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RESEARCH CENTER**

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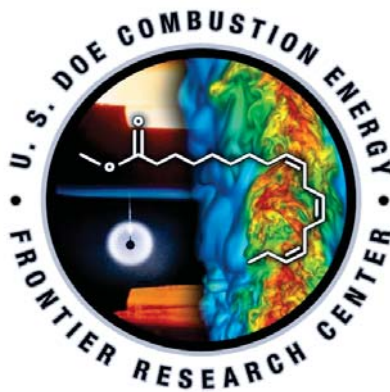


Table of Contents

1.0	Introduction and Highlights	2
2.0	Technical Status	
	2.1 Comparison of Actual Accomplishments with Goals and Objectives	3
	2.2 Technical Accomplishments	5
	2.3 Schedule Status	12
	2.4 Other Status	15
3.0	Publications and Other Products	
	3.1 Peer reviewed, archival journal publications	16
	3.2 Conference proceedings and extended abstracts	20
	3.3 Invited presentations	24
	3.4 Web site or other internet sites	27
	3.5 Networks or collaborations	27
	3.6 Technologies, techniques, inventions/patent applications	32
	3.7 Other products	32
	3.8 Outreach	32
	3.9 Developments in infrastructure	34
4.0	Cost Status	35
5.0	Staffing Data	36
 Appendices		
	A. Other Support (Current & Pending)	39
	B. Combustion Energy Research Fellows Program	50
	C. CEFRC Summer School: 2011 Session	54
	D. CEFRC Newsletter: Volume 1, Issue 2	57

1.0 Introduction and Highlights

Activities and operation of the Combustion Energy Frontier Research Center (CEFRC) are guided by four principal objectives: (1) excellence of fundamental research driven by practical energy relevance; (2) tight coordination and synergism among the individual PI-led programs; (3) leadership in the national and international combustion energy community; and (4) robust outreach program for education and information dissemination. Concerning objectives (1) and (2), the CEFRC has enlarged its scope of investigation during the second year of operation by extending our prior focus on butanol to three unifying, thrust targets that define the extensive matrix of synthetic and bio-derived alternative fuels. In particular, we aim to develop chemical reaction mechanisms for: (a) foundation fuels of the C₁-C₄ hydrocarbons; (b) alcohols especially ethanol and butanol; and (c) biodiesel. Substantial progress has been made across the entire spectrum of combustion phenomena spanning wide length- and time-scales. The following are highlights of the progress:

- A new linear-scale local multi-reference single and double excitation configuration interaction method was developed and used to compute the molecular energies of biodiesel and the reaction barriers to chemical accuracy.
- Methods were developed to handle the coupling between the many internal rotors characteristic of large fuel molecules; they play a key role in determining the entropy, heat capacity, and Arrhenius A factors of the reactions.
- A large matrix of highly accurate chemical kinetic data, relevant for the development of the three thrust mechanisms of foundation fuels, alcohols, and biodiesel, has been determined experimentally.
- *tert*-Butanol was found to have distinctively different chemical reactivity from the other three butanol isomers, namely *n*-, *sec*- and *iso*-butanol.
- The second-generation of the reaction mechanism for *n*-butanol was completed.
- A method of uncertainty minimization was developed to account for parameter uncertainties in future combustion design tools.
- Synergistic combustion through fuel blending was investigated.
- The third-body effects of water and CO₂ on syngas combustion were quantified.
- Direct numerical simulation of 3D turbulent flames indicated that the flame structure consists of mixed mode of premixed and nonpremixed burning.

Concerning objective 3, we have identified and publicized a list of Grand Challenge problems in combustion, which we believe will have a profound and permanent effect on the direction of combustion research internationally. For objective 4, the inaugural, 2010 session of our Summer School for Combustion, conducted on the Princeton campus, was an unqualified success in terms of the number of participants (122), the delivery of the lectures, and the networking opportunities for the participants. The 2011 session, scheduled for June 27 to July 1, is also shaping up to be a great one, with the number of applicants (>160) exceeding the previous one.

2.0 Technical Status

2.1. Comparison of Actual Accomplishments with Goals and Objectives

Research activities at the CEFRC are conducted through three Disciplinary Working Groups (DWGs). This structure allows focusing of the research interest and expertise of groups of the center PIs and facilitates the transitioning and synergy between them on the basis of the multi-scale aspects of combustion phenomena. Specifically, the *Chemistry-Theory* DWG derives the thermochemistry and rate coefficients in the kinetic models from elementary reaction experiments and quantum chemistry calculations, while the *Chemistry-Experiment and Mechanisms* DWG uses advanced experimental facilities to probe the combustion chemistry of fuels. The *Chemistry-Transport* DWG then integrates the chemistry information so generated into studying the structure of laminar and turbulent flames, for which transport is an integral process. The thread that links the activities of the DWGs is the three Research Thrusts of the Center, on developing the kinetic mechanisms for: 1) the foundation fuels of the H₂/CO/C₁-C₄ hydrocarbons and oxygenates; 2) alcohols; 3) biodiesel. The deliverables are the comprehensive reaction mechanisms of major classes of fuels for predictive combustion simulations. In the following, the accomplishments established for this reporting period for each DWG are compared against the goals and objectives stated in the original proposal, recognizing nevertheless that the three Research Thrusts were just identified in the past year.

2.1.1. Chemistry - Theory

The first goal of the Chemistry-Theory DWG's second year research plan is to conduct efficient MRSDCI calculations of the bond dissociation energies of larger esters. In the course of extensive validation calculations, it was found that the local truncation parameters in the L-MRSDCI method need to be adjusted in order to achieve chemical accuracy. Adjustment has been completed for linear hydrocarbons while other classes are being tested, and we are on track to complete the task before the end of Year 2. Although the group plans to compare the size-extensive local multi-reference averaged coupled pair functional (MRACPF) theory to local MRSDCI for BDE, this effort is postponed pending readjustment of the truncation parameters.

Several methyl butanoate combustion reaction paths have been studied using a combination of DFT and MRSDCI. In particular, several DFT functionals were tested, and performance for the geometry optimizations, frequency calculations, etc., were validated. The extensive validation of MRSDCI results versus experimental data has been completed as planned.

To support the goal of using high-accuracy quantum chemistry to determine definitive thermochemistry for all the expected combustion intermediates with three or fewer carbons, we completed QCISD(T) calculations for the thermochemistry of more than 100 small molecule combustion intermediates. We are now comparing these results with prior literature and experimental data, and have resolved several discrepancies.

We have also combined the MRSDCI calculations with advanced internal-rotor treatments to obtain high-accuracy thermochemistry for biodiesel and its combustion intermediates. L-MRSDCI method is operational, and we are now fine-adjusting truncation parameters. Advanced internal rotor treatments were developed and tested, with software reaching production quality. The next step is to combine the two methods to compute the thermochemistry of biodiesel species.

Regarding the goal of conducting high-accuracy calculations for the important species in combustion of other butanol isomers, we have completed a sufficient number to construct accurate detailed models for all four isomers of butanol which predict the experimental data. Currently we are analyzing these models to identify the most important species thermochemistry so that it may be refined further.

For Year 2 and continuing through Year 4, detailed calculation of the reactions identified as important by sensitivity analysis of the CEFRC kinetic mechanism are planned. These calculations have been completed for several important reactions, and the new rate coefficients almost always significantly improve the model predictions. Recent sensitivity analyses of new experiments have identified some additional reactions which need refined rate coefficients; many of these are small molecule reactions which will be addressed by the new thrust. The important reaction *n*-butanol+OH has been studied by several groups both within and outside the CEFRC, obtaining different results for H-abstraction from the γ carbon; this discrepancy will be addressed in Year 3.

The second-generation mechanism for *n*-butanol combustion was completed and presented at the US National Combustion meeting in March, 2011. The mechanism was compared with new experimental data, and errors in some of the pressure-dependent rate coefficients of the old mechanism were identified and corrected.

As planned, we continue to automate 3-D geometry estimation and spawn quantum chemistry calculations as needed during mechanism construction. Software for automatically spawning thermochemistry calculations is operational and is currently demonstrated using GAUSSIAN and (for large molecules) MM4. At present, this is the default of RMG for cyclic species, since often group additivity approach mis-estimates these species. The initial test case was application of the new software to build a kinetic mechanism for the combustion of JP-10, which is a tricyclic synthetic fuel.

For the development of a predictive reaction mechanism for the high-temperature oxidation of *iso*-butanol along with *iso*-butane, a detailed mechanism for *iso*-butanol combustion and pyrolysis was complete and was shared with the entire CEFRC team. It is now being prepared for public distribution.

2.1.2. Chemistry - Experiments and Mechanisms

During the second year in operation, the Reaction Mechanism and Experiments DWG had two goals: (1) measurements of combustion properties for components of a kinetic foundation mechanism, butanol isomers, and biodiesel surrogates including ignition delays in shock tube and rapid compression machine, flow reactor, and low-pressure laminar premixed flames; (2) using the data to validate the butanol mechanism proposed; (3) experiments and modeling study of the combustion chemistry of foundation fuels. The first two goals were met as will be discussed in Section 5. The last goal with hydrogen, syngas as well as several C₄ isomers was also accomplished. To facilitate the quantification and propagation of kinetic uncertainties across different length and time scales and among different components of the Center mechanisms, a method of uncertainty quantification by polynomial chaos expansions (MUM-PCE) was also developed and tested for ethylene combustion.

2.1.3. Chemistry - Transport

In the second year research plan for the Chemistry-Transport DWG, we had two major goals: (1) measurements of flame speeds, ignition and extinction limits, and emission properties of foundational fuels, alcohols, and methyl-esters; and (2) DNS/LES/PDF modeling of homogeneous charge compression ignition (HCCI) combustion and lifted turbulent slot jet flames.

The first goal was met and the accomplishments extend beyond the original objectives. Laminar flame speeds of the foundation fuels ($H_2/CO/C_1-C_4$) were measured up to 25 atm. Laminar flame speeds and extinction limits of C_1-C_4 alcohols, C_1-C_{10} methyl esters, C_1-C_3 ethyl esters, and C_3 and C_4 aldehydes and ketones, were obtained at atmospheric pressure. Effects of water and CO_2 third body effects on flame propagation and extinction were also examined. A new concept of radical index and transport-weighted enthalpy flux were defined and a universal relationship between fuel structure and extinction limit was obtained.

The second goal of the DNS of HCCI combustion with *n*-heptane and DME has also been met. Turbulent combustion in a canonical HCCI-like environment was modeled by using high-fidelity three-dimensional direct numerical simulation resolving the full range of time- and length-scales of turbulence and chemical kinetics directly. Extension of the PDF code (HYB2D) for plane jet flames and integration of ISAT into the LES/PDF code to incorporate realistic chemistry have been completed.

2.2. Technical Accomplishments

Technical accomplishments during the second year are summarized below for each DWG.

2.2.1. Chemistry-Theory

The Chemistry-Theory DWG has developed several new methods, and computed a large number of important thermochemical and kinetic parameters that will be key to the success of all three research thrusts. A new linear-scale local multi-reference single and double excitation configuration interaction method (L-MRSDCI) developed by Carter is being used to compute the molecular energies of biodiesel and the reaction barriers to chemical accuracy (~ 1 kcal/mole). The goal of chemical accuracy is very challenging, in part because much of the experimental data is not so accurate, making it difficult to find sufficient benchmarks (see Figure 1). This fast linear-scaling method is required to make it practical to perform high-accuracy calculations on the very large molecules (C_{16} , C_{18}) in biodiesel.

