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Development of HyChem - A Jet and Rocket Fuel Combustion Chemistry Model

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Final Report

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Development of HyChem - A Jet and Rocket Fuel Combustion Chemistry Model

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Abstract

This research project is a continuation of previous AFOSR award number FA9550-14-1-0235 entitled *Modeling Pyrolysis and Oxidation of Jet Fuels - A Hybrid Approach* FA9550-14-1-0235 with Dr. Chiping Li as Government Program Manager. Its objective is to further the development of the HyChem approach to jet fuel combustion chemistry modeling. HyChem models have been developed and published for Jet A, JP8, JP5, RP2, JP10, and other related practical liquid fuels.

Introduction

The concept, termed the HyChem approach, seeks to advance jet and rocket fuel combustion chemistry models through a physics-based understanding of the primary reaction pathways in fuel combustion. It combines an experimentally constrained fuel pyrolysis model with a detailed foundational chemistry model for the oxidation of pyrolysis products to describe and predict the combustion behaviors of real, multicomponent fuels. HyChem reaction models have been developed for Jet A, JP8, JP5, JP10 and two RP2 fuels. The accuracy of the models has been tested over a wide range of thermodynamic conditions and low-dimensional combustion phenomena, including oxidation in a flow reactor, shock-tube ignition delay and laminar flame speed and extinction strain rate. The reaction models have been released, reduced (in collaboration with T.-F. Lu of the University of Connecticut) and delivered to various AFRL and other labs for use.

The results obtained thus far allow us now to examine the remaining theoretical, modeling and experimental issues that must be resolved to improve the model predictability and define the range of applicable limits to the model. In this next stage of development, the question concerning the sensitivity of kinetic rates and pathways to different jet fuel distillation fractions will be addressed experimentally and computationally. The results from this study will be presented chronologically.

2016-2017

During the initial year of this continuation project, we targeted two areas of research. The first area was the acquisition of pyrolysis speciation data and ignition delay time (IDT) data for the ~~rocket~~ fuel JP-10. This database was used by Prof. Wang as kinetic constraints and targets in the development of a HyChem model for JP-10. The JP-10/air IDT shock tube measurements were performed at 17 at and for equivalence ratios of 0.5 to 2. The pyrolysis data were acquired at both low (1.5 atm) and high (17 atm) pressures using multiple wavelengths to measure C_2H_4 and cyclopentadiene concentration time-histories. The second area of research was the refinement of a three-wavelength, three-species diagnostic strategy to simultaneously measure ethylene, propene and iso-butene to again provide kinetic constraints on the development of a HyChem model for jet fuel. Using this strategy, high-quality species concentration time-histories for the three alkenes, as well as methane and fuel, during pyrolysis were acquired for JP-8.

As a closely coupled component of accurate HyChem models, a Foundational Fuel Chemistry Model-1 (FFCM) was released on line as the result of a collaboration with G. P. Smith of SRI. Additionally, a gas-kinetic theory formulation was developed for the molecular transport of long-chain molecules in dilute gases. The binary diffusion coefficients predicted by the theory enabled us to resolve a long-standing, unresolved issue in laminar flame modeling, namely, the difficulty of predicting the non-premixed, laminar extinction strain rates of *n*-dodecane and *n*-decane flames using detailed reaction kinetics.

2017-2018

Three areas of research were targeted. The first area was the acquisition of a standardized set of shock tube ignition delay time IDT, C_2H_4 pyrolysis yield and IR absorption spectroscopy data at conditions relevant to high-temperature HyChem models. Using this dataset, we have investigated correlations that relate the observed combustion behavior to the spectroscopic properties of the fuel vapor. We have made an important key observation. We ~~have~~ found that measurements of the ratio of infrared (IR) absorption at two wavelengths (3.410 and 3.391 mm) of the fuel vapor, strongly correlates with DCN (and thus LBO), IDT and C_2H_4 pyrolysis yields (and thus with HyChem).

These correlations show that the combustion kinetic behaviors of a wide variety of jet fuels can be characterized with a relatively simply spectroscopic test of the real fuel vapor, as a screening measure for alternative jet fuel formulations or possibly even included in the form of a fuel specification. We believe that this could be an economical yet informative screening tool for the combustion kinetics behavior of candidate alternative fuels.

