CEFRC *news*

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

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INSIDE THIS ISSUE:

Exploiting Graphics Processing Units in Reactive-Flow Simulations

By Prof. Chih-Jen Sung and Kyle Niemeyer

Chih-Jen Sung
University of Connecticut

The heavy computational demands of high-fidelity CFD simulations, caused by fine grid resolutions and time step sizes in addition to complex physical models, are the primary bottleneck preventing most researchers from performing and using such studies. Reactive-flow simulations considering detailed chemistry further pose prohibitive computational demands due to chemical stiffness, as consequences of rapidly depleting species and/or fast reversible reactions, as well as the large and ever-increasing size of detailed reaction mechanisms.

In the past, one could rely on computational capabilities improving with time, simply waiting for the next generation of central processing units (CPUs) to enable previously inaccessible calculations. However, in recent years, the pace of increasing processor speed slowed, largely due to limitations in power consumption and heat dissipation preventing further decrease in transistor size. In order to keep up with Moore's Law, processor manufacturers are embracing parallelism. Top-of-the-line CPUs used in personal computers and supercomputing clusters contain four to eight cores. Graphics processing units (GPUs), on the other hand, consist of many hundreds to thousands of - albeit fairly simple - processing cores, and fall in the category of "many-core" processors. This level of parallelism matches that of large clusters of CPUs. The explosive growth of GPU processing capabilities as well as the diminishing cost in recent years have been propelled mainly by the video game industry's demand for fast, high-quality processing, and these trends will likely continue driven by commercial demand. As researchers identify computing problems with appropriate data parallelism, GPUs are becoming popular in many scientific computing areas such as molecular dynamics, protein folding, quantum chemistry, computational finance, data mining, and a variety of computational medical techniques.

Mechanism reduction is typically performed on large mechanisms to reduce the size from hundreds or thousands of species to a manageable value (*e.g.*, <100 species). Unfortunately, high-fidelity simulations using reaction mechanisms of this size are still too demanding to be performed on average computer systems. By utilizing the massively parallel architecture of relatively low-cost GPUs, previously inaccessible reactive-flow simulations may be performed on such systems. However, while GPUs offer the potential of significant performance enhancement, researchers are only beginning to explore GPU acceleration of reactive-flow solvers. Two members of the CEFRC team, Chen and Green, pioneered GPU computing for combustion simulations. Interested readers should peruse their publications for specific details.

Most reactive-flow codes rely on the operator-splitting or fractional-step method, where the large system of governing PDEs is separated such that different physical processes are evaluated separately. For the chemistry - typically the most time-consuming portion of the simu-

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Exploiting Graphics Processing Units in Reactive-Flow (cont'd)

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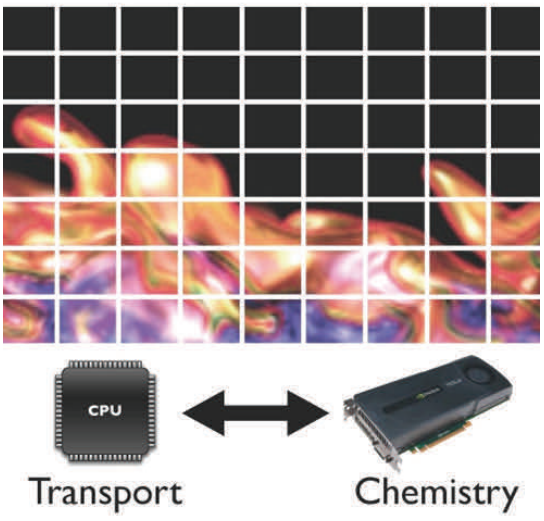
lation - this results in a system of independent ODEs for the conservation of species mass in each spatial location (*i.e.*, at each grid point or volume). Due to the independent nature of the integration for the systems of ODEs governing chemistry in each location, the entire set can be integrated simultaneously. Since the GPU-to-CPU performance ratio typically improves with increasing number of computational cells, this approach would be beneficial for large-scale simulations. The figure shown below demonstrates a concept where the chemistry integration would be performed on the GPU simultaneously with CPU transport calculations, so no portion of the calculation waits for the other to finish.

