CEFRC *news*

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

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INSIDE THIS ISSUE:

Comparison of Advanced Combustion Strategies for Transportation Engines

By Prof. Rolf D. Reitz and Adam Dempsey

Rolf D. Reitz University of Wisconsin-Madison

In an effort to reduce NOx and soot emissions in-cylinder, while maintaining high thermal efficiency, many new compression ignition combustion strategies have been proposed over the last two decades. These concepts are classified as low temperature combustion (LTC). One of the first and simplest methods of achieving LTC is homogeneous charge compression ignition (HCCI) combustion. By definition, in HCCI combustion the fuel and air are completely premixed in a relatively lean mixture ($\Phi < 0.5$) and compressed until autoignition occurs. HCCI combustion has been shown to have superior characteristics in terms of thermal efficiency and low NOx and soot emissions. However, fully premixed HCCI has no direct means to control the combustion process on a cycle-to-cycle basis.

In order to maintain control over the combustion process on a cycle-to-cycle basis there must be a coupling between the fuel injection events and the combustion event. This has prompted a large movement in the engine research community into partially premixed combustion (PPC). This concept is a hybrid between HCCI and conventional diesel combustion. To avoid high NOx and soot formation rates, the fuel must have sufficient time to mix with the air before ignition takes place. Two promising PPC strategies under investigation today are gasoline PPC and dual-fuel RCCI. Gasoline PPC premixes the majority of the fuel and direct injects the remainder of the fuel early in the cycle during the compression stroke. This provides equivalence ratio stratification in the combustion chamber and it is thought that by varying the level of stratification, the combustion process can be controlled. Dual-fuel RCCI is similar in that it premixes a high octane number fuel like gasoline, but the direct injected fuel has a low octane number, like diesel fuel, which is direct injected during the compression stroke. Thus, in addition to equivalence ratio stratification, gradients in fuel reactivity are established which have been shown to result in significant reductions in the cylinder pressure rise rate, which is related to combustion noise.

Moving forward in the development of these combustion concepts, the question will be how sensitive are these strategies to environmental conditions and can they be controlled on a vehicle on a cycle-to-cycle basis? Figure 1 shows the production version of a General Motors 1.9L diesel engine typically used for passenger car applications. A single-cylinder version of this engine was used in our current study. Figure 2 shows the combustion sensitivity of gasoline PPC and dual-fuel RCCI when

Figure 1: Light-duty experimental diesel engine

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Comparison of Advanced Combustion Strategies (cont'd)

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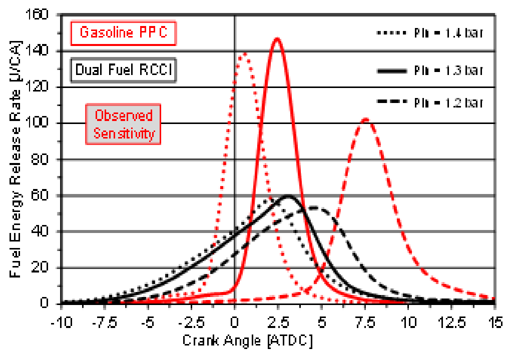
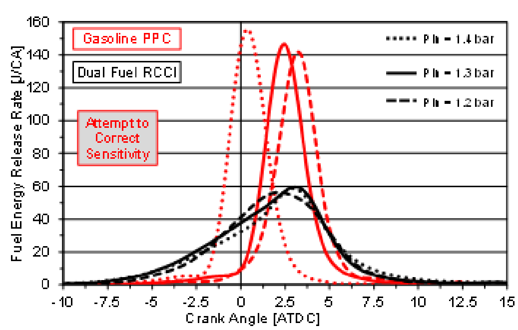


Figure 2: Combustion sensitivity of Gasoline PPC and Dual-Fuel RCCI to engine intake pressure

the engine intake pressure was perturbed, which varies widely for a turbocharged engine. As can be seen, the ignition timing of both strategies is sensitive to intake pressure, but dual-fuel RCCI to a lesser extent. The reason for this is not entirely understood and will be a topic of future engine modeling research using CFD modeling with detailed chemical kinetics and CEFRC mechanisms.

Perhaps more important for future LTC engines than the sensitivity itself, is the ability of the combustion to be controlled. Figure 3 shows the results of attempting to correct the observed combustion sensitivity to the intake pressure for both strategies by varying the percentage of premixed fuel and the direct fuel injection timing if necessary. As can be seen, for RCCI, the observed sensitivity is easily corrected through small changes in the premixed gasoline percentage. This ensures that the charge remains predominately premixed, with ultra-low NOx emissions. On the contrary, gasoline PPC struggles to retard the combustion phasing for the increased intake pressure case, and in the case of the decreased intake pressure, the equivalence ratio stratification requires such a substantial increase that the NOx emissions become unacceptably high, as summarized in the Table.

