Project 25: National Jet Fuels Combustion Program, Area #1 Shock Tube and Flow Reactor Studies of the Kinetics of Jet Fuels

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Project Lead Investigator

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University Participants

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

Project Funding Level

$285,000 from FAA with 1-1 matching funding of $285,000 from Stanford University. Includes $10,000 for travel to meetings.

Investigation Team

Prof. Ronald K Hanson, Principal Investigator, Research Direction
Prof. C Thomas Bowman, Co-Principal Investigator, Research Direction
Dr. David F Davidson, Senior Research Engineer, Research Management
Dr. Kun Wang, Post-Doctoral Research Associate, Research Assistant
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Project Overview

Provide shock tube/laser absorption and flow reactor 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

Objectives

Experiments provide an extensive fundamental kinetics database 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 Prof. 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 and flow reactor 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.

In combination with the shock tube experiments, the Stanford Variable Pressure Flow Reactor is used to provide concentration profile data for important stable intermediate and product species (see Flow Reactor Section) during fuel pyrolysis and oxidation for temperatures ranging from 900 - 1200K, for pressures up to 5 bar, and for residence times from 5 - 100 msec. These species provide critical constraints on the development of the HyChem detailed kinetic models of Prof. Hai Wang.

The range of conditions accessible in the flow reactor partially overlap those achievable in the shock tube so that the combination of shock tube and flow reactor experiments provides a comprehensive species data set over a wide range of experimental conditions that is essential for kinetic model development and validation as well as for model reduction to a size needed for implementation in the Area #4 - Combustion Model Development and Evaluation. To our knowledge, our laboratory is the only one worldwide with this combined capability.

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 Prof. 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.

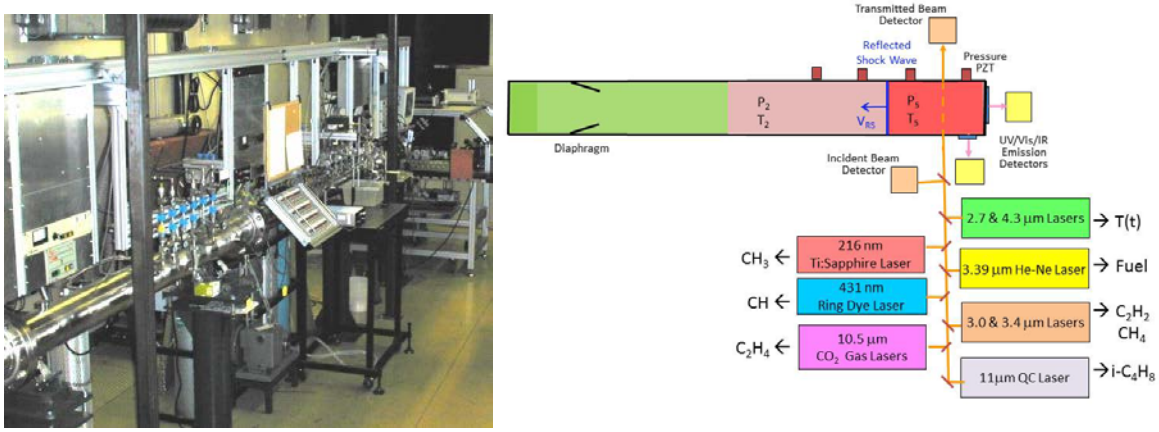


Figure 1a: Stanford 15 cm diameter shock tube. Figure 1b: Schematic of shock tube/laser absorption setup. Simultaneous measurement of multiple species time-histories and temperature with microsecond time resolution are enabled using this arrangement. Only a partial list of accessible species is indicated.

During this year of the program, using shock tube/laser absorption methods we acquired fuel, ethylene, propene, and isobutene time-histories for an investigation of several blends of FAA fuel A-2 and test fuel C-1. These pyrolysis product yield data were directly applicable to the development of the HyChem Fuel X model by Prof. Hai Wang. Representative data and HyChem simulations are shown in Figures 2a, b, and c.