We have recently demonstrated new strategies for accelerating the chemical kinetics terms in reactive-flow simulations on GPUs. Unlike prior efforts, which mainly used standard explicit integration methods and focused on nonstiff kinetics, we showed that stabilized explicit methods, such as the Runge-Kutta-Chebyshev (RKC) method, can be used in the case of moderate stiffness. Using several reaction mechanisms of increasing size and stiffness, we showed that significant performance speedup is possible, by a factor of 59–96 and 10–18 compared to equivalent single- and six-core CPU versions respectively. For moderately stiff kinetics, the GPU-based RKC algorithm was shown to be significantly more efficient than the implicit VODE solver, an integration algorithm typically used in reactive-flow simulations. However, in the presence of more severe stiffness, RKC became less favorable as compared to VODE. Therefore, for problems with severe stiffness, an integration algorithm appropriate for GPU acceleration needs to be developed—this is one area we are currently focusing on.

In closing this brief communication, it is noted that while we focused on GPUs, the developed approaches apply to future many-core processing architectures in general. There is a trend towards massively parallel processors, and GPUs are an early entry in this category. In fact, in the case of the OpenCL programming language, the same programs written for GPUs now should be useable on whatever many-core processing standard is adopted, as it is designed for executing programs on heterogeneous computing platforms.



Finding Critical Flame Features with Chemical Explosive Mode Analysis (CEMA)

By Prof. Tianfeng Lu

Tianfeng Lu
University of Connecticut

Ignition and extinction are among the most important and complex events in combustion energy applications - ignition timing is key to the operation of IC engines, while extinction can broadly affect the fuel efficiency, engine safety and emissions. However, ignition and extinction are difficult to detect and model in turbulent combustion when they are embedded in the spatial features of premixed or non-premixed flames. Diagnostics of critical flame features is further complicated by the multicomponent and multi-step nature of practical fuels, for which one or several scalars, such as temperature, progress variable, mixture fraction, or a radical concentration, are frequently not adequate to identify such crucial events because of the large number of species and combustion modes involved.

In concert with the development of laser-based diagnostics of the structure and propagation of turbulent flames in laboratory and engine environments, much can be learned through the computational diagnostics of simulated combustion events, especially recognizing the rapidly increasing computational and physical-chemical fidelity of such simulations. Furthermore, development of supercomputers has passed the petaFLOPS point and is only a few years away from the exaFLOPS era, hence representing a tremendous increase in the computing power. Consequently, the capability to conduct 3-D device-scale direct flame simulations is on the horizon. As computer power ceases to be the limiting factor in flame simulations, the lack of adequate flame diagnostics to efficiently and accurately detect critical flame features from the massive flame data, *e.g.*, hundreds of terabytes or larger, quickly becomes the new bottleneck.

As a universal tool for systematic flame diagnostics, chemical explosive mode (CEM) was found to be critical for flame features including ignition and extinction. CEM is a chemical property associated with the positive eigenvalues of the chemical Jacobian, and thus indicates the propensity of the mixture to ignite, which is a critical feature that distinguishes combustible mixtures from other substances. The role that CEM plays in ignition and extinction is demonstrated in Fig. 1, which shows that CEM is present in pre-ignition mixtures (red) and absent in post-ignition mixtures (blue) in auto-ignition, while the competition between CEM and mixing is responsible for both extinction and ignition, *i.e.* the turning points on the S-curve, in perfectly stirred reactors (PSR). Further investigation showed that CEM possesses a similar behavior in premixed flames, with eigenvalue zero-crossing occurring in the reaction zone, resulting in a robust method to pinpoint premixed flame fronts in complex flow fields.