The results of this experimental campaign suggest that not only does in-cylinder fuel blending of fuel reactivity lessen the pressure rise rate of partially premixed combustion, but it also provides a mechanism to control the combustion process, while maintaining low NOx emissions. Current research efforts are focused on studying fuel effects on RCCI combustion; namely investigating the use of ethanol and methanol as the low reactivity fuel.



	1.2 bar	1.3 bar	1.4 bar
Premixed Fuel			
RCCI	91.5%	92.6%	93.5%
PPC	65%	79.1%	94.7%
DI Fuel Timing			
RCCI	45° bTDC	45° bTDC	45° bTDC
PPC	35° bTDC	65° bTDC	65° bTDC
NOx Emissions [g/kg-fuel]			
RCCI	< 0.05	< 0.05	< 0.05
PPC	6.8	< 0.05	< 0.05

Figure 3: Results of attempting to correct for the intake pressure sensitivity on Gasoline PPC and Dual-Fuel RCCI Combustion

Measurements in Turbulent Dimethyl Ether Flames: Physical Insights and Model Validation

By Prof. Jeffrey A. Sutton

Jeffrey A. Sutton
Ohio State University

The combustion of fossil fuels was instrumental in the industrial and technological revolution(s) of the last two centuries and currently accounts for more than 85% of the world's energy usage with applications ranging from power generation to transportation to industrial processing. However, increasing concerns of environmental impacts and energy sustainability has led researchers to investigate potential alternatives to traditional petroleum-derived fuels. In terms of transportation fuels, several promising and diverse candidates exist, many of which are being investigated as part of the research within the CEFRC.

One particular fuel of interest is dimethyl ether (DME; CH_3OCH_3), which has the potential to be used as substitute for diesel fuel in compression-ignition (CI) engines. The use of DME can result in high thermal efficiencies and improved ignition properties as compared to diesel-fueled engines due to its high cetane number and can be used as a "drop-in" replacement or supplement in existing CI engines. In addition, DME has shown a propensity for cleaner engine operation with decreases in particulate formation and nitrogen oxide emissions under certain conditions.

Within the CEFRC, DME is important as it is currently the only "alternative" fuel connecting chemical kinetic development to turbulent combustion research. Chemically, DME is the simplest ether and models describing its chemistry are manageable; that is, detailed kinetic models involve less than 100 species and 500 reactions and accurate, reduced "skeletal" models involve 30 or fewer species. Such reaction mechanisms are tractable for turbulent flame simulations. In terms of experiments, DME has sufficient vapor pressures at elevated pressures such that elaborate preheating schemes are unnecessary (as in the case of larger, low-vapor pressure fuels), thus facilitating well-defined, canonical turbulent flames with repeatable boundary conditions and measurements with high precision.

As part of the CEFRC research program, measurements are underway to understand the effects of turbulent fluid mechanics on species transport and reaction chemistry, often termed "turbulence-chemistry interaction", within flames fueled by DME. A twofold strategy is taken which consists of planar imaging of targeted species such as OH and CH2O to understand turbulent DME flame structure and 1D multi-scalar measurements of temperature and major species concentrations to characterize the thermo-chemical state of turbulent DME flames.

Initial 2D imaging studies have been performed in a new set of DME/H_2/N_2 non-premixed jet flames that were formulated to match that of existing "DLR" CH_4/H_2/N_2 jet flames that serve as computational target cases within the Turbulent Nonpremixed Flame (TNF) workshop. For the DLR flames, the fuel is 22.1% CH_4, 33.2% H_2, and 44.7% N_2 and for the DME-based flames, the methane is directly replaced by the DME, resulting in a fuel mixture that is 22.1% DME, 33.2% H_2, and 44.7% N_2. Both sets of flames operate in the same facility, under the same Reynolds number conditions and are characterized by nearly identical stoichiometric mixture fractions. These operational conditions were chosen to directly examine turbulent flame structure differences when CH_4 is replaced by DME.

A comparison of instantaneous images of the reactive hydroxyl (OH) layer obtained using planar laser-induced fluorescence (PLIF) is shown in Fig. 1 for the methane-based DLR flames and DME flames at a jet Reynolds number of 22,800. It is noted that the DLR flames appear more wrinkled, with what appears

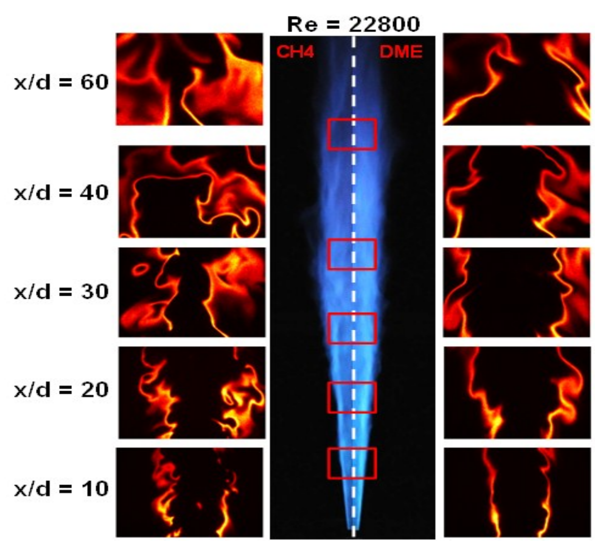


Fig. 1 – Comparison of OH PLIF images in the DLR CH_4/H_2/N_2 flames (left) and the DME/H_2/N_2 flames (right) showing the instantaneous turbulent flame structure. Visible photographs of the two flame configurations are shown in the middle column.