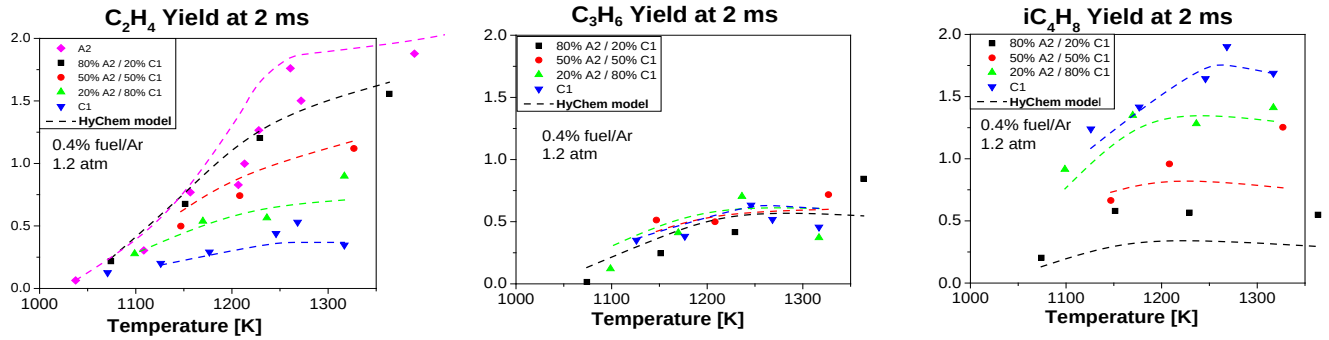


Figure 2a, b, &c: C2H4 C3H6 and iC4H8 yields acquired during the pyrolysis of blends of FAA fuels A1 & C1.

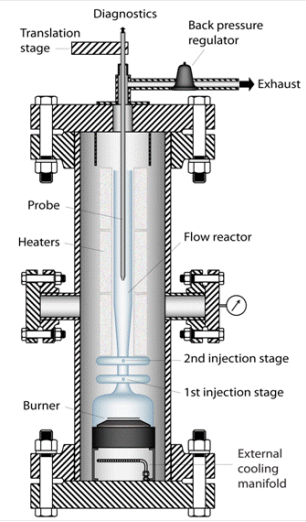
Stanford Variable Pressure Flow Reactor

A schematic diagram of the Stanford Variable Pressure Flow Reactor is shown in Fig. 3a. The facility comprises a quartz reactor tube housed in a stainless steel pressure vessel. A premixed laminar burner provides high-temperature vitiated air and this air is mixed with fuel vapor prior to entering the reactor tube. Electrical resistance heaters surrounding the reactor tube provide for nearly adiabatic reactor conditions. Gas samples are extracted by a cooled translating probe which also is used to measure gas temperature.

A variety of on-line analyzers, including a four-column gas chromatograph and a new spectrometer, obtained using AFOSR funds, are available to measure multiple stable species profiles simultaneously over reaction time scales up to 50 ms. Species that can be measured with these analyzers includes C1 - C12 alkanes, C2 - C8 alkenes, cycloalkanes, allenes,

aromatics, including benzene, toluene, and naphthalene, C1 - C3 aldehydes, H2, CO, CO2, and O2. Many of these species are not currently accessible in proposed shock tube experiments.

During this year of the program, using GC analysis we acquired a wide variety of fuel time-histories during the investigation of several blends of FAA fuel A-2 and test fuel C-1. Representative data and HyChem simulations for iso-butene and ethylene are shown in Figures 3b and c. As with the shock tube data above, these pyrolysis product yield data were directly applicable to the development of the HyChem Fuel X model by Prof. Hai Wang.