In these large molecules, and also in several of the species and reactions important in the ignition of the butanols, coupling between the many internal rotors plays a key role in determining the entropy, heat capacity, and Arrhenius A factors of the reactions. In recent years Klippenstein and Green have proposed approximate methods in handling this problem. During the past year, Truhlar has developed new methods to accurately handle these complexities, and is developing them into a software suitable for wide distribution. Green's group has performed high-accuracy thermochemistry calculations for more than a hundred small species important in the Foundation Chemistry mechanism, and has also computed many thermochemistry and reaction rates needed

to build the CEFRC's butanols mechanism. Klippenstein has performed high-accuracy calculations for some of the most important reactions in the Foundation Chemistry, including $H+HO_2$, and has collaborated with Dryer and Ju in the development of an improved H_2/O_2 model which resolves several discrepancies. Klippenstein has also trained several graduate students and postdocs supervised by other CEFRC PI's in advanced methods for computing high-accuracy reaction rates.

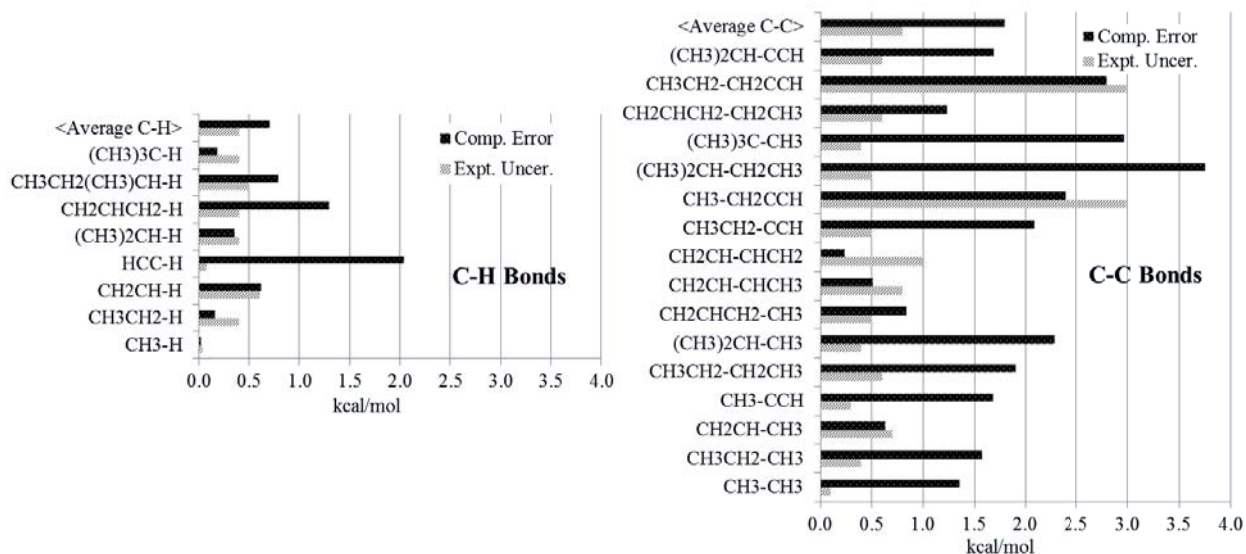


Figure 1. Comparison of experimental uncertainties and absolute errors in computed BDEs when using a minimal active space as references for CASSCF/MRSDCI.

2.2.2. Chemistry-Experimental and Mechanisms

During the second year in operation, the Reaction Mechanism and Experiments DWG has made significant progress in delivering data, tools and understanding necessary for the development of the three thrust areas. Highlights are summarized below.

2.2.2.1. Combustion of Butanol Isomers

The Center has embarked on a coordinated, collaborative study of butanol combustion reaction mechanism, which has been used as a proxy of future alcohol-based bio-gasoline. The work will facilitate the design of combustion engines using these renewable fuels in the foreseeable future. Specifically, a highly accurate experimental database of ignition delay times, species concentration time-histories is made available by shock-tube studies on the four butanol isomers, covering a wide range of temperatures, pressures, fuel loadings and equivalence ratios. This database is critical to the ongoing effort at developing a Center kinetic mechanism for butanol oxidation, using automated mechanism generation techniques and the quantum chemistry calculations described above to determine most of the parameters. For example, Figure 2 shows that the current CEFRC mechanism of butanol combustion, while correctly predicting trends with molecular structure, can be improved with respect to the data, particularly for the straight-chain alcohols. In addition, the measurement shows that the ignition time is highly sensitive to the butanol fuel structure, thus highlighting the need to tackle the underlying kinetics of these isomers at the detailed level.

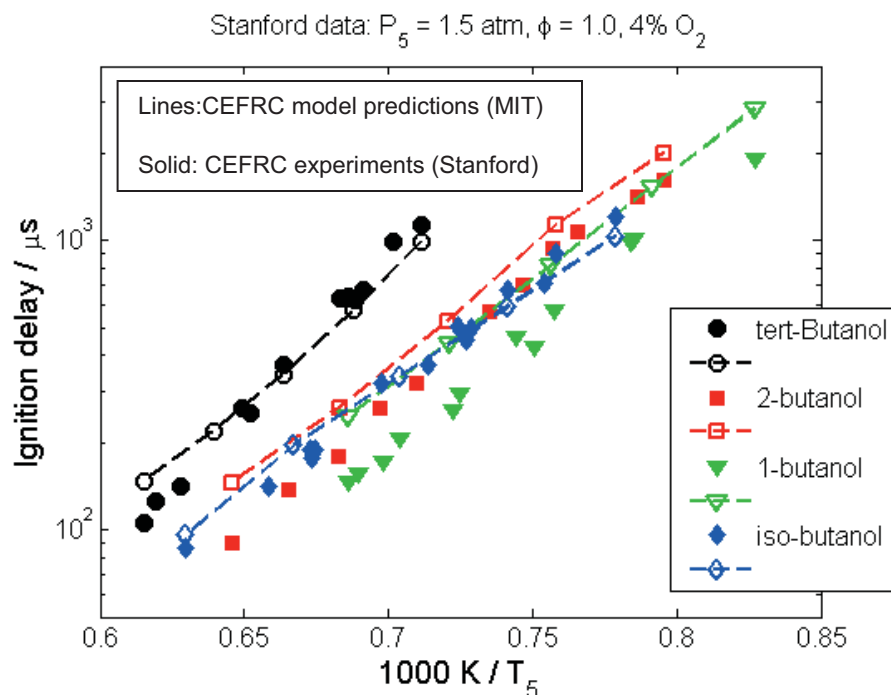


Figure 2. Ignition delay times: isomers of butanol. $P=1.5 \text{ atm}$, $X_{O_2}=0.04$, $\phi=1$, diluted in Ar.

Using the shock tube/laser absorption methodology, the time evolutions of OH, H_2O , and CH_2O during *n*-butanol pyrolysis were determined. To assist the mechanism development, the rate coefficients of H abstraction by OH in all butanol isomers were measured. Detailed experiments in low-pressure flames, measuring dozens of species including free radicals simultaneously using the Advanced Light Source (ALS), provide even more detailed test of the accuracy of the mechanisms, and identify areas where more research is needed, see for example Figure 3. The mechanism now appears accurate enough that sensitivity analysis can reliably identify the reactions and molecular properties which should be improved. Preliminary indications are that most of these reactions are those between the small molecules in the Foundation Chemistry mechanism.

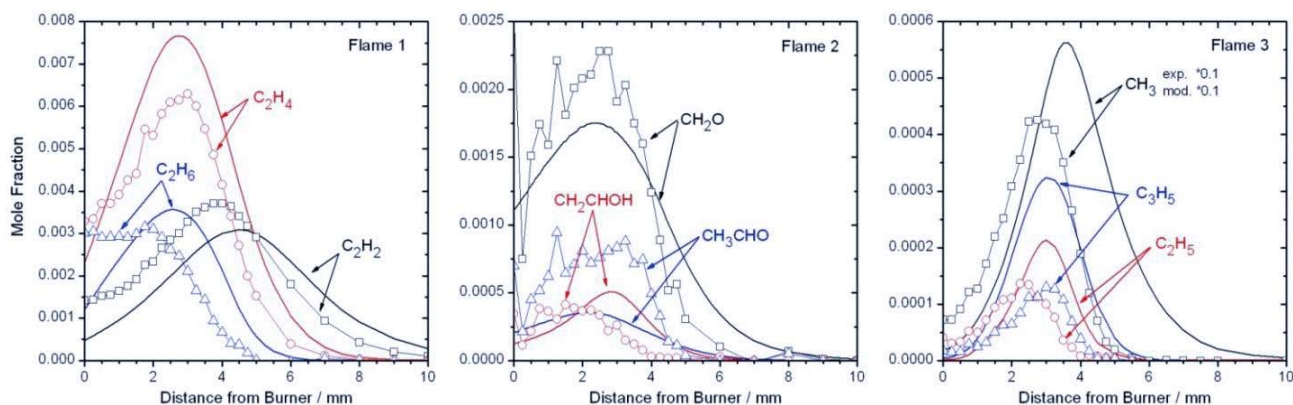


Figure 3. Intermediate species measured in three butanol premixed flames at the ALS by Nils Hansen, and the corresponding CEFRC butanol chemistry model predictions for each species.

Complementary to the shock tube and low-pressure flame experiments and to bring the Center studies to conditions closer to internal combustion engines, autoignition of *n*-butanol was studied in a heated rapid compression machine at 15 and 30 bar in the temperature range of 675–925 K, and over a range of equivalence ratio. Measurements were also made for *iso*-, *sec*-, and *tert*-butanol, 2-buten-1-ol, and *iso*-pentanol, allowing the ignition behaviors of these fuels to be compared in terms of the chemical structure and molecular size of the fuel under comparable conditions. To examine a rational blending strategy, autoignition of binary blends of *n*-butanol and *n*-heptane has also been studied. This study is currently being extended to binary blends of *n*-butanol and *iso*-octane.

The practically relevant ignition properties of the isomers of butanol when mixed with gasoline have been determined in an Ignition Quality Tester. These data show similar behavior for the normal, secondary and isomerized isomers, but show the tertiary isomer to be of unique behavior. In particular, it was determined that *tert*-butanol does not exhibit low temperature chemistry, and thus has no negative temperature coefficient behavior. Pyrolysis studies show that *iso*-propanol was observed to principally decompose to form propylene and water, the expected products of the concerted elimination reaction, $iC_3H_7OH \leftrightarrow C_3H_6 + H_2O$. These results again illustrate the complexity in bio-alcohol utilization as a transportation fuel, in that each isomer exhibits their own kinetic behavior, many of which can directly impact future engine design. In further support of the above notion, experiments conducted for ultra-rich, sooting flames of *n*-butanol and *iso*-butanol show the strong sensitivity of the kinetics of molecular weight growth and particulate formation with respect to the butanol isomer structure.

Continuing from Year 1 efforts for which a combustion reaction mechanism were proposed for all four isomers, the mechanism has undergone routine and regular updates based on the large range of work carried out by the Center PIs. For example, pressure-dependent rate coefficients in earlier version of the mechanism were improved.

