Project 025 Shock Tube Studies of the Kinetics of Jet Fuels

Stanford University

Project Lead Investigator

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University Participants

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- P.I.s: Prof. Ronald K Hanson
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- Task: Area #1 – Chemical Kinetics Combustion Experiments

Project Funding Level

$210,000 from FAA with 1-1 matching funding of $210,000 from Stanford University.

Investigation Team

Prof. Ronald K Hanson, Principal Investigator, Research Direction
Dr. David F Davidson, Senior Research Engineer, Research Management
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Project Overview

Provide shock tube/laser absorption experiments for a fundamental kinetics database for jet fuels. Experiments are expected to continue to reveal the sensitivity of combustion properties to fuel composition for the ultimate use in simplifying the alternative fuel certification process.

Task Area #1: Chemical Kinetics Combustion Experiments

Stanford University

Objective(s)

Experiments provide an extensive fundamental kinetics data for selected jet fuels. These data are used as critical input for Area #2 that seeks to develop a new hybrid and detailed kinetics model for jet fuels (HyChem). These experiments continue to reveal the sensitivity of combustion properties to variations in fuel composition for ultimate use in simplifying the alternative fuel certification process. The team works in close collaboration with Professor Hai Wang, also of Stanford University, the PI for Area #2, who uses the data acquired in our experiments. The data provided will also ensure that the combustion models developed in Area #4 - Combustion Model Development and Validation to model the extinction and ignition processes controlling lean blowout, cold ignition and high altitude relight, are chemically accurate.

Research Approach

The development, refinement and validation of detailed reaction mechanisms describing the pyrolysis and oxidation of fuels require experimental data as targets for kinetics models. Experimentally, the best way to provide these targets at high temperatures and pressures is with shock tube/laser absorption experiments, conducted over a wide range of pressure, temperature, and fuel and oxidizer composition.

Reflected shock wave experiments provide a test environment that does not introduce additional fluid mechanics, turbulence, or heat transfer effects to the target phenomena. This allows isolation of the target phenomena (ignition delay times and species concentration time-histories) in a quiescent high-temperature, high-pressure environment that is very well characterized and hence amenable to modeling. Recent work in our laboratory to develop the Constrained Reaction Volume (CRV) methodology provides an additional tool to provide shock tube data under constant-pressure constraints when needed, to significantly simplify the gasdynamic/thermodymamic models needed to properly simulate reactive reflected shock wave data.

The strength in the Stanford shock tube approach comes with the implementation of laser diagnostics that enable the simultaneous measurement of species time-histories. Using laser absorption, we are able to provide quantitative time-histories during fuel pyrolysis and oxidation of the fuel, including transient radicals (e.g., OH, CH3), stable intermediates (e.g., CH4, C2H4, iso-butene and aromatics), combustion products (including CO, CO2, and H2O), and temperature.

Measurements of the pyrolysis and oxidation systems of real fuels, rather than of surrogates or solvent surrogates, provide a direct link to actual fuel behavior. The combination of high-quality shock tube and flow reactor measurements combined with the HyChem kinetic model based on real fuel decomposition products proposed by Professor Hai Wang is meeting the FAA program objectives.

Shock Tube Experiments

Stanford has the largest and best-equipped shock tube laboratory in the U.S., perhaps in the world, with five shock tubes: three large-diameter (10, 14 and 15 cm I.D.) high-purity shock tubes (see Fig. 1a); one heated high-pressure shock tube (5 cm I.D., capable of achieving 500+ atm); and 10 cm I.D. expansion tube for generating supersonic flows. Additionally, we have unique capability for species measurements using laser absorption (see Fig. 1b) developed over the past 30 years. In these experiments, temperatures from below 500 K to above 3000 K, and pressure from sub-atmospheric (0.2 atm) to 10-500+ atmospheres can be achieved in different carrier gases, such as argon or air, with demonstrated test times up to and exceeding 50 ms at low temperatures.

