CEFRC *news*

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

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140 Students and Researchers Flocked to Princeton for Intensive Lectures in Combustion Science

In the glorious summer days of June 2011, 140 students and professionals flocked to Princeton to attend the second annual Princeton-CEFRC Summer School on Combustion – a lecture series that comprised of three 15-hour, all-day, advanced courses in combustion science. The 110 graduate students and 30 professionals came from 25 states across the U.S., six foreign countries (Canada, China, France, Mexico, Sweden, and the UK), representing 56 institutions.

Photo: F. Wojciechowski

The program, which ran from June 26 to July 1, was organized by the CEFRC and sponsored by the U.S. Department of Energy (DOE), with additional support from the Army Research Office (ARO) and the National Science Foundation (NSF). The three courses offered were *Combustion Theory, Combustion Chemistry,* and *Advanced Laser Diagnostics,* taught respectively by the eminent combustion scientists Professor Moshe Matalon of the University of Illinois at Urbana-Champaign, Professor Michael J. Pilling of the University of Leeds, UK, and Professor Marcus Aldén of Lund University, Sweden. The academic program was conducted at an accelerated pace, with daily three-hour lectures on Combustion Chemistry in the morning, followed by parallel lectures on Combustion Theory and Advanced Laser Diagnostics in the afternoon.

The program kicked off on Sunday afternoon, as participants arrived on campus and embarked on a tour of the combustion labs of Professors Dryer, Ju, and Law. The lab tour was followed by a welcome and orientation barbecue, fittingly held in the courtyard of the Engineering Quadrangle, with the enchanted early evening ambiance enlivened with sparkling white lights strung among the tree branches and tiki torches

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Science for Our Nation's Energy Future: The Inaugural EFRC Summit and Forum

On May 25-27, 2011, the U.S. Department of Energy (DOE) hosted the first Science *for Our Nation's Energy Future: Energy Frontier Research Centers Summit & Forum* in Washington D.C. (http://www.energyfrontier.us/content/agenda).

The Summit brought together scientists, students, and energy policy leaders to explore the challenges and opportunities of critical energy needs, and also highlighted early successes of the Energy Frontier Research Center. Secretary of Energy Steven Chu, John Hennessy, President of Stanford University, Mark Little, Senior VP and Director of GE Global Research and Eric Isaacs, Director of Argonne National Laboratory were among the scientific and technology leaders speaking at the Summit.

During the three-day Summit, invited guests and participants attended parallel technical sessions and poster presentations dealing with a wide range of energy topics. Thirteen CEFRC principal investigators, researchers and students attended

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140 Students and Researchers Flocked to Princeton for Intensive Lectures in Combustion Science

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lining the walkways.

Following the successful living arrangement of last year's program, the majority of the participants stayed in air-conditioned dormitory rooms on campus, and shared their meals in the cafeteria. This arrangement allowed the participants to conduct their professional and social networking beyond the classroom. Particularly memorable group activities included informal tours of the Princeton campus as well as impromptu sporting and social activities in the evenings. The week ended with a farewell dinner on Friday evening in the spacious atrium of the newly constructed chemistry building, followed by viewing the spectacular Fourth of July fireworks from the university stadium.

In this photo (l to r): Profs. Marcus Aldén, Michael J. Pilling, Chung K. Law, Moshe Matalon

(The image in the background is that of Chemistry Professor Edward C. Taylor, inventor of the chemotherapy drug Pemetrexed (brand name Alimta) for the treatment of lung cancer. Royalties for this drug enabled the construction of the new chemistry building in which the farewell party was held.)

Judging from the enthusiastic feedback of the attendees, the Combustion Summer School was again a great success. We have received many enthusiastic feedbacks and thoughtful suggestions for future sessions.

For example, **Wenjun Li**, a returning student from North Carolina State University who was in the *Combustion Chemistry* and *Advanced Laser Diagnostics* classes wrote, "Prof. Pilling's lectures were easy to understand and appreciate, making the class very enjoyable. His lectures covered a wide range of areas which gave us a broad overview picture.... Prof. Aldén did a beautiful job of including great images and animation in his slides, and providing good scientific insight into his lecture notes… he really considered the audience's background so that he explained things very clearly and was able to bring everyone into the exciting laser techniques." **Julius Corrubia**, a graduate student from Drexel University wrote, "… the *Combustion Theory* course spanned a wide range of topics from governing equations for reacting flows to laminar flames and then finally turbulent flame theory and modeling… This was great for me because it allowed me to see some new material while also getting a different perspective on material I have learned before…Dr. Matalon was great at providing the theoretical background to many of the topics we learned and he was very helpful with questions."