2.2.2.2. Foundation Chemistry Mechanism

During Year 1 of the CEFRC effort, it was recognized that the Center must embark on an activity focusing on the development of a unified, consensus chemistry mechanism for the combustion of $H_2/CO/C_xH_y$ ($x=1,..4$) fuels. This mechanism will serve as a kinetic foundation for current and future mechanism development. It will also ensure consistency of the various Center activities, extending from bio-alcohol to biodiesel. A critical element in this activity is the quantification, propagation, and minimization of the kinetic parameter uncertainties in this mechanism, in such a way that progress can be measured and quantified. For this purpose, the Method of Uncertainty Minimization by Polynomial Chaos Expansion (MUM-PCE) was developed. The method represents a major first step towards understanding the impact of parameter uncertainties in fundamental combustion research and in future combustion design tools. Figure 4 shows how the uncertainty of a previous reaction mechanism of *n*-heptane oxidation can be constrained by MUM-PCE using the recent multi-species time history data, flame speeds, and shock tube ignition delay. The method also allows for active design of new, critical experiments for combustion kinetics modeling. The importance of MUM-PCE utilizing a set of high-quality, multi-species measurements for *n*-heptane oxidation behind reflected shock waves has been demonstrated.

As a starting point of this consensus reaction mechanism, a comprehensive H_2/O_2 kinetic mechanism was developed for high pressure combustion. As part of this work, a detailed study of the kinetics of the reaction of H with HO_2 was conducted, leading to an updated kinetic-transport mechanism for the H_2/O_2 system. This mechanism also incorporates recent improvements in rate constant expressions and transport properties. In addition, new data on the collisional efficiencies of N_2 and CO_2 for the third-body reaction $H+O_2+M=HO_2+M$ have been determined. The reaction of dilute $H_2/O_2/NO$ in bath gas M (M=Ar, N_2 , CO_2 , H_2O) was also studied in a novel high pressure laminar flow reactor (HPLFR).

Concurrently, the sub-mechanism of *iso*-butane and *iso*-butene oxidation has been examined using a previous reaction mechanism against newly collected low-pressure burner-stabilized flame data using molecular-beam mass spectrometry (MBMS) in combination with single-photon synchrotron ionization, laminar flame speed, and shock tube ignition. The mechanism of *iso*-butene oxidation is of direct relevance to *iso*- and *tert*-butanol oxidation. The work identified elementary reactions currently missing from the reaction mechanism, and thus identified work critical to the third-year CEFRC effort. As a part of this foundation mechanism, the oxidation of methanol and moist syngas, hydrogen has been studied in a rapid compression machine, exploring the kinetic impact of water on fuel ignition. The experiment identified critical gaps in existing reaction mechanisms which will be filled in the coming months. Additional tests using GCMS and mid-IR absorption spectroscopy are currently conducted to follow more closely the entire reaction process after compression. Again as a component of the foundation chemistry, the oxidation of methyl formate (CH_3OCHO) has been studied in three experimental environments over a range of practical combustion conditions.

2.2.2.3. Chemistry of Biodiesel Combustion

As one of the major thrusts of the CEFRC activities, studies have been conducted for biodiesel surrogate, including methyl oleate and methyl decanoate. Specifically, ignition delay times were measured over a wide range of equivalence ratio in a second generation aerosol shock tube. These data will serve as the starting point for an accurate biodiesel reaction mechanism.

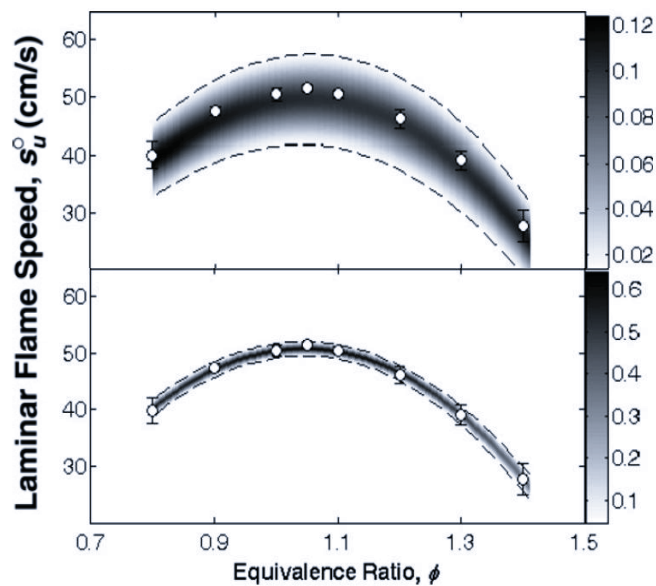


Figure 4. Probability density function of predicted flame speed of *n*-heptane-air mixture at 1 atm and 353 K. Top plot: a prior model with wide predictive uncertainties; bottom panel: a posterior model constrained by available data.

2.2.3. Chemistry-Experimental and Mechanisms

2.2.3.1. Chemistry and Transport Studies of Foundation Fuels

Flames speeds of $\text{H}_2/\text{CO}/\text{C}_1\text{-C}_4$ were measured up to 25 atm. Significant differences between experimental data and predictions at low temperature and high pressure conditions were observed (cf. Figure 5). The availability of the new experimental data led to a revisit of transport properties and development of an updated, comprehensive, high-pressure mechanism for hydrogen. Figure 5 shows that the updated high-pressure hydrogen mechanism dramatically improves the predictability of the mass burning rate of hydrogen flame at high pressures. Similar improvements in prediction were also observed for high pressure $\text{C}_1\text{-C}_2$ flames. The third-body effects of water and CO_2 on syngas combustion were also studied. The results showed that H_2O and CO_2 exhibited large collision efficiencies and enhanced the rate of chain termination reactions.

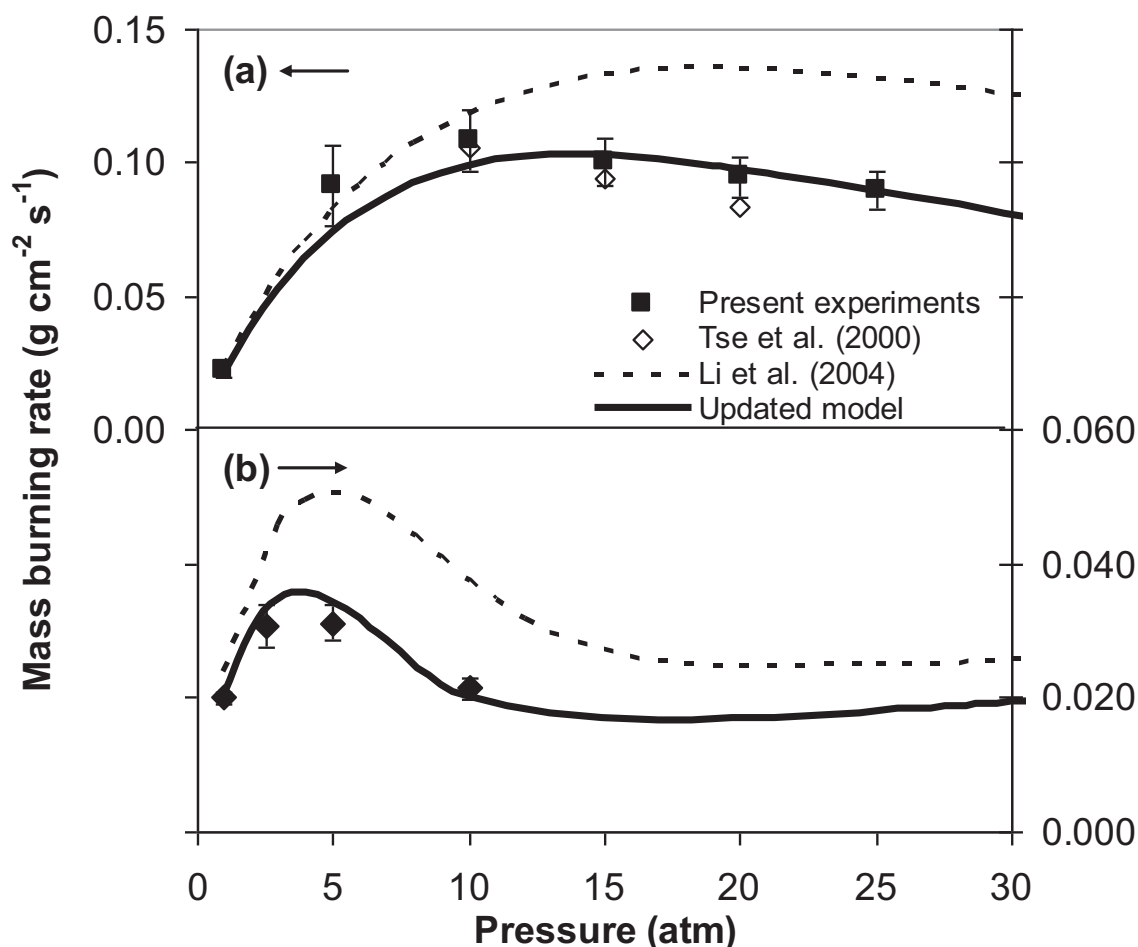


Figure 5. Comparison of measured and predicted mass burning rates for $\text{H}_2/\text{O}_2/\text{He}$ mixtures at (a) $\phi=0.85$ and (b) $\phi=0.30$ at high pressures.

2.2.3.2. Chemistry and Transport Studies of Oxygenated Fuels

Flame speeds and extinction limits of C_1 - C_4 alcohols, C_1 - C_{10} methyl-esters, C_1 - C_3 ethyl esters, and C_3 and C_4 aldehydes and ketones were measured at atmospheric pressure. It was found that fuel branching reduced the overall reactivity and flame speed. In addition, the results showed that ethyl-ester flames propagated faster than methyl-esters and that aldehydes are faster than ketones. Furthermore, *tert*-butanol extinguishes at lower strain rates than its primary intermediates. The experimental data provided important information to understand the effects of fuel functional groups on flame propagation and extinction. A new concept of radical index and transport-weighted enthalpy flux were defined and a universal relationship between fuel structure and extinction limit was obtained.

A mixing strategy for ethanol and biodiesel in petroleum diesel to reduce soot emissions and enhance overall gasification rate was explored. It was shown that there was a great potential of reducing soot emission by mixing diesel with ethanol and biodiesel, as shown in Figure 6.

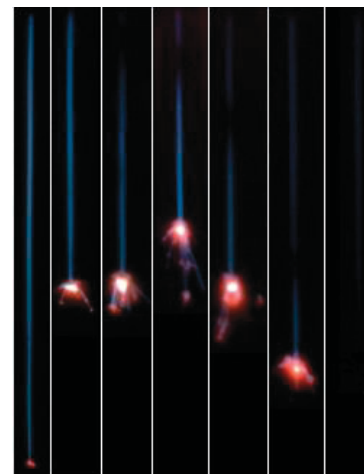


Figure 6. Flame streaks of burning droplets. Ethanol concentration increases from left to right.