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Measurements in Turbulent Dimethyl Ether Flames (cont'd)

(Continued from page 3)

to be significantly higher levels of local extinction (*i.e.,* "holes" in the OH layer) than the DME-based flames. Simply put, it appears that the local turbulence is affecting the DME-based flames much less than the DLR flames. For example, at an axial position of x/d = 10, the DME-based flame looks "laminar-like", while the DLR flame is highly strained, wrinkled, and segmented. Measurements such as these can be used to analyze the effects of turbulence on fundamental DME combustion processes since the spatial structure of the flame is a direct result of the competition between the turbulent fluid mechanics, transport processes, and finite-rate flame chemistry. Furthermore, similar experimental results will be compared to direct numerical simulation (DNS) results performed by Jacqueline Chen's group at Sandia to examine extinction/re-ignition statistics, which serves as stringent test to for the coupled kinetic and transport models in turbulent environments.

In addition to the 2D imaging studies, 1D combined Raman scattering, Rayleigh scattering, and carbon monoxide (CO) laser-induced fluorescence (LIF) diagnostics are being applied in a series of highly turbulent piloted, partially-premixed DME/air jet flames in collaboration with Dr. Robert Barlow at the Combustion Research Facility (CRF) at Sandia National Laboratories. These multi-scalar techniques are used to obtain simultaneous measurements of DME, N_2, O_2, H_2O, H_2, CO, CO_2, and temperature and deduce the important variable, the mixture fraction, which characterizes the state of mixing in turbulent flames. It is anticipated that these measurements in DME flames will be used in a similar capacity as the rich sets of data obtained in hydrogen- and methane-based flames over the last 20 years; that is, to assess turbulent combustion model performance. Within the CEFRC, the DME flame measurements will serve as benchmark data to be used as validation for LES/PDF combustion models developed by Stephen Pope's group at Cornell.

Engine combustion is characterized by highly turbulent conditions, which results in complex relationships between unsteady fluid dynamics, species transport, finite-rate chemical kinetics, and non-equilibrium thermodynamics over a broad range of spatial and temporal scales. While each of these processes have received considerable attention over the last few decades, our knowledge of the effects of their complex coupling, even in laboratory-scale turbulent flames with simple fuels, remains incomplete. This combined with the potential operation of new fuels such as DME with variations in chemical and physical properties (as compared to conventional hydrocarbons) provides a formidable challenge for controlling combustion chamber processes and developing robust and predictive computational models. To accomplish these goals will require a focused effort combining state-of-the-art experimental and computational tools such as found within the CEFRC.

Announcing the 2013 Princeton-CEFRC Summer School on Combustion

Mission

To provide the next generation of combustion researchers with a comprehensive knowledge in the technical areas of combustion theory, chemistry, experiment, computation and applications.

Program

The 2013 session will be the fourth time that the Combustion Summer School is offered. The 2013 session, scheduled for June 23 to June 28, 2013, will offer the following courses: (1) Combustion Theory; (2) Combustion Chemistry; (3) Quantitative Laser Diagnostics for Combustion Chemistry and Propulsion; and (4) Computational Turbulent Combustion. For additional information, visit http://www.princeton.edu/cefrc/combustion-summer-school/.

Course Descriptions:

Combustion Theory

Lecturer: Moshe Matalon, University of Illinois at Urbana-Champaign

Objective: The aim of this course is to provide students with an understanding of the basic principles of combustion processes, how they relate to experimental observations and how they can be used in theoretical and numerical modeling. The subject is presented in a systematic way emphasizing, in particular, the mathematical character of the various combustion problems and the advances that took place in recent years. The first four lectures cover the fundamentals of chemically reacting flows, general conservation equations and various classifications of combustion processes. One lecture is allocated to detonation waves and the remaining lectures focus on low-speed combustion, or flames. Four lectures are devoted to premixed combustion, and include the structure of a planar premixed flame and the determination of the laminar flame speed, hydrodynamic effects, stretched flames, and ignition and extinction phenomena. Three lectures are devoted to non-premixed combustion and cover the structure of a diffusion flame, the mixture fraction formulation, flame lift-off and edge flames, the burning of condensed fuels and spray combustion. The remaining three lectures are devoted to flame instability, hydrodynamic and thermo-diffusive, and to turbulence covering in particular the various regimes of turbulent combustion and the notion of the turbulent burning velocity.