Now in its second year, the Combustion Summer School reflects a deep unmet demand for what is perhaps the biggest challenge in securing the nation's energy future, according to Chung Law, Princeton's Goddard Professor of Mechanical and Aerospace Engineering and the Director of the CEFRC: "We have tapped into a powerful need… What we offer these students is a wonderful opportunity to pull together disparate areas of engineering and science needed to make a real difference for the world's energy future. Our guest lecturers are internationally renowned experts in combustion science as well as powerful and inspiring lecturers. The lectures have no doubt enriched the knowledge base of the participants and, in due time, will impact the progress of combustion and energy science through fundamental discoveries."

The lecture notes are available on the CEFRC website. The full lecture video content of the 2011 Combustion Summer School will soon be available on the CEFRC website and through iTunes U.

Seventh U.S. National Combustion Meeting: Atlanta, Georgia, March 21- 23

Principal Investigator **Stephen J. Klippenstein** of the Argonne National Laboratory gave a plenary lecture on *"Advances in Theory of Combustion Chemistry"* at the 7th U.S. National Combustion Meeting on March 20-23, 2011, in Atlanta, Georgia.

Photo: Richard West

In this photo (1st row, l to r): N. Hansen, W. Green, C. Law, F. Egolfopoulos, Y. Ju, S. Pope, C.J. Sung, M. Colket, H. Wang (2nd row, l to r): P. Zhang, G. Bansal, F. Wu, E. Dames, Y. Huang, J. Camacho, L. Wang, H. Sun, B. Webber, H. Wang, I. Stranic, S. Lieb, S. Memarzadeh, J. Mo, P. Veloo, B. Yang, Y. Shi, R. West, S. Chaudhuri

Additionally, members of the CEFRC presented 38 papers at the conference, which are listed below to illustrate the breadth and depth of the research activities being conducted at the center:

"Effect of injection angle on stabilization of a reacting turbulent hydrogen jet in cross-flow" by H. Kolla, R.W. Grout, A. Gruber and **J.H. Chen**.

"Identification of Intrinsic Low Dimensional Manifolds in turbulent combustion using an isomap based technique" by G. Bansal, A. Mascarenhas and **J.H. Chen**.

"Modeling transport and dissipation in an LES of an auto-igniting jet flame" by E. Knudsen, E.S. Richardson, Shashank, E.M. Doran, H. Pitsch, and **J.H. Chen**.

"A computational study of pulsating instabilities in externally forced 1D and 2D premixed flames" by G. Bansal and **J.H. Chen**.

"The formulation of surrogate fuels to emulate the combustion behavior of real jet aviation fuels" by S. Dooley, S.H. Won, J. Heyne, **Y. Ju, F.L. Dryer**, K. Kumar, **C.J. Sung**, H. Wang, M.A. Oehlschlaeger, T.A. Litzinger, and R.J. Santoro.

"Comprehensive H2/O2 kinetic model with assessment of commonly neglected processes" by M.P. Burke, M. Chaos, **Y. Ju, F.L. Dryer,** and **S.J. Klippenstein.**

"Methanol droplet combustion in carbon dioxide enriched environments: Extinction characteristics" by T. Farouk and **F.L. Dryer**

"High pressure burning rates and kinetic assessment of mechanisms using high hydrogen content CO2, CH4, C2H4, and C2H6 flames" by J.S. Santner, M.P. Burke, **F.L. Dryer,** and **Y. Ju.**

"Surrogate mixtures for describing real fuel combustion: Challenges and recent progress" by **F.L. Dryer.**

"Kinetic studies and experimental assessment of high temperature of methyl decanoate" by P. Diévart, S. Dooley, S.H. Won, M. Uddi, **F.L. Dryer,** and **Y. Ju.**

"Experimental data and kinetic modeling of n-decane oxidation in low- to intermediate temperature regimes" by S. Jahangirian, S. Dooley, F.M. Haas, and **F.L. Dryer.**

"A shock tube and kinetic modeling study of the autoignition of n-propylbenzene" by H. Wang, M.A. Oehlschlaeger, S. Dooley, and **F.L. Dryer.**

"A pyrolytic flow reactor study of iso-propanol" by Z. Serinyel, S. Dooley, T.I. Farouk, S. Jahangirian, H.J. Curran, and **F.L. Dryer.**

"Assessments of kinetic contribution on extinction limits of diffusion flames for large hydrocarbon fuels, a radical index" by S.H. Won, S. Dooley, **F.L. Dryer,** and **Y. Ju.**

"Combustion kinetics study of t-butanol" by J. Heyne, J. Lefkowitz, F.M. Haas, S.H. Won, S. Dooley, H.H. Kim, S. Jahangirian, **F.L. Dryer,** and **Y. Ju.**

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Dr. Jacqueline H. Chen
Combustion Research Facility
Sandia National Laboratories

Combustion Exascale Co-Design Center Established

A DOE Combustion Exascale Co-Design Center (CECDC) involving six DOE Labs -- SNL, LANL, LLNL, LBL, NREL, ORNL and five universities (Stanford, Georgia Tech, UT Austin, U. Utah and Rutgers) was awarded in 2011. The Director of the Center is CEFRC PI Jacqueline H. Chen.