The second area of research was in the advancement of jet fuel speciation and pyrolysis-product carbon counting. We have developed a new convex least-squares analysis strategy that allows deconvolution of multi-wavelength/multi-species laser absorption data to recover quantitative pyrolysis yields of direct use to the refinement of the HyChem model. Using this dataset, we have been able to provide measurements of the pyrolysis yields of the following species: C_2H_4, C_3H_6, 1-C_4H_8, i-C_4H_8, CH_4, benzene, toluene and fuel for the Cat A fuels. As the majority of the carbon in jet fuel pyrolysis products rests in alkene and aromatic products, this approach should provide near complete carbon counting for the pyrolysis products.

The third area of research is the identification and measurement of high-temperature rate constants for key reactions affecting the accuracy of CH_4 pyrolysis and oxidation models. As one example, we have identified deficiencies in current detailed reaction models (ARAMCO v.2.0 and FFCM) in their ability to predict CH_4 pyrolysis product yields at high pressures (~15 atm) and ignition delay times (IDT) at extreme pressure (~100 atm). We have also made a first attempt at measuring the rate constant of the reaction $H+C_2H_4 = C_2H_3+H_2$ using laser absorption of C_2H_4. Finally, we completed the experimental work and have two ~~emerging~~ papers describing measurements for the rate constant of the key reactions $H+O_2+M=HO_2+M$ (M=Ar, H_2O, CO_2, N_2) at elevated pressures for two temperature regimes. Introduction of these rate measurements in FFCM significantly reduce uncertainty in the foundational fuel model of Wang et al. and HyChem.

2018-2019

Work by Prof. Wang's group examined the impact of preheat-zone fuel pyrolysis of *n*-dodecane on its laminar flame propagation rate and extinction strain rate by numerical simulation with the conclusion that fuel pyrolysis has a little effect on the laminar flame speed, but it has a notable effect on flame extinction. The HyChem Jet A model has been implemented in several LES codes. The simulation results demonstrated the efficiency and accuracy of the model for predicting various turbulent flame phenomena. The principle of large component number in the combustion chemistry of complex, multicomponent fuels is further examined. The results again demonstrate the insensitivity of combustion responses to the fuel composition details when more than 12 components are present in the fuel. A bottom-up approach to kinetic modeling is demonstrated, using Keck's Rate Controlled Constrained Equilibrium (RCCE) approach. The result demonstrates the approach to be viable for modeling complex combustion chemistry when not all of the elementary reactions and their rate coefficients are available. It is suggested that the approach may be combined with the HyChem approach in such a way that the empirical features of HyChem may be removed with the RCCE principle.

Prof. Wang's group also extended their studies in the area of foundational fuel chemistry model. Critical kinetic uncertainties are examined in the context of prediction of extinction and ignition time in a perfectly stirred reactor. The results identify key reaction rate coefficients that need to be examined in future studies. A method for jointly optimizing the pre-exponential factor and activation energy was proposed. The results however show that because of the scatter in the current combustion target data, very little can be gained when the activation energy is included in uncertainty minimization.

Prof. Wang's group also extended the HyChem model to predicting NO_x and soot formation from jet fuels. In the area of NO_x formation, it was found that the extended HyChem model is capable of making good predictions against NO_x data collected in premixed stagnation flames of Jet A. Extension to soot prediction is more challenging. Nonetheless, the extended HyChem model is shown to predict soot volume fraction in Jet A flames to within a factor of two. We have also made critical advances in the area of foundational fuel chemistry model development. FFCM-2 is being prepared for release. A compact model of methane combustion in oxygen was derived from the interim version of FFCM-2 and was delivered to AFRL for wide ranging CFD simulations.

Sensitivity to HyChem related experimental uncertainties and the foundational fuel chemistry model was studied in detail. The accuracy required for the species measurements for HyChem model development is assessed. It was found that the current uncertainties of the HyChem model are largely derived from the uncertainties in the foundational fuel chemistry model. Similar sensitivity analysis was performed in DNS simulations of spherical flame kernel evolution of Jet A. The results show that the principal pathways remain~~s~~ ~~to be~~ the same ~~between~~ in ~~the~~ turbulent and laminar premixed flames under comparable conditions, except that the sensitivity spectra broadens somewhat in the turbulent flame compared to the laminar flame, and that the magnitudes of the sensitivity coefficients are larger in the turbulent flames than the comparable laminar flames, thus indicating that chemistry plays a more significant role in the total heat release rate in the turbulent flame kernel propagation.

Professor Hanson's group targeted three additional areas of research. The first area is the development of spectroscopic predicting strategies that enable the estimation of liquid fuel physical and chemical properties from their IR spectra. The second area is the study of natural gas pyrolysis and combustion kinetics. The third area is the development of laser absorption sensors for the measurement of propane and ethane concentrations.