Professor Moshe Matalon received his Ph.D. in Mechanical and Aerospace Engineering from Cornell University in 1978. After two years on the faculty of the Aerodynamics Laboratories of the Polytechnic Institute of New York he joined the McCormick School of Engineering and Applied Science at Northwestern, where he was Professor of Mechanical Engineering and of Applied Mathematics. In 2007 he joined the Department of Mechanical Science and Engineering at the University of Illinois Urbana-Champaign where he holds the College of Engineering Caterpillar Chair. His research interests are in combustion theory, theoretical fluid mechanics and applied mathematics.

Combustion Chemistry

Lecturer: Michael J. Pilling, University of Leeds

Objective: The aim of this course is to provide students with an understanding of how rate coefficients and products of elementary reactions of importance in combustion are determined experimentally, how they are used in conjunction with theoretical models and how they are incorporated in chemical mechanisms for use in combustion models. Determination of the thermodynamic properties for radical species will also be discussed. The course will be illustrated by a number of examples of relevance to high and low temperature hydrocarbon oxidation and NOx formation and control; with a discussion on the impact of combustion emissions on climate change and air quality.

Professor Michael J. Pilling received his Ph.D. in physical chemistry in 1967. He first worked in Cambridge and Oxford Universities and was appointed Professor of Physical Chemistry at Leeds in 1989. Professor Pilling has worked extensively in chemical kinetics for over 30 years, especially on laboratory measurements using laser flash photolysis. Professor Pilling's research interests center on fundamental chemical kinetics and applications in atmospheric chemistry and combustion.

Quantitative Laser Diagnostics for Combustion Chemistry and Propulsion

Lecturer: Ronald K. Hanson, Stanford University

Objective: Fundamentals of laser absorption and laser-induced fluorescence in gases, including molecular spectroscopy and photophysics. Basics of shock tubes as a primary tool for studying combustion chemistry, including recent advances. Example state-of-the-art applications of species-specific sensing for shock tube kinetics studies, and multi-parameter sensing in different types of propulsion flows and engines.

Professor Ronald K. Hanson received his Ph.D. in aeronautics and astronautics

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Announcing the 2013 Princeton-CEFRC Summer School on Combustion (cont'd)

(Continued from page 5)

from Stanford University. He has been affiliated with the mechanical engineering department at Stanford since 1972, serving as department chair from 1993-2003 and holding the Woodard Chair from 1994. He has advised over 85 Ph.D. graduates and authored or co-authored over 500 journal publications in the fields of laser diagnostics and sensors, shock wave physics, advanced propulsion and combustion chemistry.

Computational Turbulent Combustion

Lecturer: Thierry Poinsot, Institut de Mecanique des Fluides de Toulouse CNRS

Objective: This course will enable engineers and research specialists with knowledge of fluid mechanics to move to an integrated understanding of numerical combustion especially in the field of unsteady turbulent combustion. It will present basic techniques and recent progress in numerical combustion while establishing important connections with the underlying combustion basics. The course will include RANS, LES, and DNS modeling but also numerical methods adapted to these models. It will present and explore multiple examples of turbulent combustion and combustion instabilities in real combustors.

Dr. Thierry Poinsot received his Ph.D. in heat transfer from Ecole Centrale Paris in 1983 and his These d'Etat in combustion in 1987. He is a research director at IMFT (CNRS) in Toulouse, head of the CFD group at CERFACS, senior research fellow at Stanford University and consultant for various companies. Dr. Poinsot's research interests are in combustion theory, numerical methods for turbulent and laminar flames, combustion instabilities, massively parallel simulations for gas turbines, piston engines, rockets and furnaces.

Residence and Meals:

Dormitory lodging is available in air-conditioned, single-person rooms on the beautiful campus of Princeton University. Meal plans are also available to participants.

Student Scholarships:

All non-Princeton University students who are enrolled at U.S. academic institutions will receive scholarships sufficient to cover the expenses for up to 7 days of dormitory lodging from 6/22-6/29, 2013. All Princeton University students will receive scholarships sufficient to cover the expenses for 5 days of lunch, from 6/24-6/28, 2013.

Important Dates:

Application deadline: March 15, 2013

http://www.princeton.edu/cefrc/combustion-summer-school/application/

Acceptance announcement: March 29, 2013

Registration deadline: April 15, 2013

Contact:

Further inquiries on the academic program or logistics of participation may be made by contacting:

Lilian Tsang, CEFRC Program Administrator
Email: ltsang@princeton.edu
Telephone: 609.258.5041

Tsinghua-Princeton Summer School on Combustion 2013

The second annual Tsinghua-Princeton Summer School on Combustion will be held at Tsinghua University, Beijing, China from July 7-12, 2013. This year's program will feature courses in Combustion Theory, Combustion Chemistry, Laser Diagnostics in Combustion, and Gas Turbine Combustion, to be delivered respectively by Prof. Heinz Pitsch of RWTH Aachen, Prof. Hai Wang of the University of Southern California, Prof. Marcus Aldén of Lund University, and Prof. Timothy C. Lieuwen of the Georgia Institute of Technology.