2.2.3.3. DNS/LES/PDF Modeling and Turbulent Combustion

Turbulent combustion in a canonical homogeneous charge compression ignition (HCCI)-like environment was modeled by using high-fidelity three-dimensional (3D) direct numerical simulation (DNS) resolving the full range of time- and length-scales of turbulence and chemical kinetics directly. It was found that combustion phenomena in the thermally and compositionally stratified systems are controlled by mixed combustion regimes, which poses a significant challenge to LES and RANS modeling approaches. A 3D DNS was also conducted to investigate the interaction of isotropic 3D turbulence with multi-stage ignition chemistry. Figure 7 shows the heat release rate field during the second stage of ignition. In addition, an LES/PDF code with enhanced numerical accuracy and improved functionalities was developed and benchmarked in the Sandia piloted flames D and E. Systematic studies of the second-order finite-difference schemes for the convection terms on nonuniform grids in LES were performed. A new discretization scheme was proposed for better LES of turbulence and turbulent combustion. The effects of hydrodynamic, Darrieus-Landau (DL) instability on the structure and propagation of turbulent premixed flame fronts were considered. The standard turbulent premixed combustion regime diagram was modified by introducing new boundaries, limiting the domain where the instability influences the global flame shape and speed.

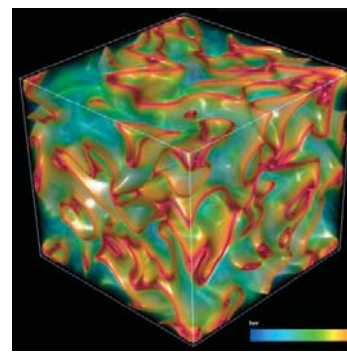


Figure 7. Heat release rate field during the second stage of ignition

2.3 SCHEDULE STATUS

Planned Research Activities	Anticipated Completion Dates	Actual Completion Dates
<p>1. Quantum Chemistry (Carter)</p> <p>a. Efficient MRSDCI calculations of BDEs in larger esters.</p> <p>b. Compare the size-extensive local multi-reference averaged coupled pair functional (MRACPF) theory to local MRSDCI for BDE.</p> <p>c. Fully study several methyl butanoate combustion reaction paths using a combination of DFT and MRSDCI.</p> <p>d. Use MRSDCI/MRACPF to characterize the reactions and intermediates important in methyl ester combustion.</p>	<p>Y2 Y3</p> <p>Y4</p>	<p>Y2– completed</p>
<p>2. Computational Thermochemistry (Carter, Green, Truhlar)</p> <p>a. Use high-accuracy quantum chemistry to determine definitive thermochemistry for all the expected combustion intermediates with three or fewer carbons.</p> <p>b. Combine the MRSDCI calculations with advanced internal-rotor treatments to obtain high-accuracy thermochemistry for biodiesel and its combustion intermediates.</p> <p>c. High-accuracy calculations for the important species in combustion of other butanol isomers.</p> <p>d. Using advanced internal-rotor methods to compute thermochemistry of the many non-rigid intermediates important in ester ignition/combustion.</p>	<p>Y2</p> <p>Y3</p> <p>Y3-Y4</p>	<p>Y2– completed</p> <p>Y2– preliminary</p>
<p>3. Elementary Reaction Rates</p> <p>a. Detailed calculations of the reactions identified as important by sensitivity analysis on the CEFRC kinetic models (Green).</p> <p>b. High-pressure ignition delay time measurements of butanol isomers including <i>sec</i>-butanol, <i>tert</i>-butanol and <i>iso</i>-butanol (Hanson, Sung).</p> <p>c. Complete measurement of detailed species concentration profiles for a series of burner-stabilized <i>iso</i>-butanol, <i>iso</i>-butene and <i>iso</i>-butane flames and carry out detailed kinetic modeling for these flames (Hanson).</p> <p>d. Pyrolysis and oxidation studies of C₃ and C₄ alcohols and measurements of rates of unimolecular decomposition (Dryer).</p> <p>e. Detailed calculations of the reactions identified as important by sensitivity analysis on the CEFRC kinetic models (Green).</p>	<p>Y2</p> <p>Y2</p> <p>Y3-Y4</p>	<p>Y2– completed</p> <p>Y2– completed</p> <p>Y2– preliminary</p>

<p>4. Kinetic Mechanisms (Green, Wang)</p> <p>a. Second-generation model for <i>n</i>-butanol combustion</p> <p>b. Assemble high-accuracy well-documented small-molecule reaction set.</p> <p>c. Automate 3-D geometry estimation and spawn quantum chemistry calculations as needed during mechanism construction.</p> <p>d. Development of a predictive reaction model for the high-temperature oxidation of <i>iso</i>-butanol along with <i>iso</i>-butane and <i>iso</i>-butane.</p> <p>e. Automate TST rate calculations for H-abstraction reactions, based on automated saddle-point finder. This will significantly reduce the time required to construct large combustion chemistry models.</p> <p>f. Refine kinetic models for the butanols based on experiments. Build models for other alternative fuels of interest.</p>	<p>Y2</p> <p>Y2</p> <p>Y3-Y4</p>	<p>Y2– completed</p> <p>Y2– completed</p> <p>Y2– preliminary</p> <p>Y2– preliminary</p>
<p>5. Flame Speeds, Ignition and Extinction Limits, and Emission Properties (Egolfopoulos, Ju, Law).</p> <p>a. Flame studies of C₁-C₄ alcohols, methyl-esters, and H₂/CO/C₁-C₄ fuels up to 30 atmospheric pressures.</p> <p>b. Ignition temperatures and laminar flame speeds determined for bio-fuels other than bio-butanols.</p> <p>c. Sooting limits determined for bio-butanol fuels.</p> <p>d. Flame ignition at pressures potentially up to 20-30 atm.</p> <p>e. Computational simulation of soot formation in bio-butanol fuels.</p> <p>f. Data and analysis on spark ignition in turbulent field.</p> <p>g. Data and analysis on flame propagation in turbulent field.</p> <p>h. High pressure jet stirred reactor with molecular beam sampling.</p> <p>i. Turbulent counterflow flame and NO_x emissions.</p>	<p>Y2</p> <p>Y2</p> <p>Y2</p> <p>Y3-Y4</p>	<p>Y2– completed</p> <p>Y2– completed</p> <p>Y2– completed</p>
<p>6. Reduced Model Development and Modeling</p> <p>a. Adaptive multi-timescale modeling approach for alcohols.</p> <p>b. Ignition to detonation transition diagram at HCCI conditions.</p>	<p>Y2</p> <p>Y3</p>	<p>Y2– completed</p>

<p>7. DNS/LES/PDF Modeling (Chen, Pope, Ju)</p> <p>a. DNS of HCCI combustion with temperature and concentration gradients.</p> <p>b. Compare DNS and LES/PDF of the lifted ethylene/air and hydrogen/air jet flames.</p> <p>c. Perform DNS of <i>n</i>-heptane and di-methyl ether in HCCI combustion.</p> <p>d. Perform DNS of expanding turbulent hydrogen/air premixed flame to examine intrinsic instabilities and compare with experiments by Law.</p> <p>e. Perform DNS of lifted <i>iso</i>-butanol jet flames in heated coflow.</p> <p>f. Compare DNS of lifted <i>iso</i>-butanol jet flame with LES/PDF calculations by Pope. Refine conditional turbulent diffusion model to account for differential mixing rates among species in partially-premixed combustion.</p> <p>g. Perform DNS of unsteady stratified laminar counterflow flames.</p> <p>h. Extend the PDF code to plane jet flames</p> <p>i. Extend LES/PDF code with 2-way coupling, molecular diffusion, and ISAT/RCCE/x2f_mpi.</p> <p>j. Demonstrate the LES/PDF capability for piloted jet flames.</p> <p>k. PDF and LES/PDF of plane lifted flames and comparison with DNS data.</p> <p>l. Perform DNS of statistically spherical turbulent premixed flame.</p> <p>m. Self-turbulization and cell size distribution in terms of imposed turbulence scales. Examine kinetic energy and scalar spectra. Compare with experiment by Law.</p> <p>n. Perform DNS of turbulent stratified counterflow flames and compare with experiments by Ju.</p> <p>o. Compare DNS of statistically spherical turbulent premixed flame with LES/PDF of same configuration. Refine turbulent diffusion model for premixed flames.</p> <p>p. Apply LES/PDF and PDF to new Sandia DNS and interrogate DNS.</p> <p>q. Apply LES/PDF and PDF to CEFRC and other stratified premixed flames.</p>	<p>Y2</p> <p>Y3-Y4</p> <p>Y3-Y4</p> <p>Y2</p> <p>Y3-Y4</p>	<p>Y2– completed</p> <p>Y2– completed</p>
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2.4 Other Status

1. Any changes in approach or aims and reasons for change
None
2. Actual or anticipated problems or delays and actions taken/planned to resolve them
None
3. Any absence or changes of key personnel or changes in teaming arrangement

James A. Miller, a principal investigator of the CEFRC retired from his employment at the Sandia National Laboratories effective December 1, 2010. After his retirement, he assumed a 25%-time appointment at the Argonne National Laboratory, where he worked in collaboration with Klippenstein, another PI of the Center. The research funding appropriated to his efforts was transferred to Argonne. On January 18, 2011, due to personal reasons, Miller resigned from the CEFRC. Miller had been working very closely with Klippenstein and as such, there was no deprivation of our scientific expertise due to this personnel change.

4. Other support (current or pending, federal and non-federal)
Please refer to Appendix A – Other Support (Current & Pending)

3.0 Publications and Other Products

3.1. Peer reviewed, archival journal publications

1. Shi, Y.; **Green, W. H.**; Wong, H. W.; and Oluwole, O. O. REDESIGNING COMBUSTION MODELING NEXT TERM ALGORITHMS FOR THE GRAPHICS PROCESSING UNIT (GPU): CHEMICAL KINETIC RATE EVALUATION AND ORDINARY DIFFERENTIAL EQUATION INTEGRATION, *Combust. Flame*, **158**, 836-847 (2011).
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3. Yang, B.; Cool, T. A.; Westbrook, Charles K.; **Hansen, N.**; and Kohse-Hoinghaus, K. FUEL-SPECIFIC INFLUENCES ON THE COMPOSITION OF REACTION INTERMEDIATES IN PREMIXED FLAMES OF THREE C₅H₁₀O₂ ESTER ISOMERS, *Phys. Chem. Chem. Phys.*, **13**, 7205-7217 (2011).
4. Dooley, S.; **Dryer, F. L.**; Yang, B.; Wang, J.; Cool, T. A.; Kasper, T.; and **Hansen, N.** AN EXPERIMENTAL AND KINETIC MODELING STUDY OF METHYL FORMATE LOW-PRESSURE FLAMES, *Combust. Flame*, **158**, 732-741 (2011).
5. Kumar, K.; and **Sung, C. J.** AUTOIGNITION OF METHANOL: EXPERIMENTS AND COMPUTATIONS, *Proc. Combust. Inst.*, **43**, 175-184 (2011).
6. Sheen, David; and **Wang, Hai** COMBUSTION KINETIC MODELING USING MULTISPECIES TIME HISTORIES IN SHOCK-TUBE OXIDATION OF HEPTANE, *Combust. Flame*, **158**, 645-656 (2011).
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9. Veloo, Peter S.; and **Egolfopoulos, Fokion N.** FLAME PROPAGATION OF BUTANOL ISOMERS/AIR MIXTURES, *Proc. Combust. Inst.*, **33**, 987-993 (2011).
10. Wang, Y. L. ; Veloo, Peter S.; **Egolfopoulos, Fokion N.**; and Tsotsis, T. T. A COMPARATIVE STUDY ON THE EXTINCTION CHARACTERISTICS OF NON-PREMIXED DIMETHYL ETHER AND ETHANOL FLAMES, *Proc. Combust. Inst.*, **33**, 1003-1010 (2011).
11. Zhang, H.; Fan, R.; Wang, S.; Tian, X.; Xu, K.; Wan, S.; and **Egolfopoulos, Fokion N.** EXTINCTION OF LEAN NEAR-LIMIT METHANE/AIR FLAMES AT ELEVATED PRESSURES UNDER NORMAL- AND MICRO-GRAVITY, *Proc. Combust. Inst.*, **33**, 1171-1178 (2011).
12. Alecu, I. M.; and **Truhlar, D. G.** COMPUTATIONAL STUDY OF THE REACTIONS OF METHANOL WITH THE HYDROPEROXYL AND METHYL RADICALS. PART I: ACCURATE THERMOCHEMISTRY AND BARRIER HEIGHTS, *J. Phys. Chem. A*, **115**, 2811-2829 (2011).