Further research has refined our understanding of the new "3.41/3.39 absorption ratio" spectroscopic predictor for estimating ignition characteristics, including derived cetane number, for hydrocarbon fuels. Its wide availability and applicability were demonstrated for a range of pure hydrocarbons, mixtures of pure hydrocarbons, and distillate and synthetic jet fuels. Spectroscopic and kinetic interpretations were provided based on the fraction of $–CH_2–$ hydrogen relative to all carbon-bonded hydrogen. These included correlations between the IR predictor and ignition delay time and C_2H_4 yield allowing the predictor to be used as a fuel screening tool.

The concept of a compact, economical FTIR-based analyzer for estimating the properties of hydrocarbon fuels properties was extended to include correlations based on broad spectral features. The high correlations between mid-IR FTIR absorption spectra of fuel vapor in the range 3300 to 3550 nm and 15 physical and chemical properties, such as density, initial boiling point, surface tension, kinematic viscosity, number of carbon and hydrogen per average molecule, and derived cetane number, for 64 hydrocarbon fuels were characterized. Lasso-regularized linear models based on linear combination of cross sections at selected wavelengths were built for each of these physical and chemical properties, yielding accurate estimations.

The pyrolysis and oxidation kinetics of natural gas (NG) were investigated using shock tube/laser absorption techniques. A wide variety of NG samples from across the United States were tested for ignition delay times, and ethylene and ethane pyrolysis yields. This study identified the strong influence that ethane content of NG has on NG ignition delay time. The performance of a sensitivity analysis to determine the influence of critical reactions on ethylene formation led to the observation that the rate for the reaction of CH_3+C_2H_6 strongly affected the C_2H_4 pyrolysis yields. Literature values for this reaction rate vary significantly at high temperatures. In separate shock tube experiments covering 1369 to 1626 K at 8.6 to 47.4 atm, this rate constant was measured with an uncertainty of +20%/-25%.

As the next major components of NG after methane are the larger alkanes, ethane and propane, efforts were made to develop sensitive laser absorption diagnostics for these two species. Currently ethane has been detected in synthetic NG at 3.35 microns in the infrared where a relatively strong absorption feature exists. Efforts have been directed to optimize the detection of propane at wavelengths near 3 microns.

2019-2020

During the reporting year, we completed the development of a HyChem model for predicting NO*x* formation from jet fuels. The extended HyChem model is capable of making good predictions against NO*x* data collected in premixed stagnation flames of Jet A. Extension of the model to soot prediction is more challenging and is ongoing. We have made critical advances in the area of foundational fuel chemistry model development. Work on FFCM-2 is continuing.

Sensitivity of the HyChem model and the foundational fuel chemistry model to experimental uncertainties was studied in detail. Comprehensive Monte Carlo analysis of model predictions with respect to species measurement was carried out using the Jet A HyChem model as the test case. We assessed the impact of the measured fuel pyrolysis products, including ethylene (C_2H_4), methane (CH_4), propene (C_3H_6), 1-butene (1-C_4H_8), iso-butene (*i*-C_4H_8), benzene (C_6H_6), and toluene (C_7H_8) on HyChem predictions using ignition delay time and laminar flame speed as the test targets. The results show that the speciation data are necessary to obtain reliable predictions for the laminar flame speed and ignition delay time at and above 1200 K. Additional measurement targets (e.g., CO and CH_2O) are proposed for future HyChem model development, especially in improving model predictions for ignition delay in the 1000 to 1200 K range.

We have also targeted two new areas of research. The first area is the measurement high-temperature and high-pressure infrared spectra of critical combustion and propulsion species. The second area is the study of natural gas pyrolysis and combustion kinetics.

A methodology for the measurement of mid-infrared absorption cross sections of gaseous molecules at high temperatures and pressures was developed. A rapid-tuning, broad-scan external cavity quantum cascade laser with a tuning rate in excess of 30,000 $cm^{-1}s^{-1}$ has been employed in the measurement of full vibrational bands (> 100 cm^{-1}) in shock-heated test gases. The approach was demonstrated with measurements of the absorption cross section of ethylene (C_2H_4) in the 8.5 to 11.7 µm region for temperatures from 800 to 1600 K and pressures from 1 to 5 atm. Decreasing peak strength with temperature was observed as well as pressure-insensitivity. The measurements were compared with existing experimental, empirical, and ab initio databases. Additionally, absorption cross section measurements of propene (C_3H_6), 1-butene (1-C_4H_8), 2-butene (2-C_4H_8), 1,3-butadiene (1,3-C_4H_6), and methanol (CH_3OH) near 1000 K and 2.3 atm were acquired.