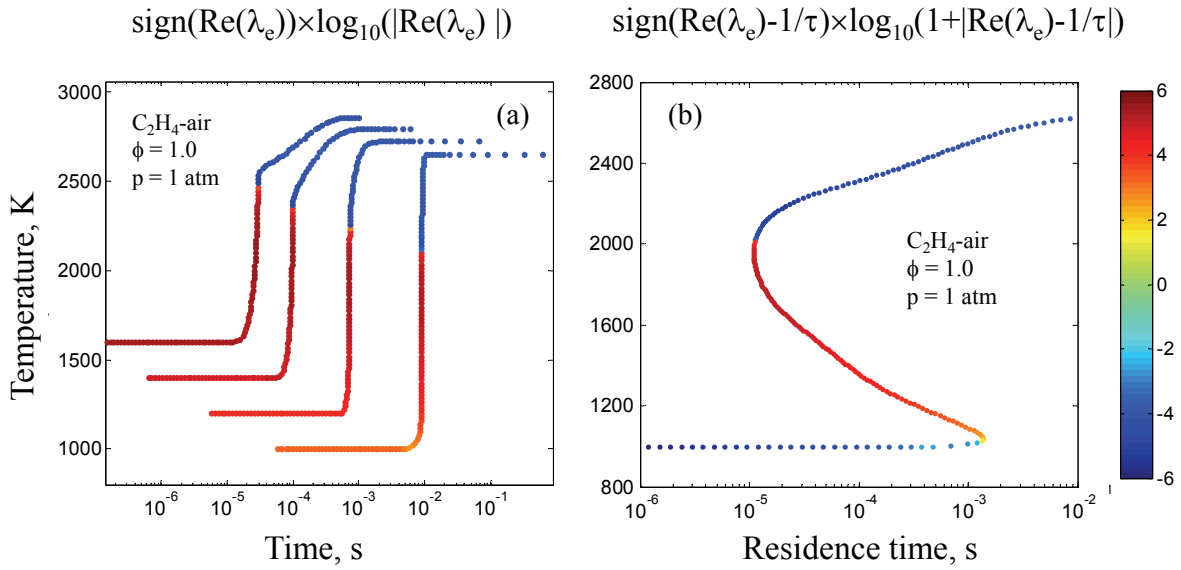


Figure 1. Timescales of CEM in (a) auto-ignition and (b) PSR, for stoichiometric ethylene-air at atmospheric pressure. In

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Finding Critical Flame Features with Chemical Explosive Mode Analysis (cont'd)

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collaboration with CEFRC PIs (Dr. J.H. Chen and Prof. C.K. Law), a chemical explosive mode analysis (CEMA) was applied to a lifted ethylene jet flame in heated coflowing air. It revealed the flame features (Fig. 2) that are difficult to observe with conventional methods, *e.g.,* weak lean premixed fronts hidden mostly in the background (the white isoline in Fig. 2), an auto-igniting layer that stabilizes the lifted flame, and controlling variables in different flame zones. The accurate identification of critical flame features renders it possible to perform subsequent on-the-fly data mining, *e.g.*, to obtain statistics conditioned on the flame features and to generate turbulent combustion models *in situ*. When applied in other flame simulations, CEMA further showed unique capability in detecting two-stage ignition at HCCI conditions, local extinction and re-ignition in premixed and non-premixed jet flames, and different modes of premixed flame propagation. Recently CEMA was built into Sandia's S3D DNS code and applied in CEFRC projects on alcohol combustion.

Another potential utility of CEMA is simplification of complex chemical kinetics of practical fuels. Since CEM plays an important role in various flame features, species and reactions that control CEM can be extracted to form a skeletal mechanism, which can be subsequently tuned to yield ultra-compact reduced models that can accurately mimic ignition and extinction behaviors of the detailed mechanism. A recent numerical experiment with dimethyl -ether (DME) shows that the reaction set in a minimal skeletal mechanism can be further halved by using the CEMA-based approach, with steady-state and transient ignition and extinction states precisely reproduced. Together with other available methods for mechanism reduction, the CEMA-based approach offers a solution to minimize the computational cost of flame simulations involving detailed chemistry, which is exploding in size nowadays.

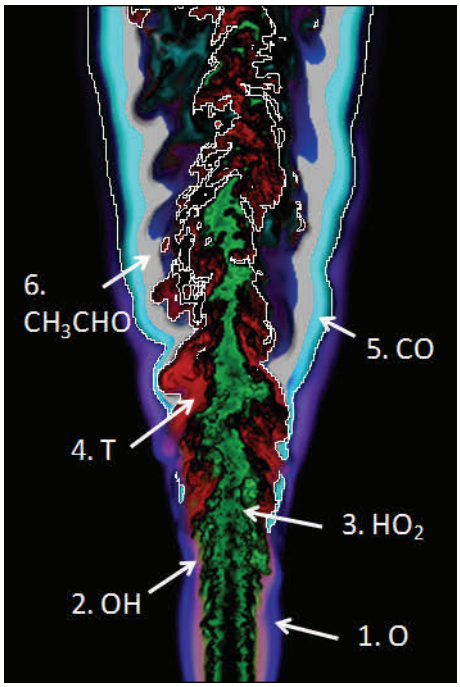


Figure 2. Controlling variables in a lifted ethylene jet flame into heated coflowing air (DNS by Yoo et al, PCI 2011). The white isoline indicates premixed flame fronts identified by CEMA.

Report by Combustion Energy Research Fellows

In this issue, we spotlight the research of Dr. Yury Suleimanov, a Combustion Energy Research Fellow co-sponsored by Professor William H. Green of MIT and Dr. Stephen J. Klippenstein of the Argonne National Laboratory. Dr. Suleimanov's research is focused on generating accurate theoretical estimates of rate coefficients using state-of-art techniques of quantum chemistry and rate theory for reactions controlling concentrations of the HO_2 radical.