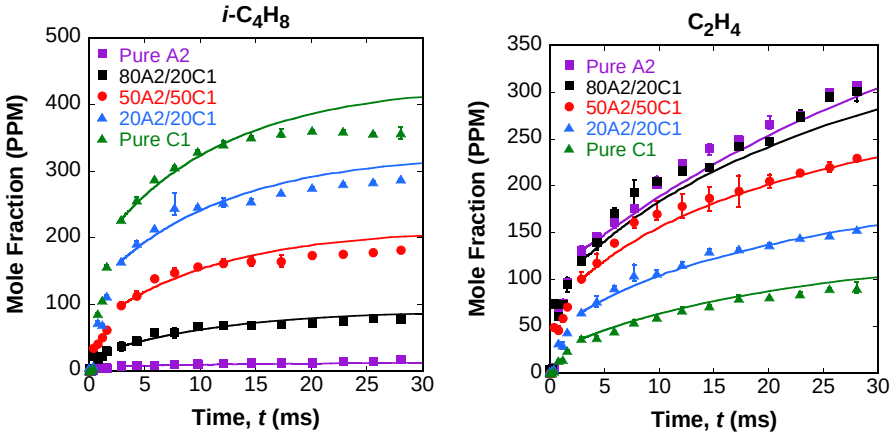


Fig. 3a: Stanford Variable Pressure Flow Reactor. Figure 3b: Species profiles during oxidative pyrolysis of A-2/C-1 fuel blends at 1 atm, ϕ=1 and initial temperature of 1030K.

Milestone(s)

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

Major Accomplishments

During this second year of this program, using shock tube/laser absorption methods we acquired fuel, ethylene, and methane, propene, and iso-butene time-histories for blends of FAA A2 & C1 fuels during pyrolysis and partial oxidation. In flow reactor experiments this set of species from the shock tube data were extended using gas chromatography measurements. These pyrolysis product yield data are directly applicable to the development of the HyChem model by Prof. Hai Wang.

Publications

Published Conference Proceedings and Archival Papers

D. F. Davidson, J. Shao T. Parise, R. K. Hanson, "Shock Tube Measurements of Jet and Rocket Fuel Ignition Delay Times," AIAA SciTech Meeting Grapevine TX, Jan. 2017, in press.

D. F. Davidson, A. Tugestke, Y. Zhu, S. Wang, R. K. Hanson, "Species Time-History Measurements during Jet Fuel Pyrolysis," 30th International Symposium on Shock Waves, Tel Aviv, Israel, November 2016, in press.

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

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 36 1-8 (2016).

D. F. Davidson, Y. Zhu, S. Wang, T. Parise, R. Sur, R. K. Hanson, “Shock Tube Measurements of Jet and Rocket Fuels,” AIAA Sci. & Tech. Forum, San Diego, Jan. 2016.

Outreach Efforts

Presentations at the AIAA Sci. & Tech. Forum, San Diego, Jan. 2016.
Upcoming presentation at AIAA SciTech Meeting Grapevine TX, Jan. 2017.

Awards

None

Student Involvement

Graduate students are actively involved in the acquisition and analysis of all experimental data.

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.

First it is necessary to evaluate the assumptions and range of validity of the HyChem and Fuel X modeling approaches. Studies will be performed to establish temperature and pressure boundaries for the validity of the HyChem modeling approach. Current in-house validation of the model is based on a small set of ignition delay time and flow reactor experiments over limited ranges of pressure, temperature, equivalence ratio, and fuel concentration. Direct testing over a wider range of test conditions, using both shock tubes and flow reactors, can provide a first-order limits of the applicability of the HyChem model. Further measurements are also planned to investigate a wide range of distillate jet fuels to evaluate the behavior of the Fuel X assumptions.

Second, an effort will be made to update the foundational fuel chemistry, paying particular attention to the i-C4H8 sub-mechanism.

Finally, we plan to seek relationships between the measured ignition delay time (IDT) and speciation data and lean blow out (LBO), high altitude relight, and other engine characteristics.