The pyrolysis and oxidation kinetics of natural gas (NG) and methane (CH_4) were investigated using reflected shock wave/laser absorption techniques. Ignition delay time (IDT) were monitored using sidewall pressure, and species time-histories were monitored using direct laser absorption diagnostics for CH_4 near 3175 nm and ethylene near 10532 nm. Stoichiometric, fuel-rich and fuel-lean mixtures of $CH_4/O_2/Ar$ over temperatures between 1450K and 1850K and pressures between 10 and 55 atm and stoichiometric mixtures of commercial natural gas blends over temperatures between 1408 to 1541K at pressures near 12 atm were studied. Of particular importance are the fuel-rich measurements, as there is a lack of literature data in this regime. To understand the effects of minor constituents (such as ethane and propane) in commercial natural gas blends, ethylene concentration was also monitored during ~~2~~ two pyrolysis experiments. The deficiency of existing kinetic models in predicting the high-temperature kinetics of natural gas blends was highlighted through these measurements. Sensitivity analysis emphasizes the importance of the reaction $CH_3+C_2H_6 \rightarrow CH_4+C_2H_5$ during natural gas pyrolysis, and the accuracy of the chemical kinetic models is significantly improved by using a revised reaction rate constant (Shao et al. 2019) for this reaction. These measurements extend the test conditions of earlier studies of methane and commercial natural gas. This work is currently being extended to include development of diagnostic schemes for larger alkanes found in NG such as ethane and propane.

2020-2021

Shock tube/laser absorption research was able to continue under the COVID restrictions. Two areas were studied: the development and application of laser absorption diagnostics for allene and propyne, and the experimental investigation of cyclopentadiene pyrolysis.

Two novel laser absorption diagnostics for allene and propyne were developed. Through examination of the high temperature spectra of the two C_3H_4 isomers via two fast-wavelength-scanning, broadband external cavity quantum cascade lasers, 1930.38 cm^{-1} and 1233.3 cm^{-1} were chosen as the wavelengths for a two-species, two-wavelength diagnostic pair that minimizes interference from other species. Absorption cross sections for allene and propyne were measured at each of these wavelengths over

1196-1502K, at 1.3-1.6 atm. Once characterized, these diagnostics were employed to measure the mutual isomerization rates of allene and propyne over the same temperature range. The rates are reported for the two reactions These rates were found to be in excellent agreement with limited past experimental determinations and recently computed rates. Using these rates, the equilibrium constant is also reported as a function of temperature.

Cyclopentadiene pyrolysis was examined behind reflected shock waves in a heated shock tube using several laser diagnostic schemes. A two-color, online-offline sensor was used to measure acetylene, while a three-color scheme of diagnostics at 10.532 μm, 10.675 μm, and 11.345 μm yielded measurements of cyclopentadiene and ethylene. Species time histories of cyclopentadiene decomposition and acetylene formation, as well as ethylene yields, were measured from 1319K to 1678 K at 1.2 - 1.5 atm. In addition, the overall decomposition rate of cyclopentadiene is reported and comparisons are made to a number of kinetic models.

A flow reactor study of the impact of vitiation on the reactivity and product distributions during the thermal decomposition of two selected real liquid jet fuels, Jet A and JP-10, was carried out, by comparison with corresponding non-vitiation conditions. The experimental results and kinetic analysis proved that the reactivity of the selected jet fuels can be both promoted by oxygen and vitiation. The addition of oxygen resulted in around 10% increase of fuel reactivity of Jet A at ~47% fuel conversion, which is primarily ascribed to the branching reaction $H + O_2 \rightarrow H + OH$. On the other hand, the vitiation increases the reactivity of Jet A and JP-10 by 300% and 200% respectively. The results from all the experiments show that the relative carbon distribution among the most important products (except that of methane) are constant at wide fuel conversion ranges, despite the varying operating conditions, such as addition of oxygen, vitiation, and change of temperature and reaction times. These results support one of the key assumptions during the development of HyChem kinetic models for multi-component, liquid, real jet fuels.

Archival Publications Supported by this Award

2021

Wang,. K., Xu, R., Bowman, C. T., Wang, H., Impact of vitiation on flow reactor studies of jet fuel combustion chemistry, Combustion and Flame 224, 66-72 (2021).