Ring polymer molecular dynamics: trajectory based method to capture quantum mechanical effects of nuclear motions

By Yury Suleimanov

The goal of this collaborative research is to improve current theoretical approaches for accurately computing chemical reaction rates. Many classes of chemical reactions exhibit significant quantum mechanical characteristics due to the effects of zero-point vibrational energy and/or tunneling through an activation barrier. For this reason, several theoretical methods have been developed in the past in an effort to approximately incorporate these important quantum effects for large polyatomic systems. Many of these methods are refinements of transition state theory (TST). TST-based methods are sensitive to the choice of the transition state dividing surface, and Klippenstein has developed sophisticated ways to define better dividing surfaces for complex reactions. Proper identification of this dividing surface becomes increasingly difficult as the dimensionality of the problem increases due to the multidimensional nature of tunneling at low temperatures and sometimes (for such systems as heavy-light-heavy reactions) the dividing surfaces suffer from many recrossings at high temperatures. As a result, TST methods are often less reliable for polyatomic reactions [1].

To overcome this problem, we employ an alternative method based on ring polymer molecular dynamics (RPMD). RPMD is an approximate quantum theory based on the isomorphism between quantum statistical properties and classical mechanics which enables the inclusion of quantum effects via classical molecular dynamics simulations in an extended phase space. The RPMD rate coefficient is rigorously independent of the choice of the transition state dividing surface used to compute it, a feature that distinguishes it from TST-based methods. Recent applications of RPMD rate theory have demonstrated that it provides systematic and consistent performance across a wide range of gas phase chemical reactions [1-4]. The RPMD rate coefficient captures almost perfectly the zero-point energy effect, and is within a factor of 2-3 of the exact rate at low temperatures in the deep tunneling regime. Furthermore, RPMD rate theory has been shown to consistently underestimate the rates for symmetric reactions and overestimate them for asymmetric reactions [3]. The systematic and consistent performance of RPMD rate theory contrasts with the performance of TST-based methods, which can vary significantly in accuracy from one reaction to another due to their sensitivity to the choice of the transition state dividing surface.

The successful application of RPMD to small systems motivated us to develop an open-source software package RPMDrate for computing bimolecular gas-phase reaction rates of arbitrary polyatomic systems [5] which is now applied to gas phase chemical kinetics studies by several research groups worldwide. The consistent and predictable accuracy of RPMDrate results makes this code extremely attractive for further application to polyatomic chemical reactions when the exact quantum mechanical calculations are impossibly expensive and TST approaches exhibit unpredictable behavior.

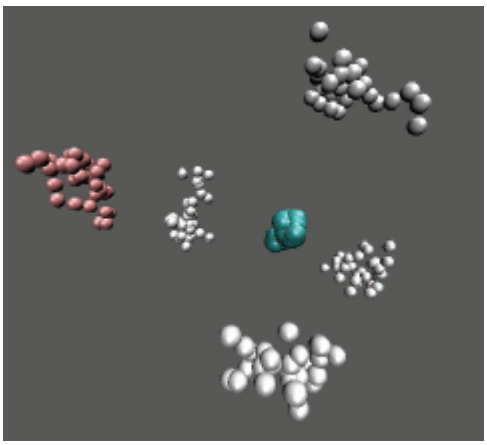


Illustration 1: Snapshot taken from the RPMD simulations of the $H+CH_4 \rightarrow H_2+CH_3$ reaction.