13. Allen, C.; Mittal, G.; **Sung, C. J.**; Toulson, E.; and Lee, T. AN AEROSOL RAPID COMPRESSION MACHINE FOR STUDYING ENERGETIC-NANOPARTICLE-ENHANCED COMBUSTION OF LIQUID FUELS, *Int. J. Chem. Kinet.*, **33**, 3367-3374 (2011).
14. Das, A. K.; Kumar, K.; Zhang, Z.; and **Sung, C. J.** LAMINAR FLAME SPEEDS OF MOIST SYNGAS MIXTURES, *Combust. Flame*, **158**, 345-353 (2011).
15. Vasu, Subith; Huynh, Lam; Davidson, David F.; **Hanson, Ronald K.**; and Golden, David REACTIONS OF OH WITH BUTENE ISOMERS: MEASUREMENTS OF THE OVERALL RATES AND A THEORETICAL STUDY, *J. Phys. Chem. A*, **115**, 2549-2556 (2011).
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17. Burke, M. P.; **Dryer, F. L.** ; and **Ju, Yiguang** ASSESSMENT OF KINETIC MODELING FOR LEAN H₂/CH₄/O₂/DILUENT FLAMES AT HIGH PRESSURES, *Proc. Combust. Inst.*, **33**, 905-912 (2011).
18. Chen, Zheng; Burke, M. P.; and **Ju, Yiguang** ON THE CRITICAL FLAME RADIUS AND MINIMUM IGNITION ENERGY FOR SPHERICAL FLAME INITIATION, *Proc. Combust. Inst.*, **33**, 1219–1226 (2011).
19. Goldsmith, C. F.; **Klippenstein, S. J.**; and **Green, W. H.** THEORETICAL RATE COEFFICIENTS FOR ALLYL + HO₂ AND ALLYLOXY DECOMPOSITION, *Proc. Combust. Inst.*, **33**, 273-282 (2011).
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21. **Ju, Yiguang**; Sun, Wenting; Burke, M. P.; Gou, Xiaolong; and Chen, Zheng MULTI-TIMESCALE MODELING OF IGNITION AND FLAME REGIMES OF N-HEPTANE-AIR MIXTURES NEAR SPARK ASSISTED HOMOGENEOUS CHARGE COMPRESSION IGNITION CONDITIONS, *Proc. Combust. Inst.*, **33**, 1245–1251 (2011).
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23. Lu, Wei; Kelley, A. P.; and **Law, C. K.** NONPREMIXED IGNITION, LAMINAR FLAME PROPAGATION, AND MECHANISM REDUCTION OF N-BUTANOL, ISO-BUTANOL, AND METHYL BUTANOATE, *Proc. Combust. Inst.*, **33**, 995-1002 (2011).
24. Memarzadeh, Saro; Tomachoff, Erik D.; Phares, Denis J.; and **Wang, Hai** PROPERTIES OF NANOCRYSTALLINE TiO₂ SYNTHESIZED IN PREMIXED FLAMES STABILIZED ON A ROTATING SURFACE, *Proc. Combust. Inst.*, **33**, 1917-1924 (2011).
25. Papajak, E.; and **Truhlar, D. G.** CONVERGENT PARTIALLY AUGMENTED BASIS SETS FOR POST-HARTREE-FOCK CALCULATIONS OF MOLECULAR PROPERTIES AND REACTION BARRIER HEIGHTS, *J. Chem. Theory Comput.*, **7**, 10-18 (2011).

26. Tang, C. K.; Huang, Z. H.; and **Law, C. K.** DETERMINATION, CORRELATION, AND MECHANISTIC INTERPRETATION OF EFFECTS OF HYDROGEN ADDITION ON LAMINAR FLAME SPEEDS OF HYDROCARBON–AIR MIXTURES, *Proc. Combust. Inst.*, **33**, 921-928 (2011).
27. **Wang, Hai** FORMATION OF NASCENT SOOT AND OTHER CONDENSED-PHASE MATERIALS IN FLAMES, *Proc. Combust. Inst.*, **33**, 41-67 (2011).
28. Wang, Haifeng; and **Pope, Stephen B.** LARGE EDDY SIMULATION/PROBABILITY DENSITY FUNCTION MODELING OF A TURBULENT CH₄/H₂/N₂ JET FLAME, *Proc. Combust. Inst.*, **33**, 1319-1330 (2011).
29. Won, Sang Hee; Dooley, S.; **Dryer, F. L.** ; and **Ju, Yiguang** KINETIC EFFECTS OF AROMATIC MOLECULAR STRUCTURES ON DIFFUSION FLAME EXTINCTION, *Proc. Combust. Inst.*, **33**, 1163-1170 (2011).
30. Yoo, C. S.; Richardson, E.; Sankaran, R.; and **Chen, J. H.** A DNS STUDY ON THE STABILIZATION MECHANISM OF A TURBULENT LIFTED ETHYLENE JET FLAME IN HIGHLY-HEATED COFLOW, *Proc. Combust. Inst.*, **33**, 1619-1627 (2011).
31. Zhang, P.; **Klippenstein, S. J.**; Sun, Hongyan; and **Law, C. K.** AB INITIO KINETICS FOR THE DECOMPOSITION OF MONOMETHYLHYDRAZINE (CH₃NHNH₂), *Proc. Combust. Inst.*, **33**, 425-432 (2011).
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34. Sun, Hongyan; and **Law, C. K.** KINETICS OF HYDROGEN ABSTRACTION REACTIONS OF BUTENE ISOMERS BY OH RADICAL, *J. Phys. Chem. A*, **114**, 12088-12098 (2010).
35. Veloo, Peter S.; Wang, Y. L.; **Egolfopoulos, Fokion N.**; and Westbrook, Charles K. A COMPARATIVE EXPERIMENTAL AND COMPUTATIONAL STUDY OF METHANOL, ETHANOL, AND N-BUTANOL FLAMES, *Combust. Flame*, **157**, 1989-2004 (2010).
36. Dooley, S.; Burke, M. P.; Chaos, M.; Stein, Y.; **Dryer, F. L.** ; Zhukov, V. P.; Finch, O.; Simmie, J. M.; and Curran, H. J. METHYL FORMATE OXIDATION: SPECIATION DATA, LAMINAR BURNING VELOCITIES, IGNITION DELAY TIMES AND A VALIDATED CHEMICAL KINETIC MODEL, *Int. J. Chem. Kinet.*, **42**, 527-549 (2010).
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39. Van Geem, K. M.; Pyl, S. P.; Marin, G. B.; Harper, M. R.; and **Green, W. H.** ACCURATE HIGH-TEMPERATURE REACTION NETWORKS FOR ALTERNATIVE FUELS: BUTANOL ISOMERS, *Ind. Eng. Chem. Res.*, **49**, 10399-10420 (2010).
40. Sun, Wenting; Chen, Zheng; Gou, Xiaolong; and **Ju, Yiguang** A PATH FLUX ANALYSIS METHOD FOR THE REDUCTION OF DETAILED CHEMICAL KINETIC MECHANISMS, *Combust. Flame*, **157**, 1298-1307 (2010).
41. Vasu, Subith; Zador, J.; Davidson, David F.; **Hanson, Ronald K.**; Golden, David; and Miller, James A. HIGH-TEMPERATURE MEASUREMENTS AND A THEORETICAL STUDY OF THE REACTION OF OH WITH 1,3-BUTADIENE, *J. Phys. Chem.*, **114**, 8312-8318 (2010).
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45. Chen, Zheng; Gou, Xiaolong; and **Ju, Yiguang** STUDIES ON THE OUTWARDLY AND INWARDLY PROPAGATING SPHERICAL FLAMES WITH RADIATIVE LOSS, *Combust. Sci. Technol.*, **182**, 124-142 (2010).
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48. Sun, Wenting; Chen, Zheng; Gou, Xiaolong; and **Ju, Yiguang** A PATH FLUX ANALYSIS METHOD FOR THE REDUCTION OF DETAILED CHEMICAL KINETIC MECHANISMS, *Combust. Flame*, (2010). [[10.1016/j.combustflame.2010.03.006](https://doi.org/10.1016/j.combustflame.2010.03.006)]
49. Veloo, Peter S.; Wang, Yang L.; **Egolfopoulos, Fokion N.**; and Westbrook, Charles K. A COMPARATIVE EXPERIMENTAL AND COMPUTATIONAL STUDY OF METHANOL, ETHANOL, AND N-BUTANOL FLAMES, *Combust. Flame*, (2010). [[10.1016/j.combustflame.2010.04.001](https://doi.org/10.1016/j.combustflame.2010.04.001)]
50. Won, Sang Hee; Sun, Wenting; and **Ju, Yiguang** KINETIC EFFECTS OF TOLUENE BLENDING ON THE EXTINCTION LIMIT OF N-DECANE DIFFUSION FLAMES, *Combust. Flame*, (2010). [[10.1016/j.combustflame.2009.11.016](https://doi.org/10.1016/j.combustflame.2009.11.016)]

3.2. Conference proceedings and extended abstracts

1. G. Bansal, and **J. H. Chen**, “*A Computational Study of Pulsating Instabilities in Externally Forced 1D and 2D Premixed Flames*,” 7th US National Technical Meeting of the Combustion Institute, March 20-23, 2011.
2. G. Bansal, A. Mascarenhas, and **J. H. Chen**, “*Identification of Intrinsic Low Dimensional Manifolds in Turbulent Combustion using an Isomap based technique*,” 7th US National Technical Meeting of the Combustion Institute, March 20-23, 2011.
3. M. P. Burke, M. Chaos, **Y. Ju**, **F. L. Dryer**, **S. J. Klippenstein**, “*Comprehensive H₂/O₂ Kinetic Model with Assessment of Commonly Neglected Processes*,” 7th US National Combustion Meeting of the Combustion Institute, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.
4. P. Diévert, S. Dooley, S-H Won, M. Uddi, **F. L. Dryer**, **Y. Ju**, “*Kinetic Studies and Experimental Assessment of High Temperature Oxidation of Methyl Decanoate*,” 7th US National Combustion Meeting of the Combustion Institute, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.
5. J. Heyne, J. Lefkowitz, F. M. Haas, S-H. Won, S. Dooley, H. H. Kim, S. Jahangirian, **F. L. Dryer**, **Y. Ju**, “*Combustion Kinetics Study of t-butanol*,” 7th US National Combustion Meeting of the Combustion Institute, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.
6. J. Heyne, J. Lefkowitz, F.M. Haas, S-H. Won, S. Dooley, H. H. Kim, S. Jahangirian, **F. L. Dryer**, **Y. Ju**, “*Combustion Kinetics Study of t-butanol and its Principal Intermediates i-Butene, Acetone, and Methane*,” 7th US National Combustion Meeting of the Combustion Institute, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.
7. J. Santner, M. P. Burke, **F. L. Dryer**, **Y. Ju**, “*High Pressure Burning Rates and Evaluation of Model Performance for C1-C2 Flames with Varied Hydrogen Content*,” 7th US National Combustion Meeting of the Combustion Institute, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.
8. Z. Serinyel, S. Dooley, T. I. Farouk, S. Jahangirian, H. J. Curran, **F. L. Dryer**, “*A Pyrolytic Flow Reactor Study of iso-Propanol*,” 7th US National Combustion Meeting of the Combustion Institute, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.
9. M. Burke, Y. Ju, **F. Dryer**, M. Chaos and S. Klippenstein, “*Kinetic Modeling of the H₂/O₂ Reaction in High Pressure Flames*,” 49th Annual Aerospace Sciences Meeting, Orlando, FL, Jan. 4-7, 2011. AIAA-2011-0093.
10. P. Dievert, S. Won, M. Uddi, S. Dooley, **F. Dryer**, **Y. Ju**, “*Measurements of Extinction Limits of Methyl Decanoate Diffusion Flames and A Kinetic Study*,” 49th Annual Aerospace Sciences Meeting, Orlando, FL, Jan. 4-7, 2011. AIAA2011-0697.
11. J. Lefkowitz, J. Heyne, F. Haas, S. Won, S. Dooley, **F. Dryer**, **Y. Ju**, “*Classical Kinetic Study of the Alternative Transport Fuel, Tertiary Butanol*,” 49th Annual Aerospace Sciences Meeting, Orlando, FL, Jan. 4-7, 2011. AIAA 2011-0698.