Xu, R., Wang, H., A physics-based approach to modeling real-fuel combustion chemistry – VII. Relationship between speciation measurement and reaction model accuracy, Combustion and Flame, 224, 126–135 (2021).

S. E. Johnson, D. F. Davidson, R. K. Hanson, Shock tube / laser absorption measurements of cyclopentadiene pyrolysis, Journal of Chemical Physics A, submitted June (2021).

S. E. Johnson, Y. Ding, D. F. Davidson, R. K. Hanson, Shock tube/laser absorption measurements of the isomerization rates of allene and propyne, Combustion and Flame, submitted March (2021).

2020

Y. Ding, W.-W. Su, S. E. Johnson, C. L. Strand, R. K. Hanson, Temperature-dependent absorption cross section measurements for propene, 1-butene, cis-/trans-2-butene, isobutene and 1,3-butadiene in the spectral region 8.4–11.7 µm, J. Quantitative Spectroscopy & Radiative Transfer 255, 107240 (2020).

S. E. Johnson, D. F. Davidson, R. K. Hanson, Shock tube/laser absorption measurements of the pyrolysis of JP-10 fuel. Combustion and Flame 216, 161–173, (2020).

Xu, R., Saggese, C., Lawson, R., Movaghar, A., Parise, T., Shao, J., Choudhary, R., Park, J.-W., Lu, T., Hanson, R. K., Davidson, D. F., Egolfopoulos, F. N., Aradi, A., Prakash, A., Mohan, V. R. R., Cracknell, R., Wang, H., A physics-based approach to modeling real-fuel combustion chemistry – **VI**. Reaction kinetic models of gasoline fuels, Combustion and Flame, submitted (2020).

Saggese, C., Wan, K., Xu, R., Tao, Y., Bowman, C. T., Park, J.-W., Lu, T., Wang, H., A physics-based approach to modeling real-fuel combustion chemistry – **V**. NOx formation from a typical Jet A, Combustion and Flame 212, 270-278 (2020); 10.1016/j.combustflame.2019.10.038 .

Wei, W., Peng, Y. W., Wang, Y., Shao, J., Hanson, R. K., Two-color frequency-multiplexed IMS technique for gas thermometry at elevated pressures, Applied Physics B 126:51 (2020); 10.1007/s00340-020-7396-4

Pinkowski, N. H., Ding, Y., Strand, C. L., Hanson, R. K., Horvath, R., Geiser, M., Dual-comb spectroscopy for high-temperature reaction kinetics, Meas. Sci. Technol. 31 055501 (10pp) (2020); 10.1088/1361-6501/ab6ecc

2019

J. Shao, R. Choudhary, A. J. Susa, D. F. Davidson, R. K. Hanson, High-speed imaging of n-heptane ignition in a high-pressure shock tube, Proceedings of the Combustion Institute 38, 911-918 (2021); 10.1016/j.proci.2020.06.158

J. Shao, R. Choudhary, Y. Peng, D. F. Davidson, R. K. Hanson, Shock Tube Measurement of the C_2H_4 + H -> C_2H_3 + H_2 Rate Constant, Phys. Chem. A 123 115-120 (2019); 10.1021/acs.jpca.8b09452

J.K. Shao, R. Choudhary, Y. Peng, D.F. Davidson, R.K. Hanson, “A shock tube study of n-heptane, iso-octane, n-dodecane and iso-octane/n-dodecane blends oxidation at elevated pressures and intermediate temperatures,” Fuel 243 541-553 (2019); 10.1016/j.fuel.2019.01.152

N. H. Pinkowski, Y. Ding, S. E. Johnson, Y. Wang, T. C. Parise, D. F. Davidson, R. K. Hanson, A multi-wavelength speciation framework for high-temperature hydrocarbon pyrolysis, J. Quantitative Spectroscopy and Radiative Transfer, 225, 180–205 (2019).

R. Choudhary, Y. Peng, J. Shao, D. F. Davidson, R. K. Hanson, Multi species time history measurements during ethanol pyrolysis behind reflected shock waves, 11th U. S. National Combustion Meeting, March 24–27, (2019), Pasadena, California.