References:
[1] J. W. Allen, W. H. Green, Y. Li, H. Guo, and Yu. V. Suleimanov, "Communication: Full dimensional quantum rate coefficients and kinetic isotope effects from ring polymer molecular dynamics for a seven-atom reaction OH + $CH_4 \rightarrow CH_3 + H_2O$", J. Chem. Phys. 138 (2013) p. 221103 (open access: http://dx.doi.org/10.1063/1.4811329)
[2] Y. Li, Yu. V. Suleimanov, M. Yang, W. H. Green, and H. Guo, "Rate constants and kinetic isotope effects of the H/D/Mu+CH_4 reactions from ring polymer molecular dynamics", J. Chem. Phys., 138 (2013) p. 094307 (http://dx.doi.org/10.1063/1.4793394)
[3] Yu. V. Suleimanov, R. P. de Tudela, P. G. Jambrina, J. P. Castillo, V. Sàez-Ràbanos, D. E. Manolopoulos, and F. J. Aoiz, "A ring polymer molecular dynamics study on the family of isotopologues of the H+H_2 reaction.", Phys. Chem. Chem. Phys., 15 (2013) pp. 3655-3665 (http://dx.doi.org/10.1039/c2cp44364c)
[4] Y. Li, Yu. V. Suleimanov, M. Yang, W. H. Green, and H. Guo, "Ring polymer molecular dynamics calculations of thermal rate constants for the $O(^3P)$ + $CH_4 \rightarrow$ OH + CH_3 reaction: Contributions of quantum effects", J. Phys. Chem. Lett. 4 (2013) pp. 48-52 (http://dx.doi.org/10.1021/jz3019513)
[5] Yu. V. Suleimanov, J. W. Allen, and W. H. Green, "RPMDrate: bimolecular chemical reaction rates for ring polymer molecular dynamics", Comp. Phys. Comm. 183 (2013) 833-840 (http://dx.doi.org/10.1016/j.cpc.2012.10.017; http://ysuleyma.scripts.mit.edu)

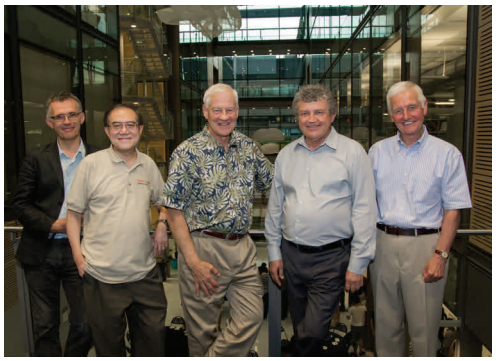
4th Annual CEFRC Summer School on Combustion Brings Students and Researchers to Princeton

2013 Princeton-CEFRC Summer School on Combustion
Photo: F. Wojciechowski

During the week of June 23-28, 2013, 180 graduate students and researchers from 11 countries, 23 states and 68 academic institutions, corporations and national laboratories attended the fourth annual Princeton-CEFRC Summer School on Combustion, hosted by Princeton University. The Summer School was fortunate to have returning lecturers Professors Moshe Matalon, from the University of Illinois at Urbana-Champaign and Michael J. Pilling, from the University of Leeds who gave the lectures for Combustion Theory and Combustion Chemistry, respectively. In addition to these two foundational courses, in response to previous years' student feedback, two new courses were added to this year's program. The first, Quantitative Laser Diagnostics for Combustion Chemistry and Propulsion, was given by Professor and CEFRC Principal Investigator Ronald K. Hanson of Stanford University. The second was a course in Computational Turbulent Combustion given by Dr. Thierry Poinsot, of the Institut de Mécanique des Fluides de Toulouse, CNRS.

The Summer School kicked off on Sunday afternoon with a tour of the combustion laboratories of Professors Frederick L. Dryer, Yiguang Ju, and Chung K. Law, followed by a welcome BBQ at the Tiger Inn, a campus eating club. The academic program consisted of daily three-hour lectures in the morning and afternoon from Monday to Friday. On Wednesday, the Summer School once again scheduled the very popular Career Panel Discussion. This year's panelists consisted of Prof. Emily A. Carter of Princeton University, John T. Farrell of ExxonMobil Research and Engineering, Prof. Ronald K. Hanson, Prof. Chung K. Law, and Dr. Thierry Poinsot. The discussion was conducted as an informal exchange, with each speaker making remarks on career prospects and market needs followed by questions from the participants.

The Summer School concluded on Friday evening with the traditional farewell dinner at the Frick chemistry building. Reading through the very positive participant feedback, it is clear that the Summer School was both educational and inspirational. **Arne Scholtissek**, from the Technische Universitaet Bergakademie Freiberg wrote, "The lecture of Dr. Poinsot was fun - I like his teaching style, combining broad and deep knowledge with humor. He tells a story but still comes straight to the point, which makes it easy to follow although the topic is very complicated. I was amazed at the LES-visualizations and the research examples that he showed. I suppose that even for non-numericists the lecture was very interesting because the problems he discussed were closely connected to technical applications." **Anna Oldani** of the University of Illinois at Urbana-Champaign wrote, "I think the instructors are one of the greatest aspects of this program. Where else is there such close access to leaders of their respective fields? Not only do students



In this photo (l to r): Dr. Thierry Poinsot, Profs. Chung K. Law, Ronald K. Hanson, Moshe Matalon, and Michael J. Pilling.
Photo: D.K. Crow

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4th Annual CEFRC Summer School (cont'd)

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have the opportunity to attend 15 hours of lecture over the course of the week, but they can also interact with professors at several other opportunities made possible by the nature of the program."