The objective of the CECDC is to perform the multi-disciplinary research required to simultaneously redesign all aspects of the combustion simulation process from algorithms to programming models to hardware architecture in order to make exascale combustion simulation a reality by 2018.

Power and cost constraints are driving future exascale computer architectures to be radically different than the current generation of HPC architectures that have evolved iteratively over the last two decades, culminating in today's petascale computer architectures. Absorbing such sweeping changes into software and making sure the hardware is developed (managed) to meet the mission requirements of DOE in combustion is the subject of co-design for this center. Exascale computing will enable combustion scientists to perform first principles direct numerical simulation at higher pressure, higher Reynolds number, and with greater chemical complexity. Such work is essential to the U.S. to meet pollutant and greenhouse gas emissions targets, reduce dependence on petroleum, and promote economic competitiveness. The design and implementation of numerical algorithms, data management, fault tolerance, and their evaluation on proposed exascale architectures is critically important to combustion research and to determining the appropriateness of proposed exascale architectures to appear in the 2018 time-frame.

The development of efficient combustion technology is critical for US energy security, and a central justification for DOE investments in exascale computation. The center will combine the talents of combustion scientists, mathematicians, computer scientists, and hardware architects working in integrated teams to address critical themes in the co-design process. The goal of this work is to develop a combustion modeling capability that combines simulation and analysis, develop the necessary computer science tools to facilitate the development of these applications, and quantify hardware constraints for an effective exascale system. The team has assembled a comprehensive roadmap to reinvent combustion modeling for the next decade and lead the way to using co-design methods to define the hardware and software for exascale computing.

Mitchell D. Smooke
Professor, Yale University

Transforming Combustion Research Through Cyberinfrastructure: An NRC Report

The National Research Council (NRC) has released its report *Transforming Combustion Research through Cyberinfrastructure.* The report explains the need for a combustion cyberinfrastructure and the relationships between combustion science, the mathematical sciences, and computer science required to implement such a cyberinfrastructure. It also presents a strategic view for the development of the cyberinfrastructure.

This report is the result of two years deliberation by the *Committee on Building Cyberinfrastructure for Combustion Research,* chaired by Professor Mitchell Smooke of Yale University. It concludes with several recommendations of the committee concerning the importance of such a cyberinfrastructure for research and education, its funding requirements, its benefits to the combustion and other scientific communities, and key steps for planning it. The report identifies the movement of data and the sharing among different research communities as the primary function of a combustion cyberinfrastructure. The report recommends that three outreach teams—one connecting with the many chemistry oriented subcommunities providing fuel data, one connecting with the reacting flow and turbulent flame communities, and one connecting with the industrial engine and fuel R&D communities—should work closely with a central team for the design and construction of the combustion cyberinfrastructure.

The report is available as a free pdf file at:
http://www.nap.edu/catalog.php?record_id=13049

Combustion Chemistry of Biodiesel

By Yiguang Ju, Stephen Dooley, and Pascal Diévart

Yiguang Ju
Professor, Princeton University

With the increasing concerns of energy sustainability and climate change, researchers worldwide are looking for clean burning renewable fuels for the transportation sector, which contributes about one quarter of the global CO_2 emissions. Biodiesel, a mixture that is much less volatile and has a higher lubrication capability than the C_1-C_4 bio-alcohols, has attracted significant attention as a sustainable fuel produced from biomass that can be used as a drop-in replacement or supplement to diesel fuel.

In 2009 about 0.3 million barrels of biodiesel were produced worldwide from major renewable feedstocks (~90% of total production) of vegetable oils and animal fats. Significant research and development has led to a second generation of biodiesel production, by considering additional feedstocks such as Jatropha and various strains of algae. These additional feedstocks produce much higher levels of triglyceride than animal and vegetable fat processing, and do not compete for land or other resources inherent to food production.