S. Wang, R. K. Hanson, Quantitative 2-D OH Thermometry using Spectrally-Resolved Planar Laser-Induced Fluorescence, Optics Letters. 44 578-581 (2019); 10.1364/OL.44.000578

S. J. Cassady, A. J. Susa, A. M. Ferris, C. L. Strand, R. K. Hanson, A Two-wavelength Ethylene-Absorption Temperature Diagnostic, Measurement Science and Technology, 30 035206 (2019); 10.1088/1361-6501/ab02cf

Strand, C. L., Ding, Y., Johnson, S. E., Hanson, R. K., Measurement of the Mid-Infrared Absorption Spectra of Ethylene (C2H4) and Other Molecules at High Temperatures and Pressures, Jour. Quant. Spectrosc. Radiat. Transfer, 222-223 122-129 (2019); 10.1016/j.jqsrt.2018.10.030

W. Wei, W. Peng, Y. Wang, R. Choudhary, S. Wang, R. K. Hanson, Rejection of Non-Absorbing Interference using Wavelength Modulation Spectroscopy in High-pressure Shock Tubes, J. Phys. B 125, 9 (2019). 10.1007/s00340-018-7118-3

Wang, Y.,Ding, Y., Wei, W., Cao, Y., Davidson, D. F., Hanson, R. K., On estimating physical and chemical properties of hydrocarbon fuels using mid-infrared FTIR spectra and regularized linear models, Fuel 255, 115715 (2019); 10.1016/j.fuel.2019.115715

Wei, W., Peng, Y. W., Wang, Y., Choudhary, R., Wang, S., Shao, J., Hanson, R. K., Demonstration of non-absorbing interference rejection using wavelength modulation spectroscopy in high-pressure shock tubes, Applied Physics B 125, 9 (2019); 10.1007/s00340-018-7118-3

Xu, C., Poludnenko, A., Zhao, X., Wang, H., Lu, T.-F., Structure of strongly turbulent premixed n-dodecane–air flames: direct numerical simulations and chemical explosive mode analysis, Combustion and Flames 209, 27–40 (2019); 10.1016/j.combustflame.2019.07.027

Y. Ding, C. L. Strand, R. K. Hanson, High-temperature Mid-infrared Absorption Spectra of Methanol (CH3OH) and Ethanol (C2H5OH) between 930 & 1170 cm^{-1}, Fuel 224, 396-402 (2019) 10.1016/j.jqsrt.2018.11.034.

Y. Wang, D.F. Davidson, R.K. Hanson, A New Method of Predicting Derived Cetane Number for Hydrocarbon Fuels, Fuel 241, 319-326 (2019); 10.1016/j.fuel.2018.12.027

Zhao, X., Tao, Y., Lu, T., Wang, H., Sensitivities of direct numerical simulations to chemical kinetic uncertainties: spherical flame kernel evolution of a real jet fuel, Combustion and Flame 209, 117-132 (2019); 10.1016/j.combustflame.2019.07.021

2018

Book Chapter: H. Wang, Uncertainty Quantification and Minimization, Elsevier Computer Aided Chemical Engineering Series: Mathematical Modeling of Gas-Phase Complex Reaction Systems: Pyrolysis and Combustion, submitted (2018).

Book Chapter: S. Wang, D. F. Davidson, R. K. Hanson, Shock tube techniques for kinetics target data to improve reaction models, Elsevier Computer Aided Chemical Engineering Series: Mathematical Modeling of Gas-Phase Complex Reaction Systems: Pyrolysis and Combustion, accepted May (2018)

A. Felden, L. Esclapez, E. Riber, H. Wang, B. Cuenot, Including real fuel chemistry in large-Eddy simulations, Combustion and Flame 193, 397–416 (2018).

H. Wang, R. Xu, K., Wang, C. T. Bowman, R. K. Hanson, D. F. Davidson, K. Brezinsky, F. N. Egolfopoulos, A Physics-based approach to modeling real-fuel combustion chemistry. **I**. Evidence from experiments, and thermodynamic, chemical kinetic and statistical considerations, Combustion and Flame (2018); 10.1016/j.combustflame.2018.03.019.

J. Shao, D. F. Davidson, R. K. Hanson, A shock tube study of ignition delay times in diluted methane, ethylene, propene and their blends at elevated pressures, Fuel 225 370-380 (2018).

J. Shao, R. Choudhary, A. Susa, D. F. Davidson, R. K. Hanson, Shock tube study of the rate constants for $H+O_2+M=HO_2+M$ (M=Ar, H_2O, CO_2, N_2) at elevated pressures, Proceedings of the Combustion Institute 37 (2018).

J. Smolke, F. Carbone, F. N. Egolfopoulos, H. Wang, Effect of n-dodecane decomposition on its fundamental flame properties, Combustion and Flame, 190, 65-73 (2018).