Three primary types of shock tube experiments are performed.

The first primary shock tube experiments are species concentration time-history measurements obtained during fuel pyrolysis. These data are used to place strong constraints on the reaction mechanism and the individual reaction rates and pathways. Laser absorption techniques, many pioneered at Stanford, are used to measure these species time-histories. The following species time-histories measurements have been acquired and used in the development of the HyChem model: fuel at a wavelength of 3.39 microns, and the stable fuel decomposition products: ethylene, methane, and iso-butene, at wavelengths of 10.53, 3.1754 and 11.3 microns, respectively. We also are able to measure the transient radical OH (in the UV at 306 nm), the combustion products CO, CO2 and H2O (in the IR at 2.7, 4.6 and 2.5 microns, respectively) as well as other product species.

Representative data acquired using these methods are shown in Figures 2a, b, and c. These measurements of the major jet fuel decomposition products during pyrolysis (fuel, ethylene, propene, and isobutene time-histories) were directly applicable to the development of the HyChem Fuel X model by Prof. Hai Wang.

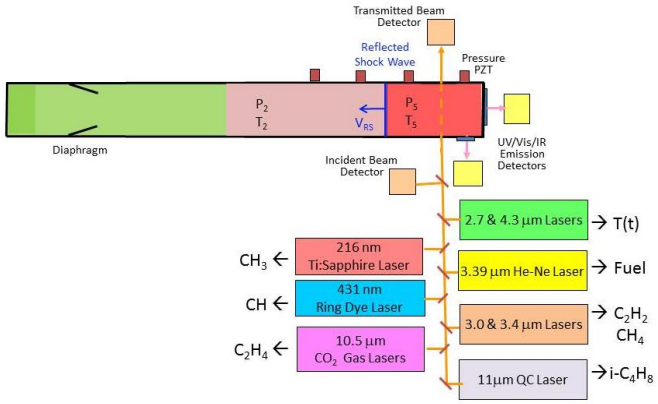

Figure 1a: Stanford 15 cm diameter shock tube. **Figure 1b:** Schematic of shock tube/laser absorption setup. Simultaneous measurement of multiple species time-histories and temperature with microsecond time resolution are enabled using this arrangement. Only a partial list of accessible species is indicated.

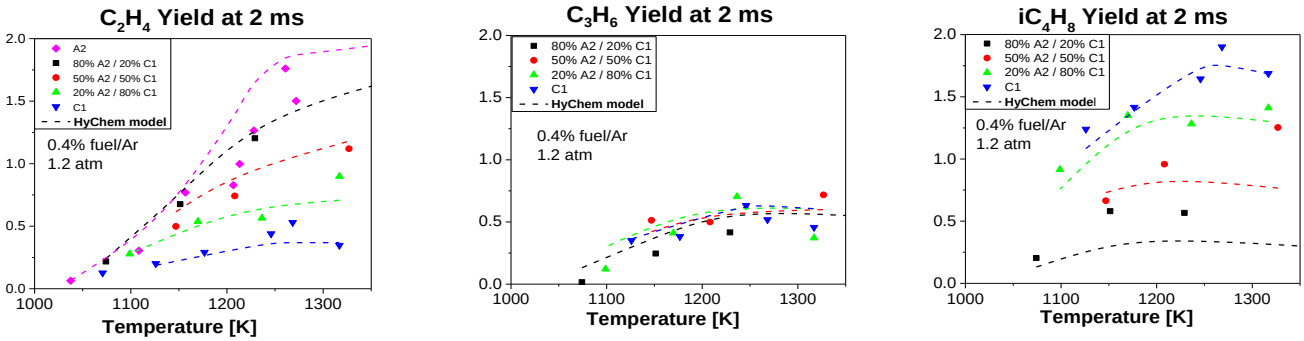

Figure 2a, b, & c: C2H4 C3H6 and iC4H8 yields acquired during the pyrolysis of blends of FAA fuels A1 & C1.