Biodiesel is made through the transesterification of triglyceride with alcohols, typically methanol (or ethanol), to produce long-alkyl-chain methyl esters (16-20 carbon atoms) with a terminal methyl (or ethyl) ester functional group. The heating value of biodiesel is about 38 MJ/kg depending on the feedstock and synthesis process, which is only 10% lower than petroleum n-based diesel fuel but 20% higher than ethanol. As a result of the long alkyl chain, biodiesel has much better ignition characteristics compared to ethanol and thus can be used in diesel engines either as the sole fuel or blended with petroleum diesel in any proportion. However, biodiesel components may separate from the diesel fuel and form a wax, therefore limiting their blending potential in cold climates. This temperature limitation, along with the oxygen content of diesel, prevents its use in aircraft gas turbine applications at the cold high-altitude conditions of air transportation.

Since the chemical composition of biodiesel is different from that of petroleum derived diesel, its combustion properties are also different. The incorporation of the methyl ester functional group produces complicated thermochemical and chemical kinetic differences compared to similar alkanes. This is exhibited by significant differences in biodiesel bond dissociation energies (BDEs) for carbon-carbon and carbon-hydrogen bonds. These effects propagate to alkyl radical β-scission reactions and low temperature alkylperoxy radical reactions, producing significantly different combustion kinetic phenomena relative to those of the similar molecular weight alkanes typical of petro diesel. For example, research at the CEFRC has shown that biodiesel forms much more carbon monoxide (CO) and formaldehyde (CH_2O) at much lower flame temperatures than typical alkanes, explaining why biodiesel flames are much less resistant to extinction than equivalent alkane flames such as those of n-heptane. These differences will affect engine performance and emission properties so it is essential that they are understood in order to effectively control the combustion of these fuels.

To help control combustion emissions and improve efficiency via both fuel and engine designs, the CEFRC team is committed to developing a predictive kinetic model for biodiesel combustion. There is already a large database available for the combustion, thermochemistry and reaction kinetics of alkane fuels. Since a biodiesel molecule consists of a long alkyl chain with a methyl or ethyl ester functional group, the team's strategy is to take advantage of the database and focus on improving the reactions that describe the combustion kinetics of the much less studied methyl ester functional group. The team's effort differs from previous kinetic model development for biodiesel by integrating expertise on quantum chemically derived elementary reaction kinetics and thermochemical calculations, advanced laser diagnostics to measure important transient reaction intermediates, and the variety of high pressure kinetic experimental studies (flow reactors, shock tubes, various flame configurations) available to the team. This integration provides both accurate physical constants required for model input construction and validation of the constructed models across a wide range of pressure, temperature, and equivalence ratio.

Our strategy is to understand the uniqueness of the oxidative reactivity of the methyl ester functional groups in the isolated environments of small (~C_5) model methyl esters. In this scenario the ester-specific elementary processes are of much more importance to the prediction of measurable quantities and combustion phenomena than in the much larger and more complex true biodiesel reacting systems.

If the model molecules are properly selected, the knowledge obtained can be extended to describe the larger reacting environments of biodiesel methyl esters by chemical group additivity. The determined rate constants and thermochemical parameters will be tested and constrained by detailed speciation measurements gathered by the entire CEFRC team in shock tubes, flow reactors and flames, stressing different parts of the oxidation model in a systematic manner.

The first iteration of this modeling evolution has just been completed. A combustion model for methyl decanoate has been constructed from the combustion knowledge available for the similar but smaller and much more easily studied C_5 ester, methyl butanoate. The combustion model (http://engine.princeton.edu) shows very promising predictive performance against available experimental data such as the ignition delay time as well as global burning properties such as the flame speed and diffusion flame extinction limit. Analysis of the model performance has allowed the most important uncertain model inputs to be identified, providing a road map to guide the entire CEFRC team to improve the model inputs and evolve the model. This cycle repeats and the kinetic model is refined, optimized, and released to research and industrial communities.

Seventh U.S. National Combustion Meeting: Atlanta, Georgia, March 21- 23

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"Oxidation of small methyl and ethyl esters in flames" by Y.L. Wang, C.K. Westbrook, T.T. Tsotsis and **F.N. Egolfopoulos**.

"Effect of water vapor addition on the extinction of premixed and nonpremixed H2/CO/air flames" by O. Park, P.S. Veloo, and **F.N. Egolfopoulos**.

"Flame propagation of C3 and C4 hydrocarbon/air mixtures" by O. Park, P.S. Veloo, and **F.N. Egolfopoulos**.

"The effect of carbon-carbon double bonds on the combustion chemistry of fatty acid esters" by B. Yang, T.A. Cool, C.K. Westbrook, **N. Hansen**, and K. Kohse-Höinghaus.