The Combustion Institute Summer School 2013

The Combustion Institute together with local host National Centre for Combustion Science and Technology (CECOST) will hold the first Combustion Institute Summer School (CISS) in Lund, Sweden from August 19-23, 2013. This pilot program will feature courses in Chemical Kinetics, Turbulent Combustion, and Diagnostics, to be delivered respectively by Prof. Henry Curran of NUI Galway, Prof. Norbert Peters of RWTH Aachen, and Prof. Marcus Aldén of Lund University.

Reports by Combustion Energy Research Fellows

In this issue, we spotlight the research of Dr. Damir Valiev, a Combustion Energy Research Fellow co-sponsored by Dr. Jacqueline H. Chen, Sandia National Laboratories and Professor Chung K. Law, Princeton University. Dr. Valiev is investigating various aspects of high-pressure combustion by means of direct numerical simulation (DNS) and theoretical modeling.

Direct Numerical Simulations of High-Pressure Combustion

By Damir Valiev

As a result of recent advances in petascale high-performance computing, multi-dimensional direct numerical simulations (DNS) employing detailed chemistry mechanisms has become a powerful tool for providing fundamental theoretical insight into multi-scale combustion problems. We are particularly interested in the combustion of biofuels in transportation environments at low-temperature, high-pressure conditions. At these conditions there exist strong 'turbulence-chemistry' interaction due to the overlap of finite-rate ignition chemistry and local mixing rates, the complexities associated with thermal/composition stratifications, and the prevalence of intrinsic flame instabilities that exacerbate the ability to implement combustion control. At high pressures, experimental differentiation of these factors on flame propagation still remains extremely difficult. With DNS it is possible to study each of these effects in isolation.

The goal of the collaboration between the research groups of the CEFRC PIs Jacqueline H. Chen and Chung K. Law is to improve the theoretical insight into high-pressure combustion by employing state-of the-art high-fidelity numerical methods and high-quality combustion experiments. Carefully designed DNS and experiments enable detailed comparisons of flame instabilities and flame-turbulence interaction. The objective of this joint computational/experimental project is to perform DNS and to extend the theory and modeling of premixed flames at high pressures accounting for intrinsic flamefront instabilities, which include diffusive-thermal pulsating instability (Le>1), diffusive-thermal cellular instability (Le<1), and hydrodynamic Darrieus-Landau (DL) cellular instability. In particular, the effects of an unsteady flow field on the intrinsic diffusive-thermal pulsating instability of a premixed strained flame were studied using detailed hydrogen-air [1] and hydrocarbon-air chemical kinetics.

Another problem of interest is the self-acceleration of flames due to diffusive-thermal and DL cellular instabilities, and the potential for self-turbulization and the eventual DDT (deflagration-to-detonation transition) in both confined and free spaces. The simulations were compared to experiments on spherical flames at nearly constant pressure [2]. A parallel study is also being conducted on the coupling of DL instability and turbulence, which is studied in collaboration with Andrea Gruber, SINTEF Energy research, Norway. It was shown that DL instability is related to fuel-injection flashback safety for stationary power generation [3], actively contributing to flame acceleration by the creation of near-wall regions of reverse flow ahead of the flame sheet (Illustration 1) and maintaining high flame propagation velocities. This problem requires a fundamental investigation of the role of hydrodynamic instability on the regime of flame front propagation in turbulent flow.

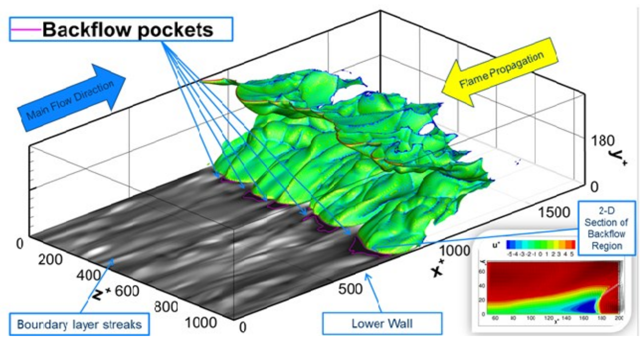

Illustration 1: DNS of premixed lean hydrogen-air flame flashback in turbulent channel flow. Flame is represented by progress variable isosurface, with blue regions characterized by lower heat release rate. Greyscale flooded contours show streamwise velocity, darker color corresponds to lower velocity. Image courtesy of A. Gruber.