J. J. Girard, R. Choudhary, R. K. Hanson, Collisional-induced Broadening and Shift Parameters of OH with Ar and N2 near 308.6 nm, Measured at T = 1300 – 2000K and P = 20 – 100 atm, J. Quant Spectrosc. Radiat. Trans. 221, 194-201 (2018); 10.1016/j.jqsrt.2018.10.007

K. Wang, C. T. Bowman, H. Wang, Kinetic analysis of distinct product generations in oxidative pyrolysis of four octane isomers, Proceedings of the Combustion Institute, (2018).

K. Wang, R. Xu, T. Parise, J. K. Shao, D. J. Lee, A. Movaghar, Y. Gao, T.-F. Lu, F. N. Egolfopoulos, D. F. Davidson, R. K. Hanson, C. T. Bowman, H. Wang, "A Physics-based approach to modeling real-fuel combustion chemistry - **IV**. HyChem modeling of combustion kinetics of a bio-derived jet fuel and its blends with a conventional Jet A, Combustion Flame, (2018).

L. Esclapez, P. C. Ma, E. Mayhew, R. Xu, S. Stouffer, T. Lee, H. Wang, M. Ihme, "Fuel effects on lean blowout in a realistic gas turbine combustor," Combustion and Flame 181, 82-89 (2017).

M. Janbozorgi, H. Wang, Bottom-up modeling using the rate-controlled constrained-equilibrium theory: the n-butane combustion chemistry, Combustion and Flame 174, 223-232 (2018).

R. Xu, H. Wang, "Principle of large component number in multicomponent fuel combustion – a Monte Carlo study," Proceedings of the Combustion Institute, (2018).

R. Xu, K. Wang, S. Banerjee, J. Shao, T. Parise, Y. Zhu, S. Wang, R. Zhao, D. J. Lee, A. Movaghar, X. Han, Y. Gao, Y., T. Lu, K. Brezinsky, F. N. Egolfopoulos, D. F. Davidson, R. K. Hanson, C. T. Bowman, H. Wang, A

Physics-based approach to modeling real fuel combustion chemistry. **II**. Reaction models of jet and rocket fuels. Combustion and Flame (2018); 10.1016/j.combustflame.2018.03.021

S. Wang, D. F. Davidson, R. K. Hanson, "Shock tube measurements of OH concentration time-histories in benzene, toluene, ethylbenzene and xylene oxidation," Proceedings of the Combustion Institute 37 (2018).

S. Wang, R.K. Hanson, Ultra-sensitive Detection of OH Radical in High-temperature Transient Reactions, Optics Letters 43, 3518-3521 (2018), doi.org/10.1364/OL.43.003518

T. C. Parise, D. F. Davidson, R. K. Hanson, Development of a two-wavelength IR laser absorption diagnostic for propene and ethylene, Measurement Science and Technology 29 055202 (8pp) (2018).

X. Han, M. Liszka, R. Xu, K. Brezinsky, H. Wang, A high-pressure shock tube study of the pyrolysis of real jet fuel Jet A," Proceedings of the Combustion Institute 37, (2018).

Y. Tao, G. P. Smith, H. Wang, Critical kinetic uncertainties in modeling hydrogen/carbon monoxide, methane, methanol, formaldehyde, and ethylene combustion, Combustion and Flame, (2018); 10.1016/j.combustflame.2018.02.006.

Y. Tao, H. Wang, Joint probability distribution of Arrhenius parameters in reaction model optimization and uncertainty minimization, Proceedings of the Combustion Institute, (2018).

Y. Tao, R. Xu, K. Wang, J. Shao, S. E. Johnson, A. Movaghar, X. Han, J. W. Park, T. Lu, K. Brezinsky, F. N. Egolfopoulos, D. F. Davidson, R. K. Hanson, C. T. Bowman, H. Wang, A Physics-based approach to modeling real-fuel combustion chemistry – **III**. Reaction kinetic model of JP10. Combustion and Flame, 198, 466–476 (2018).

2017

A. M. Tulgestke, S. E. Johnson, D. F. Davidson, R. K. Hanson. High-speed imaging of inhomogeneous ignition in a shock tube, Shock Waves 28, 1089–1095 (2018).

S. Wang, T. Parise, S. E. Johnson, D. F. Davidson, R. K. Hanson, A new diagnostic for hydrocarbon fuels using 3.41-µm diode laser absorption, Combustion and Flame 186, 129-139 (2017).