"High-temperature oxidation chemistry of n-butanol in low-pressure premixed flames" by **N. Hansen**, M. R. Harper, and **W. H. Green**.

"Shock tube measurements of ignition delay times for the butanol isomers" by I. Stranic, D. Chase, J. Harmon, S. Yang, D.F. Davidson, and **R.K. Hanson**.

"Kinetic effects of nonequilibrium plasma on partially premixed flame extinction" by W. Sun, M. Uddi, S.H. Won, and **Y. Ju.**

"Droplet combustion of ethanol, diesel, castor oil biodiesel, and their mixtures" by M. L. Botero, Y. Huang, D.L. Zhu, A. Molina, and **C. K. Law**.

"Further study on effects of hydrogen addition on laminar flame speeds of fuel-air mixtures" by F. Wu, A.P. Kelley, D. Zhu, and **C.K. Law**.

"Secondary channels in the thermal decomposition of monomethylhydrazine (CH3NHNH2)" by P. Zhang, H. Sun, and **C. K. Law**.

"Thermal decomposition of monomethylhydrazine: Reaction mechanism and kinetic modeling" by H. Sun, P. Zhang, and **C. K. Law**.

"Modification of turbulent combustion regime diagram and turbulent flame speed by Darrieus-Landau instability" by S. Chaudhuri, V. Akkerman, and **C.K. Law**.

"Parametric PDF studies of turbulent premixed stratified flames" by H. Wang and **S.B. Pope**.

"A rapid compression study of the butanol isomers at elevated pressure" by B.W. Weber and **C.J. Sung**.

"A mechanistic study of Soret diffusion in n-heptane/air flames" by Y.X. Xin, **C. . Sung**, and **C.K. Law**.

"Modeling the pressure dependence of H2/O2/diluent mass burning rates" by D.A. Sheen and **H. Wang**.

"Experimental and modeling study of the oxidation of isobutane and isobutene" by B. Yang, H. Wang, E. Dames, **N. Hansen**, S.A. Skeen and T.A. Cool.

"Combustion kinetic modeling using multispecies time-histories in shock-tube oxidation of heptanes" by D.A. Sheen and **H. Wang**.

"Molecule/particle beams detection by fast superconducting bolometers" by S. Gao, D.J. Phares and **H. Wang**.

"Scattering of noble gas molecules and transition metal nanoparticles: A molecular dynamics study" by S. Koumlis and **H. Wang**.

"Combustion kinetic modeling using multispecies time-histories in shock-tube oxidation of n-dodecane" by R. Tangko, D.A. Sheen and **H. Wang**.

"Formation of soot in laminar premixed n-butanol and isobutanol flames" by J. Camacho, S. Lieb and **H. Wang**.

"A comparative study of the sooting properties of laminar premixed flames of C6 hydrocarbons" by J. Camacho, S. Lieb and **H. Wang**.

RECENT CEFRC RESEARCH

In each issue of the CEFRC News, we highlight the research being conducted by some of the Center's students and research associates. In this issue, we spotlight the research of **Dr. Peng Zhang,** a Combustion Energy Research Fellow who is being co-sponsored by Dr. Stephen J. Klippenstein, Argonne National Laboratory, Professor Chung K. Law, Princeton University, Professor Stephen B. Pope, Cornell University, and Professor Hai Wang, University of Southern California.