12. J. Santner, M. Burke, **Y. Ju**, **F. Dryer**, “*High Pressure Burning Rates and Model Comparisons for High-Hydrogen CO, CH₄, C₂H₄, C₂H₆ Mixtures*”, 49th Annual Aerospace Sciences Meeting, Orlando, FL, Jan. 4-7, 2011. AIAA-2011-0242.
13. P. S. Veloo, **F. N. Egolfopoulos**, “*Studies of Non-Premixed Flames of C₃ and C₄ Saturated Alcohols*,” Paper No. 10S-019 Spring Technical Meeting, Western States Section/Combustion Institute, University of Colorado at Boulder, Boulder, Colorado, March 21-23, 2010.
14. P. S. Veloo, C. K. Westbrook, **F. N. Egolfopoulos**, “*Combustion characteristics of C₃ and C₄ aldehydes and ketones*,” Paper 1F01, 7th US Combustion Meeting, Atlanta, Georgia, March 20-23, 2011.
15. Y. L. Wang, C. K. Westbrook, T. T. Tsotsis, **F. N. Egolfopoulos**, “*Oxidation of small methyl and ethyl esters in flames*,” Paper 1F02, 7th US Combustion Meeting, Atlanta, Georgia, March 20-23, 2011.
16. O. Park, P. S. Veloo, **F. N. Egolfopoulos**, “*Effect of water vapor addition on the extinction of premixed and non-premixed H₂/CO/air flames*,” Paper 1E13, 7th US Combustion Meeting, Atlanta, Georgia, March 20-23, 2011.
17. O. Park, P. S. Veloo, and **F. N. Egolfopoulos**, “*Flame propagation of C₃ and C₄ hydrocarbon/air mixtures*,” Paper 2D12, 7th US Combustion Meeting, Atlanta, Georgia, March 20-23, 2011.
18. J. Lefkowitz, J. Heyne, F. Haas, S-H Won, S. Dooley, **F. L. Dryer**, **Y. Ju**, “*Chemical Kinetic Study of the Alternative Transport Fuel, tertiary-Butanol*,” AIAA-2011-698, 49th AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition, Orlando, Florida, Jan. 4-7, 2011.
19. J. S. Santner, M. P. Burke, **F. L. Dryer**, **Y. Ju**, “*High pressure burning rates and kinetic assessment of mechanisms using high hydrogen content CO₂, CH₄, C₂H₄, and C₂H₆ flames*,” Paper 1E14, 7th U.S. National Combustion Meeting, March 20-23, 2011, Georgia Institute of Technology, Atlanta GA.
20. S-H Won, S. Dooley, **F. L. Dryer**, **Y. Ju**, “*Assessments of kinetic contribution on extinction limits of diffusion flames for large hydrocarbon fuels: a radical index*,” Paper 3C01, 7th U.S. National Combustion Meeting, March 20-23, 2011, Georgia Institute of Technology, Atlanta GA.
21. B. Yang, **H. Wang**, E. Dames, **N. Hansen**, S. Skeen, and T. A. Cool, “*Experimental and Modeling Study of the Oxidation of Isobutane and Isobutene*,” 7th US National - Combustion Meeting, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.
22. B. Yang, T. A. Cool, C. K. Westbrook, **N. Hansen**, and K. Kohse-Höinghaus, “*The Effect of Carbon-Carbon Double Bonds on the Combustion Chemistry of Fatty Acid Esters*,” 7th US National Combustion Meeting, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.
23. **N. Hansen**, M. R. Harper, and **W. H. Green**, “*High-Temperature Oxidation Chemistry of n-Butanol in Low-Pressure Premixed Flames*,” 7th US National Combustion Meeting, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.

24. R. D. Cook, R. Sur, I. Stranic, D. F. Davidson, **R. K. Hanson**, M. R. Harper, **W. H. Green**, “*Measurements of OH and H₂O Time-Histories in n-Butanol Pyrolysis*,” Paper 66, 7th International Conference on Chemical Kinetics, Cambridge MA, July 7-14, 2011.
25. M. Campbell, D. F. Davidson, **R. K. Hanson**, “*A Second-Generation Aerosol Shock Tube and its Use in Studying Ignition Delay Times of Large Methyl Esters*” Presentation, Thermo Sciences Affiliates Meeting, Stanford CA, Feb 2-4, 2011.
26. D. P. Chase, I. Stranic, J. T. Harmon, S. Yang, D. F. Davidson, **R. K. Hanson**, “*Shock Tube Measurements of Ignition Delay Times for Butanol Isomers*,” 7th US Combustion Meeting, Atlanta GA, March 20-23, 2011.
27. M. Campbell, D. F. Davidson, **R. K. Hanson**, “*A Second-Generation Aerosol Shock Tube and its Use in Studying Ignition Delay Times of Large Methyl Esters*,” 28th International Symposium on Shock Waves, Manchester UK, July 17-22, 2011.
28. R. Cook, **R. K. Hanson**, D. F. Davidson “*Multi-Species Laser Measurements for Validation of Oxygenated Fuel Mechanisms*,” 28th International Symposium on Shock Waves, Manchester UK, July 17-22, 2011.
29. M. L. Botero, D. L. Zhu, A. Molina, **C. K. Law**, “*Combustion characteristics of biodiesel/alcohol droplets*,” Paper No. W2P101, 33rd International Symposium on Combustion, Beijing, China, August 1-6, 2010.
30. Z. Y. Luo, C. S. Yoo, E. S. Richardson, **J. H. Chen**, **C. K. Law**, T. F. Lu, “*Chemical explosive mode analysis for a turbulent lifted ethylene jet flame in highly-heated co-flow*,” Paper No. W5P021, 33rd International Symposium on Combustion, Beijing, China, August 1-6, 2010.
31. **C. K. Law**, “*Fuel options for next generation chemical propulsion*,” Conference Dryden Lecture, Paper No. 2011-1, 49th AIAA Aerospace Sciences Meeting, Orlando, FL., Jan. 4-7 2011.
32. M. L. Botero, Y. Huang, D. L. Zhu, A. Molina, **C. K. Law**, “*Droplet combustion of ethanol, diesel, castor oil biodiesel, and their mixtures*,” Paper No. 1D07, 7th US National Combustion Meeting, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.
33. F. Wu, A. P. Kelley, D. Zhu, **C. K. Law**, “*Measurements and correlation of laminar Flame speeds of CO and C₂-hydrocarbons with hydrogen addition at atmospheric and elevated pressures*,” Paper No. 1E10, 7th US National Combustion Meeting, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.
34. P. Zhang, H. Sun, **C. K. Law**, “*Secondary channels in the thermal decomposition of monomethylhydrazine (CH₃NHNH₂)*,” Paper No. 2A01, 7th US National Combustion Meeting, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.
35. H. Sun, P. Zhang **C. K. Law**, “*Thermal decomposition of monomethylhydrazine: reaction mechanism and kinetic modeling*,” Paper No. 2A04, 7th US National Combustion Meeting, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.

36. S. Chaudhuri, V. Akkerman, **C. K. Law**, “*Turbulent flame speed and its modification by Darrius-Landau instability*,” Paper No. 2C07, 7th US National Combustion Meeting, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.
37. H. Wang and **S. B. Pope**, “*Parametric PDF studies of turbulent premixed stratified flames*”, 7th US National Combustion Meeting, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011.
38. H. Wang and **S. B. Pope**, “*LES/PDF Modeling of Turbulent Lifted Jet Flames in a Vitiated Co-Flow*”, 13th international conference on numerical combustion, Corfu, Greece, April 27-29, 2011.
39. H. Wang, P. P. Popov, V. Hiremath, S. R. Lantz, S. Viswanathan, **S. B. Pope**, “*Large-eddy simulation/probability density function modeling of local extinction and re-ignition in Sandia flame E*”, 63rd Annual Meeting of the APS Division of Fluid Dynamics, Long Beach, California, November 21-23, 2010.
40. H. Wang, **S. B. Pope**, “*LES/PDF modeling of a turbulent $CH_4/H_2/N_2$ jet flame*”, poster in: Thirty-third International Symposium on Combustion, Beijing, China, August, 2010
41. H. Wang, **S. B. Pope**, “*Development of an LES/PDF Code and Its Application to Flame D*”, in: TNF10 workshop, Tsinghua University, Beijing, China, July, 2010
42. **C. J. Sung**, A.K. Das, “*Ignition Delay Study of Moist Syngas/Oxidizer and Hydrogen/Oxidizer Mixtures using a Rapid Compression Machine*,” Forty-Ninth Aerospace Sciences Meeting, AIAA Paper No. 2011-91 (2011).
43. Y. Zhang, K. Kumar, **C. J. Sung**, “*Autoignition of Binary Fuel Blends of n-Butanol and n-Heptane in a Rapid Compression Machine*,” Forty-Ninth Aerospace Sciences Meeting, AIAA Paper No. 2011-92 (2011).
44. B. W. Weber, K. Kumar, **C. J. Sung**, “*Autoignition of Butanol Isomers at Low to Intermediate Temperature and Elevated Pressure*,” Forty-Ninth Aerospace Sciences Meeting, AIAA Paper No. 2011-316 (2011).
45. B. W. Weber, **C. J. Sung**, “*A Rapid Compression Study of the Butanol Isomers at Elevated Pressure*,” Seventh Joint Meeting of the U.S. Sections of the Combustion Institute, Atlanta, GA, 2011.
46. Y. X. Xin, **C. J. Sung**, **C. K. Law**, “*A Mechanistic Study of Soret Diffusion in n-Heptane/Air Flames*,” Seventh Joint Meeting of the U.S. Sections of the Combustion Institute, Atlanta, GA, 2011.
47. **D. G. Truhlar**, I. M. Alecu, “*Computational Study of the Reactions of Methanol with the Hydroperoxyl and Methyl Radicals*,” 240th ACS National Meeting, Boston, August 22-26, 2010, abstract PHYS-360.
48. **D. G. Truhlar**, I. M. Alecu, “*Computational Study of the Reactions of Methanol with the Hydroperoxyl and Methyl Radicals*,” Joint Meeting: Multi-Agency Coordinating Committee for Combustion Research (MACCCR) Fuels Research Review and Combustion Energy Frontier research Center (CEFRC) First Annual Meeting, Plainsboro, NJ, Sept. 23, 2010.