References:

[1] Valiev D.M., Zhu M., Bansal G., Kolla H., Law C.K., Chen J.H., "Pulsating Instability of Externally Forced Premixed Counterflow Flame", Combustion and Flame 160(2) (2012) pp. 285–294 , (http://dx.doi.org/10.1016/j.combustflame.2012.10.014)

[2] Wu F., Jomaas G., Law C.K., "An experimental investigation on self-acceleration of cellular spherical flames", Proceedings of the Combustion Institute 34 (2013) pp. 937 – 945 (http://dx.doi.org/10.1016/j.proci.2012.05.068)

[3] Gruber A., Chen J.H., Valiev D., Law C.K., "Direct numerical simulation of premixed flame boundary layer flashback in turbulent channel flow", Journal of Fluid Mechanics 709 (2012) pp. 516 – 542 (open access: http://dx.doi.org/10.1017/jfm.2012.345)

CEFRC People in the News

In August 2012, **Prof. Emily A. Carter** delivered the keynote lecture, entitled "Quantum Mechanical Design and Evaluation of New Solar Energy Conversion Materials" at SPIE Optics & Photonics, 2012. In October, 2012, **Prof. Carter** received the degree of Docteur Honoris Causa from L'École Polytechnique Fédérale de Lausanne, Switzerland.

Dr. Jacqueline H. Chen received the O.W. Adams Award, named after Bill Adams, DOE's original CRF sponsor. **Dr. Chen** was recognized for her research in direct numerical simulations (DNS) of turbulence-chemistry interactions in gas-phase combustion.

Prof. Ronald K. Hanson is listed as number 16 on Applied Optics Journal's list of 50 most published authors in the last 50 years (60 papers as of 1/6/2012). In December 2012, the American Institute of Aeronautics and Astronautics (AIAA) awarded M. Gamba, G. Mungal and **Ronald K. Hanson** AIAA Best Paper Award in Propellants and Combustion for the paper "Ignition and Near-Wall Burning in Transverse Hydrogen Jets in Supersonic Crossflow".

In October 2012, **Prof. Chung K. Law** received the degree of Doctor of Engineering *Honoris Causa* from the Hong Kong Polytechnic University. Also in October, **Prof. Law** was elected a Fellow of the American Association for the Advancement of Science (AAAS). **Fujia Wu**, a graduate student in Prof. Law's group and engaged in CEFRC research, won Best Presentation Award at the First International Education Forum on Environment and Energy Science, hosted by the Academy for Co-creative Education of Environment and Energy Science (ACEEES) at Tokyo Institute of Technology. His talk was entitled "New Understandings of Flame Chemistry and Dynamics from Experimentation on Expanding Premixed Flames".

Prof. Chih-Jen Sung was elected a Fellow of the American Society of Mechanical Engineers (ASME) in November, 2012.

Prof. Donald G. Truhlar received the 2012 Chemical Dynamics Award of the Royal Society of Chemistry "for his many fundamental contributions to the modeling and understanding of chemical reaction dynamics." Additionally **Prof. Truhlar** delivered the following invited lectures: "New Density Functionals with Broad Applicability for Molecules and Solids and Charge Penetration Effects in Electrostatic Modeling and QM/MM Calculations" at the Symposium on Bridging the Gap between ab initio and Classical Simulations, 244th National ACS Meeting, August, 2012; and "Variational Transition State Theory for Complex Reactions," at the 21st IUPAC International Conference on Physical Organic Chemistry (ICPOC) organized by the Royal Society of Chemistry (RSC) in September 2012.

New Appointments of Combustion Energy Research Fellows

Two new appointments to the CEFRC's Combustion Energy Research Fellows Program were made: Colin Smith and Aaron Vandeputte. Each will begin two-year research positions, co-sponsored by two of the Center's principal investigators.

Colin Smith received his Ph.D. in Mechanical Engineering from the University of Texas at Austin in 2012. He is co-sponsored by Dr. Nils Hansen of Sandia National Laboratories and Prof. Ronald K. Hanson of Stanford University. His area of research focuses on tunable diode laser absorption spectroscopy for thermometry in low-pressure, burner-stabilized flames.

Äăron Vandeputte received his Ph.D. in Chemical Engineering from Ghent University in 2012. He is co-sponsored by Prof. William H. Green of MIT and Dr. Stephen J. Klippenstein of Argonne National Laboratory. His area of research focuses on quantifying the effect of roaming mechanisms during combustion.

Where Are They Now?

Subsequent to their association with the CEFRC, our alumni have gone on to do great things in academia and industry. We are justifiably proud of them!

CEFRC Combustion Energy Research Fellows (aka Roving Post-docs)

• Dr. Ionut Alecu is Manager of Research and Development at Hydrotex Partners Ltd. He was co-sponsored by Profs. William H. Green of MIT and Donald G. Truhlar of the University of Minnesota.

• Dr. Mruthunjaya Uddi is a post-doctoral associate in Prof. Ahmed F. Ghoniem's group at MIT. Dr. Uddi was co-sponsored by Profs. Yiguang Ju of Princeton University and Chih-Jen Sung of the University of Connecticut.