Ab Initio Kinetics for the decomposition of α-Hydroxybutyl Radical of n-butanol

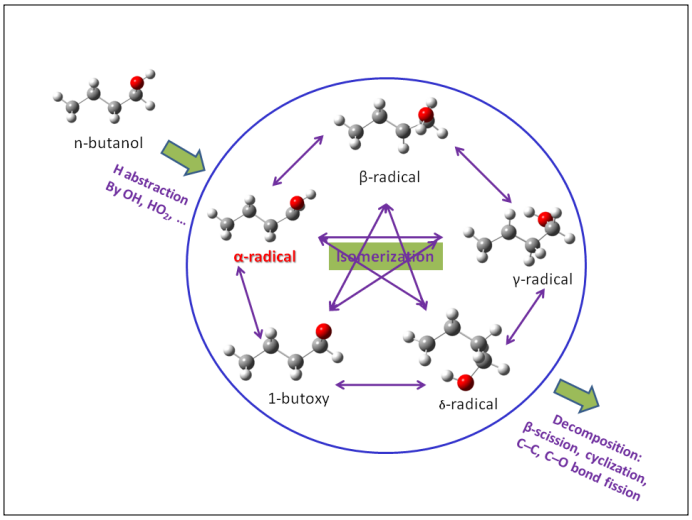
By Dr. Peng Zhang

Currently, the CEFRC is focusing on developing accurate models for the oxidative chemistry of butanol. The α-hydroxybutyl radical ($CH_3CH_2CH_2C{\cdot}HOH$) is the most important product of hydrogen abstraction reactions of n-butanol by small radicals such as the hydroxyl (OH) and hydroperoxy (HO_2) radicals (see accompanying figure). This radical can isomerize to three other hydroxybutyl radicals, namely the β- ($CH_3CH_2C{\cdot}HCH_2OH$), γ- ($CH_3C{\cdot}HCH_2CH_2OH$) and δ- ($C{\cdot}H_2CH_2CH_2CH_2OH$) radicals, as well as the 1-butoxy radical ($CH_3CH_2CH_2CH_2O{\cdot}$). These radicals are also products from the hydrogen abstraction reactions of n-butanol and differ from the α-radical by the position of the unpaired electron. They further decompose mainly through beta-scission, leading to a number of major chain initiation reactions. Thus, their decomposition is crucial to predicting the ignition properties of n-butanol.

By studying the decomposition of hydroxybutyl radicals, we aim to find answers to the following questions. What are the major decomposition products? How to accurately calculate the rate coefficients for the reaction channels leading to these products? What are the branching ratios of the rate coefficients? How does temperature and pressure affect the rate coefficients and the branching ratios?

Experiments are often used to answer these questions, although they are restricted to limited ranges of temperature and pressure. Theoretical chemical kinetics enables us to overcome such a limitation and extend the answers to wider ranges of temperature and pressure, for example, from the room temperature to the flame temperature and from the collisionless condition to the high-pressure limit. In the present theoretical study on the decomposition kinetics of the hydroxybutyl radicals, we used the *ab inito* transition state theory based multi-well master equation analysis. The theoretical method was developed by Dr. Stephen Klippenstein and Dr. Jim Miller in recent years and has been proven to be a quantitatively accurate prediction tool for many chemical reactions in atmospheric and combustion chemistries.

According to our preliminary results, the most important decomposition products for the α-radical decomposition are the ethyl radical ($CH_3C{\cdot}H_2$) and ethenol (CH_2CHOH), which dominate over other products such as butanal ($CH_3CH_2CH_2CHO$) and 1-butenol ($CH_3CH_2CH{=}CHOH$) for all the temperatures of interest (300K-2500K). At low temperatures, the isomerization reaction of the α-radical to the δ-radical becomes more important than the decomposition reactions. The decomposition products for the β-radical are overwhelmingly 1-butene ($CH_3CH_2CHCH_2$) and the hydroxyl radical (OH). The γ-radical most likely decomposes to propene (CH_3CHCH_2) and the hydroxymethyl radical ($C{\cdot}H_2OH$), while it tends to isomerize to the 1-butoxy radical at low temperature. For the δ-radical, the dominant pathway is the isomerization to the 1-butoxy radical, for which the dominant decomposition products are the propyl radical ($CH_3CH_2C{\cdot}H_2$) and formaldehyde (CH_2O). Currently, we are focusing on calculating the temperature- and pressure-dependent reactions rates. The final results will be fitted into functions of temperature and pressure, which can be directly used to build up the CEFRC mechanism for butanol.



Pathways for the Formation, Isomerization and Decomposition of Hydroxybutyl Radicals

Science for Our Nation's Energy Future

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the Summit in various roles of participation. In particular, Director **Chung K. Law** anchored a director's poster on "Combustion Energy Frontier Research Center" on behalf of the center, while CEFRC Co-Director **Emily A. Carter** was among a panel of scientists to present "A View from Senior EFRC Representatives". In addition, each of the three coordinators of the Disciplinary Working Groups and the thrust leaders in mechanism development presented position talks:

William H. Green: "Combustion Chemistry of a New Biofuel: Butanol" .

Yiguang Ju: "Development of Kinetic Models for Methyl-Ester Molecules for Biodiesel Modeling" .

Hai Wang: "Multiscale Kinetic Knowledge Propagation - Combustion Chemistry of Small Hydrocarbons".

Posters on group activities were also presented by **Ionut Alecu**, **Enoch Dames, Stephen J. Klippenstein**, **Joseph Lefkowitz, Victor Oyeyemi, and Stephen B. Pope.**

CEFRC People In The News

Professor Emily A. Carter was named member of the International Advisory Board of the Winton Programme for the Physics of Sustainability, Cambridge University. In March 2011, **Carter** gave the Davidson Lecture at the University of North Texas. The title of her lecture was "How quantum mechanics can help solve our energy problems." **Carter** also gave the Jerome B. Cohen Distinguished Lectures in Materials Science and Engineering at Northwestern University on June 1-3. The lectures were entitled: "Contributing to efficient power generation: atomic-scale insight into thermal barrier coatings from quantum mechanics", "Quantum mechanical evaluation of energy conversion materials for generating electricity", and "Quantum simulations of materials at the mesoscale: physics, algorithms, and applications".