The CEFRC plans to offer the Combustion Summer School in 2014. Interested participants should check the CEFRC website for information on the 2014 session in January.

The 2013 Princeton-CEFRC Summer School is primarily funded by the U.S. Department of Energy, with additional support from the National Science Foundation and the Air Force Office of Scientific Research.

Photo: D.K. Crow

In these photos, participants gather for a farewell dinner at the Frick chemistry building.
Photo: D. K. Crow

2nd Tsinghua-Princeton Summer School on Combustion

Following the successful, inaugural Tsinghua-Princeton Summer School on Combustion held in China in 2012, the Center for Combustion Energy at Tsinghua University hosted the 2nd Summer School on July 7-12. It was attended by over 320 participants, coming from practically every part of China as well as other Asian countries including Korea, Japan and Saudi Arabia (KAUST). The academic program follows that of the well-established Princeton-CEFRC Summer School, except at a larger scale which demanded special logistical considerations. Lectures were given by Prof. Heinz Pitsch on Combustion Theory, Prof. Hai Wang on Combustion Chemistry, Prof. Tim Lieuwen on Gas Turbine Combustion, and Prof. Marcus Alden on Combustion Diagnostics. For many participants this was their first exposure to such a powerful group of master lecturers in combustion. The impact that this Summer School will have in advancing combustion science and technology in this rapidly developing part of the world can hardly be estimated.

2013 EFRC PI Meeting in Washington DC, July 18-19

Our sponsor, the DOE-BES, called an EFRC-wide Principal Investigators' Meeting in Washington DC in July to review progress. Each center was allocated nine attendees. The CEFRC sent seven PIs (Chen, Egolfopoulos, Green, Klippenstein, Law, Sung and Wang,), a roving post-doc (Enoch Dames) and a graduate student (Ting Tan). Each PI either presented a podium talk or prepared and then manned a poster, listed in the following, highlighting the breadth and depth of the research activities being conducted at the Center.

Podium Talks

Jacqueline H. Chen: "High-Fidelity Simulations of Turbulence-Chemistry Interactions Towards Predictive Models for Energy Conversion Devices with Alternative Fuels"

William H. Green: "Predicting the Performance of Alternative Fuels"

Posters

- "Development of Predictive Combustion Kinetics for Model Biodiesel Fuels", by Emily A. Carter, **Fokion N. Egolfopoulos**, Nils Hansen, Ronald K. Hanson, Yiguang Ju, Stephen J. Klippenstein, Chung K. Law, Chih-Jen Sung

- "Contributions from Theory to Butanol and Biodiesel Combustion Modeling", by Emily A. Carter, Donald G. Truhlar, William H. Green, Chung K. Law, **Stephen J. Klippenstein**

- "Unraveling Chemistry-Transport Coupling in Flames" by Jacqueline H. Chen, Frederick L. Dryer, Fokion N. Egolfopoulos, Yiguang Ju, **Chung K. Law**, Stephen B. Pope, Rolf D. Reitz

- "Experimental Insights into Chemical Kinetics of Biofuel Combustion", by Frederick L. Dryer, Nils Hansen, Ronald K. Hanson, Yiguang Ju, **Chih-Jen Sung**

- "Uncertainty Quantification and Propagation in Reaction Kinetics and Kinetic Models", by S. J. Klippenstein, K. Kumar, C. J. Sung, D. A. Sheen, Y. Tao, O. Park, F. N. Egolfopoulos, **H. Wang**

A sixth poster, prepared by PI Professor Chih-Jen Sung and his graduate students Kyle Brady and Nicholas Curtis and shown in the next page, was submitted and displayed in response to the call for "EFRC Science in Only Ten-Hundred and One Words Challenge". The objective of this Challenge was to use only a list of the 1001 most commonly used words in the English language to describe and highlight an EFRC-centric theme, meant for a general audience. You may find all the entries at http://www.energyfrontier.us/posters.

During the two-day conference the attending CEFRC PIs also held extensive meetings among ourselves to discuss the mission and strategy for the next phase of the CEFRC, in anticipation of the preparation of the renewal proposal for the Center. Reviewing all the CEFRC activities in the past four years, the PIs unanimously felt a strong sense of satisfaction with our various aspects of accomplishments, and look forward with excitement to do the additional science in CEFRC-II.