• Dr. Bin Yang, is Associate Professor at the Center for Combustion Energy and the Department of Thermal Engineering, Tsinghua University, China. Dr. Yang was the CEFRC's first roving post-doc, and was co-sponsored by Dr. Nils Hansen of Sandia National Laboratories and Prof. Hai Wang of the University of Southern California.

• Dr. Peng Zhang is Assistant Professor at Hong Kong Polytechnic University. He was co-sponsored by Profs. Chung K. Law of Princeton University, Stephen B. Pope of Cornell University and Hai Wang of the University of Southern California and Dr. Stephen J. Klippenstein of Argonne National Laboratory.

CEFRC Post-Doctoral Associates

• Dr. Apurba Das, formerly with Prof. Chih-Jen Sung's group at the University of Connecticut, is a Thermal Engineer at Alstrom Power, Inc.

• Dr. Stephen Dooley, formerly with Prof. Frederick L. Dryer's group at Princeton University, is a Senior Research Scientist at the University of Limerick.

• Dr. Shaokai Gao, formerly with Prof. Hai Wang's group at the University of Southern California, is a Postdoctoral Fellow at the University of California, Riverside.

• Dr. Hossam El-Asrag, formerly with Prof. Yiguang Ju's group at Princeton University, is a Senior Technical Engineer at ANSYS Inc.

• Dr. Yun Huang, formerly with Prof. Chung K. Law's group at Princeton University, is an Assistant Professor at the Chinese Academy of Sciences, Beijing, China.

• Dr. Michele Pavone, formerly with Prof. Emily A. Carter's group at Princeton University, is an Assistant Professor of Physical Chemistry at the University of Naples "Federico II", Italy.

• Dr. Haifeng Wang, formerly with Prof. Stephen B. Pope's group at Cornell University, is an Assistant Professor at Purdue University.

• Dr. Richard West, formerly with Prof. William H. Green's group at MIT, is an Assistant Professor in the Department of Chemical Engineering at Northeastern University.

CEFRC Graduate Students

• Dr. Michael Harper, formerly with Prof. William H. Green's group at MIT, is a Senior Engineer at Exxon Mobil Corporation.

• Dr. Gregory Magoon, formerly with Prof. William H. Green's group at MIT, is a Senior Engineer, Aerodyne Research, Inc.

• Dr. Saro Nikraz, formerly with Prof. Hai Wang's group at the University of Southern California, continues his tenure there as a Postdoctoral Fellow.

• Dr. Ewa Papajak, formerly with Prof. Donald G. Truhlar's group at the University of Minnesota, is a postdoctoral associate with Dr. Judit Zádor at the Combustion Research Facility, Sandia National Laboratories.

• Dr. David Sheen, formerly with Prof. Hai Wang's group at the University of Southern California, is an NRC Fellow at the National Institute of Standards and Technology (NIST).

• Dr. Erik Tolmachoff, formerly with Prof. Hai Wang's group at the University of Southern California, is in an internship with the USC Stevens Institute.

• Dr. Peter Veloo, formerly with Prof. Fokion N. Egolfopoulos at the University of Southern California, is a Postdoctoral Fellow with Prof. Frederick L. Dryer at Princeton University.

Message from the Director

Over a glass of beer someday I will tell you how I accidentally became involved in combustion research – a lucky break as combustion is such a *scientifically beautiful, intellectually challenging,* and *technologically important* discipline that it has sustained my pursuit ever since. The above characterization of combustion is abundantly illustrated by the three technical articles that appear in this issue of the Newsletter. Specifically, Damir Valiev, a CEFRC research fellow, and graduate student Yuxuan Xin have been performing DNS (direct numerical simulation) of expanding laminar flames. One of the goals is to explore if the continuously developing inherent flamefront cellular instability over an otherwise smooth surface, and the corresponding increase in the flame surface area, can lead to self-turbulization and perhaps even the eventual transition to detonation. The images below show the two faces of such an expanding laminar flame, with and without surface wrinkling – I think both the science and the images are *beautiful*.

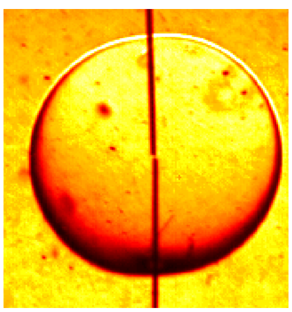

Image I: Laminar, stable, hydrogen-air premixed flame of equivalence ratio: 4.0 at 5atm pressure. Vertical line images are the spark ignition electrodes.

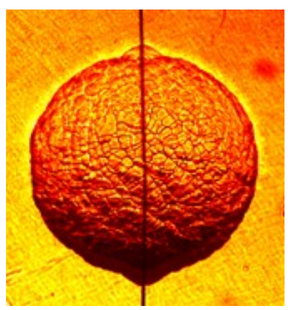

Image II: Laminar, diffusion-thermally unstable, hydrogen-air premixed flame of equivalence ratio: 0.6 at 5atm pressure.