Professor Frederick L. Dryer was elected to Fellow of the American Society of Mechanical Engineers (ASME).

Professor William H. Green hosted the 7th International Conference on Chemical Kinetics, July 10-14, 2011 at MIT.

Invited speakers from the CEFRC were **Donald G. Truhlar** who presented "Multi-Structural Variational Transition State Theory" and **Stephen J. Klippenstein** who presented "The Kinetics of Roaming Radical Reactions".

Klippenstein also delivered a plenary lecture at the First Topical Workshop on Methods for Model Simplification, Evaluation, and Improvement, Jun 28, 2011 in Cardiff, entitled "Model Improvement via Uncertainty Driven Theoretical Studies".

Professor Ronald K. Hanson delivered the CeNIDE Lecture, University of Duisburg-Essen in July. **Hanson** has also been appointed to a Duisburg-Essen, Honorary Guest Professorsorship (2011-2013). **Hanson** received the R. I. Soloukhin Award, from the International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS), 2011.

The paper, "Effects of non-equilibrium plasma discharge on counterflow diffusion flames extinction", was selected as a Distinguished Paper in the New Technology Colloquium of the 33rd International Symposium on Combustion. The authors are: **Yiguang Ju**, Mruthunjaya Uddi (a CEFRC Combustion Energy Research Fellow), Tim Ombrello, Sang Hee Won and Wenting Sun.

Professor Chung K. Law delivered the Dryden Lecture in Research on Tuesday, January 4, at the 2011 AIAA Aerospace Sciences Meeting. The title of the lecture was "Fuel options for next generation chemical propulsion". The Lectureship emphasizes the importance of basic research in aeronautics and astronautics and is a salute to research scientists and engineers.

Dr. Andrey Starikovskiy received the Best Paper Award for "Flow Separation Control on Airfoil with Pulsed Nanosecond Discharge Actuator", by A. Starikovskiy, G. Correale, I. Popov, A. Rakitin, S. Hulshoff, and L. Veldhuis presented at the 49th AIAA Aerospace Sciences Meeting, Orlando, Florida, January 2011.

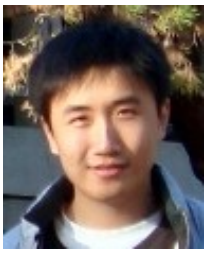
Professor Chih-Jen Sung was elected to the Connecticut Academy of Science and Engineering in February 2011.

Professor Donald G. Truhlar was awarded the Distinguished Alumnus Award from St. Mary's University of Minnesota, 2011, "in recognition as a world-renowned physical chemist who has advanced and transformed chemistry and chemical physics as a distinguished professor, author, and researcher". In March, **Truhlar** gave the Kenneth Wiberg Honorary Lecture at Yale University, entitled "Density Functional Theory: Status and Advances" and the Distinguished McElvain Lecture in Physical Chemistry at the University of Wisconsin, entitled "Density Functional Theory: Introduction and Current Status". In July, **Truhlar** delivered the Keynote Lecture, "Density Functionals for Catalysis," at the Biennial Meeting of The Royal Society of Chemistry of Spain in Valencia, Spain.

Yue Yang, a Combustion Energy Research Fellow, was awarded the Chapman Thesis Prize at the California Institute of Technology.

New Appointments of Combustion Energy Research Fellows

Bret Windom obtained his Ph.D. from the University of Florida in 2009 and joined the CEFRC in May, 2011. Dr. Windom is co-sponsored by Professor Fokion N. Egolfopoulos of the University of Southern California and Professor Yiguang Ju of Princeton University. Using optical diagnostics, his goal is to characterize flames by measuring temperatures, flow velocities, and stable and radical species concentrations for flames under pressures typically experienced in practical applications. Using simple and carefully designed counterflow and spherically expanding flame configurations this data is expected to aid in the development and confirmation of high-pressure combustion models. Simple fuels will be investigated to create a framework of data for which complex high-pressure combustion models can be validated and built upon.