CEFRC Science in 1001 Words (A DOE-EFRC Challenge)

CEFRC People in the News

Prof. Emily A. Carter gave the Francis Clifford Phillips Lectures on May 1-2 in the Department of Chemistry of the University of Pittsburgh. The titles of her lectures were: "A Quantum Search for Fuels from Sunlight" and "Quantum Mechanics without Wavefunctions." **Carter** also gave the Tedori-Callinan Lecture in April, 2013 at the Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania and was honored for "pioneering discoveries in theoretical and computational materials research, and for advancing sustainable energy solutions through innovative research combining chemistry and mechanics. The title of her lecture was "Quantum Mechanics and the Future of the Planet." Also in 2013, **Carter** gave the W. Allan Powell Lecture at the Virginia Section of the American Chemical Society, University of Richmond. The title of her lecture was "The Role of Science in Moving the Planet to Green Energy and a Sustainable Future."

Congratulations to **Prof. Fokion N. Egolfopoulos** for his appointment to the William E. Leonhard Professorship in Engineering at the University of Southern California.

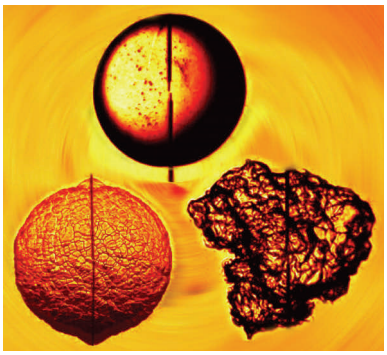
Congratulations to **Profs. William H. Green and Donald G. Truhlar** whose recently accepted article "New Pathways for Formation of Acids and Carbonyl Products in Low-Temperature Oxidation: The Korcek Decomposition of γ-ketohydroperoxides (DOI: 10.102/ja4034439) was featured in the Journal of the American Chemical Society (JACS) Spotlights in August 2013.

In June 2013, **Prof. William H. Green** gave the keynote lecture at the Frontiers in Chemical Reaction Engineering Symposium to inaugurate the new Laboratory for Chemical Technology at the University of Ghent. The title of his lecture was "Understanding and Predicting Complex Gas Phase Kinetics."

Prof. Ronald K. Hanson was the co-winner of the SAE Arch T. Colwell Merit Award in April 2013. Also in April, Hanson delivered the Edison Engineering Lecture at Notre Dame University. The title of his lecture was "Laser-Based Diagnostics for Combustion and Propulsion: Absorption and Fluorescence." **Prof. Hanson** was also recognized by the Applied Optics Journal as the 16th "Most Published Authors of the Past 50 Years".

Congratulations to **Prof. Yiguang Ju**, who was named at Princeton University to the Robert Porter Patterson Professorship in July, 2013. Additionally, the Institute of Mechanics of the Chinese Academy of Sciences presented **Prof. Ju** the Hsue-Shen Tsien Professorship of Engineering Sciences upon the delivery of a lecture entitled "The Challenges and Opportunities of Combustion Research."

Prof. Yiguang Ju and **Prof. Chung K. Law**'s research groups won First Places in the Combustion Art Competition at the 2013 National Combustion Meeting. The artwork by Ju's group, entitled "Turbulent Flame is a Beauty of Art!" won first place for "Artistic Merit", and one by Law's group, entitled "Three Faces of an Expanding Flame" won first place for "Scientific Merit".



First Place for Scientific Merit:
Three Faces of an Expanding Flame

First Place for Artistic Merit:
Turbulent Flame is a Beauty of Art!

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CEFRC People in the News (cont'd)

(Continued from page 10)

In May 2013, **Prof. Donald G. Truhlar** was honored by the International Symposium on Organic Reaction Mechanism in celebration of Bob Grubbs, Ken Houk, Paul Schleyer and Don Truhlar as "four of the great chemists of our time," at Peking University, Shenzhen Graduate School.

Dr. Yue Yang, a Combustion Energy Research Fellow who has been conducting research with Professor Stephen B. Pope and Dr. Jacqueline H. Chen, has been appointed Assistant Professor at Peking University.

Dr. Bret Windom, a Combustion Energy Research Fellow who has been conducting research with Professors Yiguang Ju and Fokion N. Egolfopoulos, has been appointed Assistant Professor at the University of Colorado at Colorado Springs (UCCS).

We wish Dr. Windom and Dr. Yang all the best as they embark on the next phase of their scientific career.