C. Liu, R. Zhao, R. Xu, F. N. Egolfopoulos, H. Wang, H., Binary diffusion coefficients and non-premixed flames extinction of long-chain alkanes, Proceedings of the Combustion Institute 36, 1523–1530 (2017).

D. F. Davidson, J. Shao, T. Parise, R. K. Hanson, Shock Tube Measurements of Jet and Rocket Fuel Ignition Delay Times, 55th AIAA Aerospace Sciences Meeting, paper 1798, (2017).

D.F. Davidson, Y. Zhu, J. Shao, R. K. Hanson, Ignition Delay Time Correlations for Distillate Fuels, Fuel 187, 26–32 (2017). 10.1016/j.fuel.2016.09.047

J. Shao, Y. Zhu, S. Wang, D.F. Davidson, R.K. Hanson, Shock Tube Study of Jet Fuel Pyrolysis and Ignition at Elevated Pressure, Paper 1F05, 10th US Combustion Meeting, College Park (2017).

K. Wang, R. Xu, T. Parise, J. K. Shao, D. J. Lee, A. Movaghar, D. F. Davidson, R. K. Hanson, H. Wang, C. T. Bowman, F. N. Egolfopoulos, Combustion Kinetics of Conventional and Alternative Jet Fuels using a Chemistry (HyChem) Approach, Paper 2A15, 10th US Combustion Meeting, College Park MD, April 23-26, (2017).

K. Wang, R. Xu, T. Parise, J.K. Shao, D. F. Davidson, R. K. Hanson, H. Wang, C. T. Bowman, Evaluation of a Hybrid Chemistry Approach for Combustion of Blended Petroleum and Bio-derived Jet Fuels, Paper 2A16, 10th US Combustion Meeting, College Park MD, April 23-26, (2017).

R. Xu, D. Chen, K. Wang, Y. Tao, J.K. Shao, T. Parise, Y. Zhu, S. Wang, R. Zhao, D.J. Lee, F.N. Egolfopoulos, D.F. Davidson, R. K. Hanson, C. T. Bowman, H. Wang, HyChem Model: Application to Petroleum-Derived Jet Fuels, Paper 2A11, 10th US Combustion Meeting, College Park MD, April 23-26, (2017).

R. Xu, H. Wang, D. F. Davidson, R. K. Hanson, C. T. Bowman, F. N. Egolfopoulos, Evidence Supporting a Simplified Approach to Modeling High-Temperature Combustion Chemistry, Paper 2A10, 10th US Combustion Meeting, College Park MD, April 23-26, (2017).

2016

C. K. Law, F. Wu, F. N. Egolfopoulos, V. Gururajan, V., H. Wang, On the rational interpretation of data on laminar flame speeds and ignition delay times, Combustion Science and Technology 187, 27-36 (2015).

C. Liu, R. Zhao, R. Xu, F. N. Egolfopoulos, H. Wang, “Binary diffusion coefficients and non-premixed flames extinction of long-chain alkanes, Proceedings of the Combustion Institute (2016).

C. Liu, Z. Li, H. Wang, H., Drag force and transport property of small cylinder in free molecule flow: a gas-kinetic theory analysis, Physical Review E 94, 023102 (2016).

D. F. Davidson, Y. Zhu, S. Wang, T. Parise, R. Sur, and R. K. Hanson, Shock tube measurements of jet and rocket fuels, Paper AIAA 2016-0178 54th AIAA Sciences Meeting, San Diego CA, January (2016).

H. Wang, Key phenomena enabling direct simulation of real fuel combustion chemistry, PacifcChem Conference, Honolulu, HI, December (2015).

S. Banerjee, R. Tangko, D. A. Sheen, H. Wang, C. T. Bowman, An experimental and kinetic modeling study of n-dodecane pyrolysis and oxidation, Combustion and Flame 163, 12-30 (2016).

T. Parise, D. F. Davidson, R. K. Hanson, “Shock tube/laser absorption measurements of the pyrolysis of a bimodal test fuel,” Proceedings of the Combustion Institute, (2016).

Xu, R., Chen, D., Wang H., Hybrid approach to combustion chemistry of jet fuels,” poster presentation at the 36th International Symposium on Combustion, Seoul, Korea, August (2016).

Y. Gao, R. Shan, S. Lyra, G. Li, H. Wang, J. H. Chen, T. Lu, On lumped-reduced reaction model for combustion of liquid fuels, Combustion and Flame 163, 437–446 (2016).