49. B. Yang, **H. Wang**, **N. Hansen**, S. Skeen, T. A. Cool, "Experimental and modeling study the oxidation of isobutane and isobutene," 7th US National Meeting of Combustion, Atlanta, Georgia, March 20-23, 2011, paper 1A13.
50. J. Camacho, S. Lieb, **H. Wang**, "*Formation of soot in laminar premixed n-butanol and isobutanol flames*," 7th US National Meeting of Combustion, Atlanta, Georgia, March 20-23, 2011, paper 2H08.
51. J. Camacho, S. Lieb, **H. Wang**, "*A comparative study of the sooting properties of laminar premixed flames of C6 hydrocarbons*," 7th US National Meeting of Combustion, Atlanta, Georgia, March 20-23, 2011, paper 3H01.
52. S. Memarzadeh, C. Thompson, **H. Wang**, "*Dependence of TiO₂ crystal phase on flame synthesis conditions*," 7th US National Meeting of Combustion, Atlanta, Georgia, March 20-23, 2011, 3F06.
53. S. Memarzadeh, D. J. Phares, **H. Wang**, "*Dye sensitized solar cells fabricated by flame stabilized on a rotating surface*," 7th US National Meeting of Combustion, Atlanta, Georgia, March 20-23, 2011, 3F05.
54. R. Tangko, D. A. Sheen, **H. Wang**, "*Combustion kinetic modeling using multispecies time-histories in shock-tube oxidation of n-dodecane*," 7th US National Meeting of Combustion, Atlanta, Georgia, March 20-23, 2011, paper 2A18.
55. D. A. Sheen, **H. Wang**, "*Modeling the pressure dependence of H₂/O₂/diluent mass burning rates*," 7th US National Meeting of Combustion, Atlanta, Georgia, March 20-23, 2011, paper 1B07.
56. D. A. Sheen, **H. Wang**, "*Combustion kinetic modeling using multispecies time-histories in shock-tube oxidation of heptane*," 7th US National Meeting of Combustion, Atlanta, Georgia, March 20-23, 2011, paper 1A14.
57. S. Koumlis, **H. Wang**, "*Scattering of noble gas molecules and transition metal nanoparticles: A molecular dynamics study*," 7th US National Meeting of Combustion, Atlanta, Georgia, March 20-23, 2011, paper 2F10.
58. S. Gao, D. J. Phares, **H. Wang**, "*Molecule/particle beams detection by fast superconducting bolometers*," 7th US National Meeting of Combustion, Atlanta, Georgia, March 20-23, 2011, paper 2H15.

3.3. Invited presentations

Carter

1. "How Quantum Mechanics Can Help Solve Our Energy Problems," Davidson Lectureship, Department of Chemistry, University of North Texas, Denton, TX, March 4, 2011.

2. “Fast Yet Accurate Algorithms for Multireference Ab Initio Electron Correlation Treatment of Large Molecules,” Department of Chemistry, University of North Texas, Denton, TX, March 3, 2011.
3. “Fast Yet Accurate Algorithms for Multireference Ab Initio Electron Correlation Treatment of Large Molecules,” at the Pacificchem 2010 Congress, Honolulu, HI, December 20, 2010.
4. “How Quantum Mechanics Can Help Solve Our Energy Problems,” at the Frontiers in Renewable Energy Sciences and Technologies Workshop, Cambridge, MA, September 30, 2010.
5. “Multireference Correlated Wavefunction Calculations and Reaction Flux Analyses of Methyl Ester Combustion,” at the Annual Conference for the Combustion Energy Frontier Research Center, Princeton, NJ, September 23, 2010.
6. “How Quantum Mechanics Can Help Solve Our Energy Problems,” at the Meeting of the National Research Council Board on Chemical Sciences and Technology, Woods Hole, MA, August 26, 2010.
7. “Efficient Ab Initio Multireference Electron Correlation Methods for Ground and Excited States,” at the Molecular Quantum Mechanics 2010 Conference, Berkeley, CA, May 27, 2010.

Chen

8. Plenary Invited Presentation “Petascale Direct Numerical Simulation of Turbulent Combustion –Fundamental Insights Towards Predictive Models,” Beijing, 2010. Proc. Combust. Inst. 33(2011) 99-123.

Dryer

9. “Surrogate Mixtures for Describing Real Fuel Combustion: Challenges and Recent Progress”, 7th US National Combustion Meeting of the Combustion Institute, Georgia Institute of Technology, Atlanta, GA, March 20-23, 2011. Invited Topical Paper.

Ju

10. “Fuels chemistry and surrogate modeling,” Workshop on Combustion Science in an Energy-Constrained World, Tsinghua University, China, July 31, 2010.
11. “A Dynamic Multi-Timescale Method for Kinetic Model Reduction and Direct Numerical Simulation of HCCI Combustion,” Combustion and Fuels Workshop, Shanghai Jiaotong University, China, Aug.9-10, 2010.

Klippenstein

12. "*Theoretical rate coefficients for allyl + HO₂ and allyloxy decomposition*", 33rd International Symposium on Combustion – The Combustion Institute, Atlanta, GA, August 1-6, 2010.

Green

13. "*Comprehensive Reaction Mechanism for n-Butanol Pyrolysis and Combustion*", AIChE Annual Meeting, Salt Lake City, UT, November 7-12, 2010.
14. "*Accurate Reaction Networks for Alternative Fuels: Butanol Isomers*", 21st International Symposium on Chemical Reaction Engineering, Philadelphia, PA, USA, June 13- 6, 2010.
15. "*Redesigning Combustion Modeling Algorithms for the Graphics Processing Unit (GPU): Chemical Kinetic Rate Evaluation and Ordinary Differential Equation Integration*", 7th US National Technical Meeting of the Combustion Institute, Atlanta, GA, March 20-23, 2011.
16. "*A multi-approach algorithm for enabling efficient application of very large, highly detailed reaction mechanisms in multi-dimensional HCCI engine simulations*", 7th US National Technical Meeting of the Combustion Institute, Atlanta, GA, March 20-23, 2011.

Hansen

17. "*High-temperature oxidation chemistry of n-butanol in low pressure premixed flames*", 7th US National Technical Meeting of the Combustion Institute, Atlanta, GA, March 20-23, 2011.

Law

18. "*Some recent advances in combustion science for propulsion applications*", Annual Advanced Propulsion Meeting, Office of Naval Research, Arlington, VA, June 24, 2010.
19. "*Ignition, propagation, and morphology of expanding spherical flames*", Keynote Lecture, Workshop on Fuels and Combustion, Wu Zhen, China, August 9, 2010.
20. "*Fuel options for next-generation chemical propulsion*", Dryden Lecture, Aerospace Sciences Meeting, AIAA, Orlando, FL, Jan. 3-7, 2011.

Pope

21. "*Stochastic Lagrangian Models for Turbulent Flows*" Georgia Institute of Technology, Aerospace Engineering, October 21, 2010.

22. "Advances in Computer Simulations of Turbulent Combustion" University of Southern California, Mechanical Engineering, February 23, 2011.
23. "Advances in Computer Simulations of Turbulent Combustion" California Institute of Technology, GALCIT, February 24, 2011.

Sung

24. "Rapid Compression Machine Studies on Autoignition of Next Generation Fuels," Argonne National Laboratory, Washington, DC, August 24, 2010.

Truhlar

25. "Computation of Accurate Thermochemical and Rate Parameters for Complex Combustion Reactions" Joint Meeting: Multi-Agency Coordinating Committee for Combustion Research (MACCCR) Fuels Research Review and Combustion Energy Frontier research Center (CEFRC) First Annual Meeting, Plainsboro, NJ, Sept. 23, 2010.
26. "Density Functional Theory for Kinetics, Catalysis, and Organometallic Complexes," invited lecture, National ACS Meeting, Boston, Aug. 24, 2010.

3.4. Web site or other internet sites

- CEFRC Intranet: The intranet for the CEFRC is set up as a wiki, which is intrinsically easier to use than conventional shared Web space. Researchers and their groups can upload, download and read shared files on the wiki. Whereas our extranet is our WWW face to the whole world, the intranet is for internal sharing and communication. It is password protected, and Center researchers are registered users who can login to use the wiki. Center PI Donald G. Truhlar and Jingjing Zheng at the University of Minnesota manage it. The intranet URL is <https://cefrchem.umn.edu/groups/cefrwiki/>. When a user logs in, there is a help page that tells him or her how to add a file and how to register the members of their research group. The pages for sharing information contain key Center documents, Center preprints and publications, Center presentations, current Center projects, and progress reports of Center groups.
- CEFRC Website: The CEFRC was redesigned in January 2011 to incorporate a fully functional application, registration and reporting system to support the Princeton-CEFRC Summer School. The website address is <http://www.princeton.edu/cefr/>.

3.5 Networks or collaborations

Carter

- Established a collaboration with Theresa Windus and Mark Gordon at Iowa State University, via a small DOE-ASCR grant to the ISU PIs, to work together to port her fast MRSDCI code to work with GAMESS and to parallelize the code so that it can scale on

DOE supercomputers. A parallel, scalable MRSDCI code will allow much faster throughput to evaluate bond dissociation energies and activation energies of the many species involved in biodiesel combustion.

Chen

- Collaboration with computer scientists, Valerio Pascucci of U. Utah and Kwan-Liu Ma of UC Davis, through DOE ASCR grant on Petascale Data Discovery from Combustion Simulation, to provide analytics and visualization tools to extract physical insight from petascale simulated combustion data. Collaboration with Suresh Menon, Heinz Pitsch, James Sutherland, and Ed Knudsen to perform a posteriori validation of combustion models for large-eddy simulation of turbulent combustion using DNS data. Collaboration with Ray Grout of NREL, Ramanan Sankaran of ORNL, and John Levesque of Cray Research to refactor direct numerical simulation code, S3D, for hybrid petaflop architectures.

Dryer

- Collaboration with Steve Klippenstein at Argonne. Through the role as the Principal Investigator of an AFOSR MURI on the development of surrogate fuels provides coordination between researchers at CEFRC and this MURI program.

Egolfopoulos

- Through the role as the Principal Investigator of an AFOSR IPT program provides coordination between researchers at CEFRC and this program.
- Internal collaborations within include the research groups of Wang, Law, and Ju. More specifically, issues associated with small hydrocarbon kinetics are addressed with the input of Wang and there is a long-standing collaboration between the two PI's as the record shows. The collaboration with Law includes issues associated with the experimental determination of laminar flame speeds. The two research groups are using different (stagnation flames and spherically expanding flames) but yet complementary experimental approaches and while frequently agreements exist between independently determined sets of data, this is not always the case especially on the fuel lean side. Given that the experimental data should be unique for each reacting mixture, the two groups are working closely in order to assess ways to consolidate the results obtained using the two different experimental approaches. The collaboration with Ju just initiated through a newly appointed roving postdoc who will be working on alternative experimental approaches to study flame kinetics at high pressures that are of relevance to internal combustion engines.
- External collaborations include Westbrook of the Livermore National Laboratories. Westbrook is a pioneer of combustion kinetics and his most recent work is largely focused on the pyrolytic and oxidation kinetics of oxygenated fuels, such as alcohols, ketones, aldehydes, and esters, which are key target compounds to the CEFRC program.