To study such problems with any sense of reality - to be qualitatively correct and quantitatively predictive as these are the requirements of exact science, is immensely *intellectually challenging* because combustion is a multi-physics and multiscale discipline. It involves the two major branches of nonlinear science: fluid mechanics and chemical kinetics, whose temporal and spatial variations can span many decades. The challenge is particularly severe for turbulent flows, requiring the deployment of the big guns in modern scientific investigation: DNS and LES (large eddy simulation) in computational simulation and state-of-the-art laser diagnostics in experiments such as those on DME (dimethyl ether) flames reported by Jeff Sutton, who recently joined the CEFRC as a senior investigator.

The piece by CEFRC PI Rolf Reitz and his student Adam Dempsey then highlights the *technological importance* of combustion, particularly the potential benefit of low-temperature and high-pressure combustion in internal combustion engines. With combustion accounting for about 85% of the world's energy production, and with the corresponding environmental implications, it is without a question the dominant technology affecting humanity for at least the foreseeable decades.

The CEFRC held its third annual conference on Nov. 14-16, 2012 at the Combustion Research Facilities (CRF) of the Sandia National Laboratories in Livermore, CA. The meeting site was selected to facilitate the interaction between the Center activities on basic combustion energy sciences with the engine research activities of the CRF. Talks were given by CRF scientists John Dec, Lyle Pickett and Craig Taatjes on their respective activities, followed by an overview by Rolf Reitz on industry needs and connecting the CEFRC activities with the engine user community. There was also considerable focused discussion on the directions for future research, not just for the CEFRC but also the community at large. We will be reporting our collective thoughts in future issues of the newsletter.

An important mission of the CEFRC is to educate the next generation of researchers in combustion energy. In the newsletter we have listed the post-CEFRC activities of our doctoral and post-doctoral alumni; it is gratifying to see that they are all well launched in their respective career paths.

In the last newsletter we reported that the concept of the combustion summer school, initiated with our CEFRC program, had gone global with the inauguration of the Tsinghua-Princeton Summer School in China last summer. I am pleased to report that we now have a third member in this summer school activity as the Combustion Institute has decided to join force, and will be offering a Summer School in Europe this July. Details of the three summer schools are given elsewhere in the newsletter. It appears that we have succeeded beyond our wildest dreams when we first started the Princeton-CEFRC Summer School in 2010, with an initially planned enrollment of only 25! The real heroes of the success of the summer schools are the instructors who have expended tremendous effort in the preparation of their lecture notes and the subsequent 3-hour/day delivery; we all owe them a great debt of gratitude. For the participants of the summer schools, I encourage you to personally thank them when you meet them at conferences as a token gesture of appreciation.

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

Chung K. Law

Upcoming Events

April, 2013

14th Int. Conference on Numerical Combustion (SIAM NC13)
http://www.siam.org/meetings/nc13
April 8-10, San Antonio, TX

May, 2013

7th Int. Seminar on Fire and Explosion Hazards
https://www.seeuthere.com/rsvp/invitation/invitation.asp?donotrefresh=1
May 5-10, Providence, RI

8th U.S. National Combustion Meeting
http://www.combustion2013.utah.edu
May 19-23, Salt Lake City, UT

9th Asia Pacific Conference On Combustion
http://www.aspacc2013.com
May 19-22, Gyeongju, Republic of Korea

June, 2013

Engine Research Center (ERC) Symposium
http://www.erc.wisc.edu/symposium2013.php
June 5-6, Madison, WI

4th Int. Workshop on Model Reduction in Reacting Flows (IWMRRF)
http://modelreduction.net
June 19-21, San Francisco, CA

Princeton-CEFRC Summer School on Combustion
http://www.princeton.edu/cefrc/combustion-summer-school
June 23-28, Princeton, NJ

6th European Combustion Meeting (ECM2013)
http://www.ecm2013.lth.se
June 25-28, Lund, Sweden

July, 2013

Tsinghua-Princeton Summer School on Combustion
http://www.cce.tsinghua.edu.cn/en/school2013
July 7-12, Beijing, China

8th Int. Conference on Chemical Kinetics
http://www.icck2013.us.es
July 8-12, Seville, Spain

24th ICDERS
http://www.icders2013.tw
July 28-Aug 2, Taipei, Taiwan

August, 2013

Combustion Institute Summer School
http://www.cecost.lth.se/ciss.html
August 19-23, Lund, Sweden

September, 2013

8th Mediterranean Combustion Symposium
http://www.ichmt.org/mcs-13
September 8-13, Cesme, Izmir, Turkey

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Editors: C.K. Law, N. Hansen, L. Tsang
Contact: Lilian Tsang, ltsang@princeton.edu