individual “strong-minded” investigators, we have instituted a 2D interaction matrix (see figure), with three disciplinary working groups on chemistry theory, chemistry experiment, and flames, interwoven with the development of three thrust mechanisms of the C\(_3\)-C\(_4\) fuels, the alcohols especially butanol, and biodiesel. The resulting synergy has been amazing, leading to accomplishments that can be truly considered as “the whole is greater than the sum of the parts”.

It is also becoming increasingly apparent that the Center has established two signature outreach programs that could serve as models for the development of high-level interdisciplinary scientific manpower: the roving post-doc program that ensures the joint and cross-fertilizing training of a post-doc fellow by two or more PIs at their respective sites; and the annual Summer School which offers intense, advanced-level courses on subject areas that are disciplinarily distinct but are crucial components of an interdisciplinary activity. The success of these initiatives is reported in this newsletter; it is believed that in due time these educational outreach programs would evolve to be the legacies of our Center.

I am also pleased to announce the addition of Professor Rolf Reitz of the University of Wisconsin at Madison as a PI of our Center. Professor Reitz is a world leader in the development and simulation of internal combustion engines. He directs the Engine Research Center at Wisconsin, is the editor of the International Journal of Engine Research, and the recipient of many honorific recognitions in engine-related R&D. His participation rounds off the technical coverage of the Center - from quantum mechanical calculations of reaction dynamics to the simulation of the combustion processes in engines. He will also serve as the Center’s liaison with the engine community, facilitating the transfer of the knowledge that we generate, including the various reaction mechanisms, to the engine community, hence fulfilling our overarching goal of: “Developing a validated, predictive, multi-scale, combustion modeling capability to optimize the design and operation of evolving fuels in advanced engines for transportation applications.”

I wish you continued success and intellectual fulfillment in your research.

Chung K. Law

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