While parallel efforts on kinetics are ongoing within CEFRC, additional input from members that are external to the center and of the scientific caliber of Westbrook are considered at a minimum as beneficial and complementary. Several manuscripts have been co-authored with Westbrook.

Green

- Organizer of the 7th International Conference on Chemical Kinetics, providing networking opportunities for the Center PIs who will be attending this conference as well as other international participants on chemical kinetics.
- Greg Magoon (Green group) tested and improved the new CEFRC capability to automatically spawn quantum chemistry calculations of thermochemistry while constructing kinetic models through a collaboration with Aerodyne Research funded by the Navy on synthetic fuel JP-10.
- Methyl Formate (smallest methyl ester): collaboration with Nabiha Chaumeix (CNRS, Orleans) and Laurent Catoire (ENSTA ParisTech), with several interactions with Stephen Dooley (Dryer group, Princeton).
- David Sheen (Wang's recent student, now at UVa and NIST) visited Green group, gave a seminar and discussed on issues of uncertainty.
- Joint oral presentation will be given at ICCK (July 2011) on "Combustion of the butanol isomers: Reaction pathways at elevated pressures from low-to-high temperatures" by several CEFRC PIs plus a non-CEFRC collaborator: Michael R. Harper, William H. Green (MIT), Kevin M. Van Geem (Ghent), Bryan W. Weber, Chih-Jen Sung (UConn), Ivo Stranic, David F. Davidson, Ronald K. Hanson (Stanford)
- Collaborators trained to use the RMG mechanism-construction software through visits to MIT: Stijn Vranckx (Aachen), Pierre-Alexandre Glaude and Xavier Grandmougin (CNRS Nancy), Nick Vanderwiele (Ghent), Rajesh Parmar (Queens U. Canada), Subith Vasu (Sandia Livermore CRF, scheduled for May 2011), Mani Sarathy & Marco Mehl (LLNL, scheduled for July 2011)
- Franklin Goldsmith (Green group) published one joint paper with Stephen Klippenstein, second manuscript in preparation.

Ju

- Collaborations with Carter, Dryer, Kippenstein, and Hai to develop a biodiesel surrogate model. Collaboration with Egolfopoulos, Hansen, and Law to obtain flame properties for kinetic validation. Team with Chen and Pope to develop multiscale models for turbulence modeling.

Klippenstein

- Collaboration with Law, Pope, and Wang, through the roving post-doc appointment of Peng Zhang. Collaboration with Dryer at Princeton, Green at MIT, and Ju at Princeton. Through the role as Principal Investigator of a DOE FWP on high pressure combustion chemistry provides coordination between researchers at the CEFRC and the combustion chemistry groups at Argonne and Sandia.

Law

- Collaboration with Klippenstein, Pope and Wang on high-pressure combustion through the roving post-doc appointment of Peng Zhang, with Chen on effects of flamefront pulsating and cellular instabilities on the turbulent flame structure, and with Egolfopoulos on the laminar flame structure.
- As the director of the CEFRC, the PI also coordinates closely with the Center for Combustion Energy at Tsinghua University in China, and the Clean Combustion Energy Center of the King Abdullah University of Science and Technology in Saudi Arabia, in a global alliance on clean combustion energy.

Hansen

- Within the CEFRC, collaboration with Green on the combustion chemistry of n- and iso-butanol, with Wang on the C4 (n-butane, iso-butane, and iso-butene) chemistry, and with Ju on developing a mechanism for methylbutanoate.
- External to CEFRC, collaboration with Terry Cool (Cornell), Charlie Westbrook (LLNL), and Katharina Kohse-Höinghaus (Bielefeld) on the chemistry of simple ester fuels. Collaborates with Jim Miller (Argonne), Hope Michelsen (Sandia), and Angela Violi (Michigan) on aromatics and soot formation chemistry in hydrocarbon flames.

Hanson

- Collaboration with Christof Shultz Universitat Duisburg on developing refined reaction mechanisms for oxygenated fuels based on time-dependent speciation data acquired at both Duisburg and Stanford. Current work focuses on 3-pentanone oxidation and pyrolysis.
- Collaboration with Peter Lindstedt of Imperial College London on the role of individual reaction rate constants (in particular reactions of OH+alcohols) in the refinement of reaction mechanisms for higher alcohols including butanol.
- Collaboration (and visit) with Aamir Farooq of KAUST (King Abdullah University of Science and Technology) Saudia Arabia on the development of a quantitative laser diagnostic for carbon monoxide for use in the acquisition of time-dependent speciation data for CO during methyl ester pyrolysis and oxidation.

Sung

- Autoignition of 2-buten-1-ol

Buten-1-ol is an important intermediate in the combustion of *n*-butanol, and has been found by several studies in the literature, especially under engine-relevant conditions. Moreover, 2-buten-1-ol has some potential as an additive in, or replacement for, gasoline. In collaboration with Green of MIT, this investigation aims at understanding the autoignition chemistry of this fuel.

- Autoignition of iso-Pentanol

iso-Pentanol produced from biological sources presents several advantages over ethanol and butanol including higher energy content and lower water solubility, which makes it a promising alternative to petroleum-derived gasoline fuels. Autoignition of *iso*-pentanol will be investigated using our rapid compression machine under both SI- and HCCI-relevant conditions over a wide range of pressure and temperature conditions. Experimental data will then be used to validate the detailed mechanism developed by William Pitz of Lawrence Livermore National Laboratory and Henry Curran of the National University of Ireland.

- IR Absorption Spectroscopy in Rapid Compression Machine

In situ absorption spectroscopy of important species such as CO, H₂O, and H₂O₂ will be conducted in the PI's rapid compression machine for various fuel systems. The evolution/consumption history of the species will be recorded and compared with reaction mechanism for better evaluation of the chemical kinetic model. This work is in collaboration with Ju of Princeton University.

Pope

- Organizer of the MACCCR Workshop on Collaboration for Turbulent Combustion Model Development and Validation, Georgia Institute of Technology, March 20, 2011; and of the International Workshop on the Measurement and Computation of Turbulent Nonpremixed flames.
- Collaboration with Chen at Sandia on turbulent combustion simulations through the roving post-doc Yue Yang. Collaborating with Law on premixed turbulent combustion through the roving post-doc Peng Zhang. Ongoing collaboration with Alex Klimenko (U. of Adelaide, Australia) on modeling turbulent combustion; Peyman Givi (U. of Pittsburgh) on LES/PDF modeling; P.K. Yeung (Georgia Tech) on large-scale turbulence simulations.

Truhlar

- Used new density functional methods to find the lowest-energy conformer of methyl butanoate and to calculate all the bond dissociation energies for comparison to Carter's results obtained by multireference configuration interaction.

- Collaborating with Green through a CEFRC Postdoctoral Fellow, John Alecu. John is learning theoretical methods and calculating rate constants in my group, and he will carry out related experiment experiments next year in Green's lab.
- Collaborating with Ahren Jasper of Sandia. The goal is to interface the POLYRATE program with a two-dimensional master equation that resolves the dynamics with respect to both the energy and rotational state of the system. The main bottleneck with the project is coding the method in a general and efficient way. This could potentially also involve collaboration with the Argonne group.
- Collaborating with Rex Skodje and the Argonne group on reactions important for their work on the butanol oxidation mechanism. Close contact with Green's group to keep abreast of work on butanol mechanisms.
- Collaborating with Orlando Roberto-Neto and coworkers in Brazil on rate constant calculations relevant to the CEFRC mission.

Wang

- Collaboration with Dryer, Klippenstein, Green, Ju, Hansen, Hanson and others to develop a foundation fuel chemistry model. Collaborates with Hansen on the chemistry of isobutane and isobutene combustion through the roving postdoc appointment of Bin Yang.

3.6. Technologies, techniques, inventions/patent applications

None

3.7. Other products

- Videos of the 2010 summer school lectures by Professor Norbert Peters on Combustion Theory, and by Drs. Stephen J. Klippenstein and Charles K. Westbrook on Combustion Chemistry were produced and are available to the public at iTunes University, <http://deimos.apple.com/WebObjects/Core.woa/Browse/princeton.edu.4746982603.04746982605> and at <http://www.princeton.edu/engineering/video/combustion-2010/>. Refer to Section 3.8 and Appendix C for additional information on the Princeton-CEFRC Summer School on Combustion.

3.8. Outreach

The CEFRC continued its efforts in each of three major outreach programs, namely the Combustion Energy Research Fellows (the roving post-docs) program, the Princeton-CEFRC Summer School on Combustion, and the bi-annual CEFRC Newsletter. Each of these functions is headed by a team of PIs, both in execution and oversight.

- **Combustion Energy Research Fellows Program**

The Combustion Energy Research Fellows Program offers two-year appointments for co-sponsored postdoctoral or more senior research associates to perform joint, high-risk/high-payoff research projects with at least two principal investigators of the Center at their respective locations, providing synergy and continuous rejuvenation of research directions. These Combustion Energy Research Fellowships are highly competitive appointments which provide rigorous training for the next generation of leaders in combustion science and technology. Appointments are made three times a year. Thus far, four rounds of selection have been conducted, resulting in the appointment of six fellows. We anticipate the next round of appointments should complete the eight slots allocated for this program. Refer to the CEFRC website <http://www.princeton.edu/cefr/combustion-research-fello/combustion-research-fello/> for a description of the appointees as well as Appendix B for a listing of the Combustion Energy Fellows currently in residence.

- **Princeton-CEFRC Summer School in Combustion**

Following on the success of the inaugural session of the Princeton-CEFRC Summer School on Combustion held in June, 2010, planning for the 2011 session of the Summer School is well underway. The Combustion Summer School is a one-week seminar series hosted on the Princeton University campus and held annually, during which advanced graduate students and researchers in combustion and energy will take two courses of 15 hours each. For the 2011 session, the Combustion Theory lectures will be delivered by Professor Moshe Matalon of the University of Illinois at Urbana-Champaign; the Combustion Chemistry lectures will be delivered by Professor Michael J. Pilling of the University of Leeds, U.K.; and an advanced course on Combustion Laser Diagnostics will be delivered by Professor Marcus Aldén of Lund University, Sweden. Based on the positive feedback to the video tapings of the 2010 lectures, which have been made available to the public at iTunes University on the Princeton University website at <http://deimos.apple.com/WebObjects/Core.woa/Browse/princeton.edu.4746982603.04746982605> and <http://www.princeton.edu/engineering/video/combustion-2010/> respectively, we will once again video tape the week-long lectures.

The call for applications to the 2011 session has surpassed that of last year, with 133 applicants admitted thus far. With a growing waiting list, we are making arrangements to move the classes to an even larger venue, so as to allow the maximum number of applicants the opportunity to attend this summer's session.

Scholarships are available to domestic students to cover travel and local expenses. Refer to Appendix C for the announcement and syllabus of the 2011 session.

- **CEFRC Newsletter**

The second issue of the Center's newsletter, *CEFRCnews*, was published and distributed January 2011. Refer to Appendix D for the newsletter.