Yue Yang obtained his Ph.D. from the California Institute of Technology in 2011 and joined the CEFRC in March. Dr. Yang is co-sponsored by Dr. Jacqueline H. Chen of Sandia National Laboratories and Professor Stephen B. Pope of Cornell University. Dr. Yang is working on advanced simulations of turbulent combustion. The goal of his research is to assess and to improve the capabilities of LES/PDF by making detailed comparisons with DNS of the same flames and developing advanced SGS models. The performance of the LES/PDF will be assessed via posteriori comparisons with DNS in turbulent lifted jet flames, premixed and stratified jet flames, and future simulations focusing on biofuels for transportation under engine conditions.

Upcoming Events and Announcements

August 2011

2nd Annual Conference of the CEFRC, August 17-19, 2011, Princeton, NJ

242nd ACS National Meeting & Exposition, August 28-Sept 1, Denver, CO

October 2011

Eastern States Technical Meeting, October 09-12, 2011, Storrs, CT

Western States Technical Meeting, October 16-18, 2011, Riverside, CA

November 2011

64th Annual Meeting of the APS's Division of Fluid Dynamics, November 20-22, 2011, Baltimore, MD

ASME 2011 International Mechanical Engineering Congress and Exposition, November 11-17, 2011, Denver, CO

January 2012

34th International Symposium on Combustion, Deadline for Submission of Papers: January 3, 2012, Midnight Pacific Standard Time (GMT-5hrs)

A Message from the Director

I am pleased to report that research at the CEFRC is making significant progress on all fronts as the center enters its third year of operations. As evidence of our sustained performance, the CEFRC PIs and their associates presented a total of 38 CEFRC-sponsored papers at the 7th U.S. National Combustion Conference held at Georgia Tech on March 21-23, 2011, which also matches the number of published CEFRC-papers in the proceedings of the 33rd International Combustion Symposium held in 2010.

In terms of research directions, in the past year the CEFRC has decided to expand its effort in mechanism development to include three classes of fuels, namely: (1) C0-C4 foundation fuels, (2) alcohols especially butanol, and (3) biodiesel. The need for a community C0-C4 mechanism has been long advocated as it is the building block for mechanisms of practically all hydrocarbon fuels. Unfortunately at present a rigorously developed, extensively validated, and generally accepted C0-C4 mechanism does not exist, leading to considerable uncertainty and confusion in the study of fuel chemistry in combustion. The decision to develop mechanisms for alcohols and biodiesel is timely as they represent the two major classes of biofuels in terms of oxidation kinetics and applications. You will find a write-up on biodiesel by Yiguang Ju and his associates in this issue. Progress on these three thrust fuels by the CEFRC PIs will be presented at the upcoming annual conference of the center in mid-August, and will be posted on our web-site thereafter.

The Princeton-CEFRC Summer School on Combustion just had its second session of operation. The number of participants, 140, exceeded last year's 120, and a new course on combustion laser diagnostics was added. Highlights of the program are separately reported in this issue and the details can be found on http://www.princeton.edu/cefrc/combustion-summer-school. The feedbacks from the participants are overwhelmingly enthusiastic, expressing their appreciation of the opportunity to take these classes and to network with their peers. At the personal level, it was an inspirational experience for me to recognize the immense personal effort of the instructors in preparing and delivering the lectures, and the attentiveness of the students in absorbing them.

The Combustion Energy Research Fellows program has reached steady state, with eight appointees and with the first class of appointees about to "graduate" by the end of this year. We look to them to play a leadership role in combustion energy research.

I am also pleased to note that interest and support for combustion and fuels research appear to be on the rise, especially in the U.S. The Department of Energy has initiated a program on high-pressure combustion anchored at Argonne Laboratory, established a Combustion Exascale Co-Design Center with CEFRC PI Jacqueline Chen being its director (see separate write-up in this issue), and showed interest in developing predictive simulation capabilities of combustion engines burning evolving fuels. The National Research Council has also completed a study on cyberinfrastructure in combustion, https://www.combustioninstitute.org/pages/page121.php, chaired by Professor Mitchell D. Smooke of Yale University, with CEFRC PIs J.H. Chen, W.H. Green and C.K. Law, and CEFRC advisors M.B. Colket and C.K. Westbrook, as committee members.

While such increases in interest are encouraging, it is nevertheless noted that the total amount of funding available for combustion research is far from being adequate relative to the disproportionately large share, ~85%, of combustion as an energy source. Furthermore, there also appear to be isolated instances of the de-emphasis of combustion programs in some funding agencies and academic institutions, posing threat to the long-term supply of scientific talents needed for breakthrough discoveries in combustion energy. These are unfortunate developments, and I urge you to be proactive in getting these messages out to our scientific colleagues and policy makers in academia and government, for the prosperity of all!

With best wishes,

Chung K. Law

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