Milestones

Major milestones included regular reporting of experimental results and analysis at monthly meetings for both the Kinetics Working Group and the Steering Working Group, as well as reporting at FAA Quarterly and ASCENT annual meetings.

Major Accomplishments

During this third year of this program, we made advances in several areas.

We have developed infrared laser diagnostics schemes for propene at 10.975 microns and for fuel at 3.41 microns. These diagnostics provide quantitative, sensitive, low-noise detection of key species involved in the combustion of jet fuels.

Using these new diagnostics schemes and our existing systems for ethylene, methane and isobutene, we have acquired refined multi-species data for Cat A and C1 fuels using a six-IR-wavelength strategy.

In the analysis of this multi-species/multi-wavelength approach we have also assessed the role of minor interfering species (e.g. 1-butene, 2-butene, and allene) on the measured iso-butene and propene pyrolysis yields.

In separate experiments we measured ignition delay times (IDT) of a series of jet fuels with varying cetane number and showed the variation of IDT with CN.

We have also performed IDT measurements of a series of Air Force jet fuels from geographically varying locations to investigate the range of commercially available jet fuel performance.

Finally, we are currently developing a diagnostic scheme to measure aromatics yields during fuel pyrolysis. These measurements will enable us to close the carbon balance of jet fuel pyrolysis products.

Publications

Peer-reviewed journal publications

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

Published conference proceedings

R. Xu, D. Chen, K. Wang, Y. Tao, J.K. Shao, T. Parise, Y. Zhe, S. Wang, R. Zhao, D.J. Lee, F.N. Egolfopoulos, D.F. Davidson, R.K. Hanson, C.T. Bowman and H. Wang, "HyChem Model for Petroleum-Derived Jet Fuels," 10th U. S. National Combustion Meeting, April 23-26, 2017, College Park, Maryland.

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," 10th U. S. National Combustion Meeting, April 23-26, 2017, College Park, Maryland.

J.K. Shao, D.F. Davidson and R.K. Hanson, "Shock Tube Study of Jet Fuel Pyrolysis and Ignition at Elevated Pressure," 10th U. S. National Combustion Meeting, April 23-26, 2017, College Park, Maryland.

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," 10th U. S. National Combustion Meeting, April 23-26, 2017, College Park, Maryland.

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 and F.N. Egolfopoulos, "Combustion Kinetics of Conventional and Alternative Jet Fuels using a Hybrid Chemistry (HyChem) Approach," 10th U. S. National Combustion Meeting, April 23-26, 2017, College Park, Maryland.

Outreach Efforts

Ignition delay time measurements of a series of jet fuels with varying cetane number from the Army Research Laboratory (ARL) providing fuel characterization data of use to both the FAA and the ARL.

Ignition delay time measurements of a series of jet fuels from geographically varying locations from the Air Force/Wright Patterson Airbase providing fuel characterization data of use to both the FAA and the AFOSR.

Awards

None

Student Involvement

Graduate students are actively involved in the acquisition and analysis of all experimental data. Tom C. Parise is preparing to defend his Ph.D. thesis based on work performed under this contract.

Plans for Next Period

Advances in the HyChem model development based on the experimental and theoretical work so far indicate that there are several important issues that should be addressed as the model is further developed and validated. 1) The HyChem model will be tested on a wide range of jet fuel types to establish temperature and pressure boundaries for the validity of the HyChem modeling approach. 2) Efforts will be made to update the foundational fuel chemistry, paying particular attention to the i-C4H8 sub-mechanism, that is the basis of the oxidation sub-mechanism of HyChem. 3) Shock tube/laser absorption measurements will be used to investigate the relationship of Cetane Number (CN) and ethylene yields during pyrolysis. 4) Efforts will also be made to completely characterize jet fuel using shock tube/laser absorption measurements by completing the carbon balance of fuel pyrolysis products.