Upcoming Events

SEPTEMBER 2013
8th Mediterranean Combustion Symposium
www.ichmt.org/mcs-13/
Çeşme, İzmir, Turkey
September 8-13, 2013

MUSAF II Colloquium
http://www.cerfacs.fr/musaf/
Toulouse, France
September 18-20, 2013

OCTOBER 2013
2013 Western States Fall Technical Meeting
www.eecl.colostate.edu/combustioninstitute
Fort Collins, CO
October 7-8, 2013

2013 Eastern States Fall Technical Meeting
www.clemson.edu/ces/me/essci/essci2013.html
Clemson, SC
October 13-16, 2013

Air Quality IX: Int. Conf. on Environmental Topics Associated with Energy Production
http://www.undeerc.org/AQ9/
Arlington, VA
October 21-23, 2013

DECEMBER 2013
35th International Combustion Symposium
Deadline for paper submission
December 5, 2013

Message from the Director

With this newsletter the DOE-EFRC program, including the CEFRC, enters its fifth and final year of funding. With renewal of the program currently being considered by Congress and our sponsor the DOE-BES, it is instructive to review what has been accomplished by the EFRC as a whole and by the CEFRC in particular. Regarding the former, a directors' session was convened with the BES management at the EFRC PIs meeting in DC in July to jointly identify the criteria defining success of the EFRC. In addition to the obvious criteria based on the number and quality of publications and patents, and the merit of Team Science – the whole is greater than the sum of the parts, the following specific attributes of the EFRC were highlighted: focus on energy, involving students, post docs and PIs on a unified mission; dual focus on science and technology; long term and size of the collaboration, accelerating rate of scientific discovery; tackling of big problems; coupling of experiment, computation and theory; facilitating collaboration between academic institutions and government labs, for example the use of the advanced light source; team science covering wide disciplines; director providing coordination and focus; and availability of advisory committee for guidance.

To assess the accomplishments of the CEFRC, let us first review our mission statement: "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." To accomplish this goal, we have been following a 2D matrix of investigation, consisting of the study of chemically reacting flows through chemistry-theory, chemistry-experiments, and flames, which are interwoven with the specific target of developing reaction mechanisms for the foundation, alcohol and biodiesel fuels. Based on the above goal, it is quite evident that we have made extensive and critical contributions to combustion energy science over the past four years, as substantiated by the large number of publications in high-level journals. A surprising consensus that has emerged from our investigations and frequent discussions among the Center PIs is that there exist substantial deficiencies in the theoretical and experimental methodologies currently employed in the study of chemical kinetics. This in turn has led to considerable uncertainties in the published and subsequently adopted reaction mechanisms of various fuels. Their inherent detrimental impact on the development of combustion science is particularly alarming by further recognizing the recent proliferation of papers reporting experimental and computed kinetics data, as well as follow-on studies using these data, apparently without sufficient attention paid to their limitations in many of these studies. In response to such a concern, we have decided to undertake the mammoth task of preparing critical review/position papers highlighting such limitations. We believe that these documents would serve not only as a credible accounting of our performance on behalf of the CEFRC, but even more importantly they would provide critical assessments of the published data as well as guideline for further improvement in the theoretical and experimental methodologies.

As in almost every branch of science, computation has become an essential tool in combustion research. The challenge in simulations involving complex chemical reactions is the computation load due to the large number of species and reactions as well as the associated stiffness. Furthermore, even if the flow field and the myriad chemical entities can be resolved, we are still faced with the daunting task of abstracting out the physics from the massive data generated. In this newsletter we report two new developments in this area: PI Professor Chih-Jen Sung of the University of Connecticut reports on "Exploiting Graphic Processing Units in Reactive Flow Simulations," and guest contributor Professor Tianfeng Lu, also of the University of Connecticut, reports on the computational diagnostics technique using CEMA (Chemical Explosive Mode Analysis).

A signature program of the CEFRC is the Summer School on Combustion. In June the CEFRC held its 4th session at Princeton, attended by over 180 participants. In addition to the foundational courses of Combustion Theory and Combustion Chemistry, two new courses, on Laser Diagnostics and Computational Turbulent Simulation, were added. The attendee were uniformly enthusiastic with the lectures and the networking opportunities. A sister summer school, held at Tsinghua University in Beijing in July, attracted over 320 attendees and was equally successful. Both summer schools will surely be offered again in 2014.

In the next few months members of the worldwide combustion community will be busily involved in the preparation of papers for submission to the 2014 international combustion symposium. I wish you all the best in your scientific discovery and the preparation of stellar papers in reporting them.

Chung K. Law

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