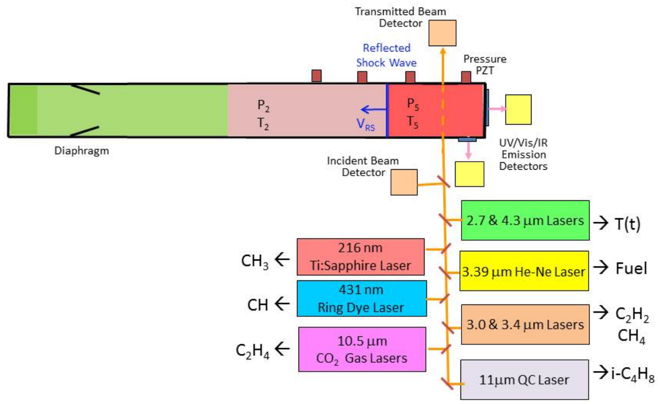
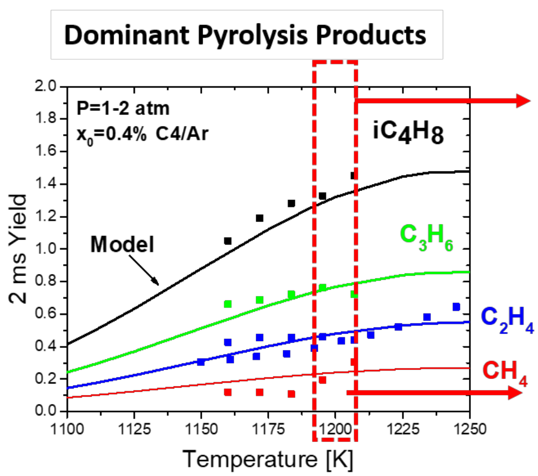


Figure 1a. Stanford 15 cm diameter shock tube. **Figure 1b.** Schematic of shock tube/laser absorption setup. Simultaneous measurement of multiple species time-histories and temperature with microsecond time resolution are enabled using this arrangement. Only a partial list of accessible species is indicated.



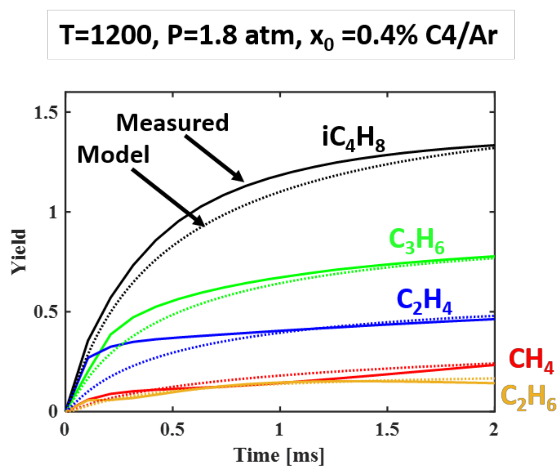


Figure 2a. Variation of the CH4, C2H4, C2H6, C3H6 and iC4H8 pyrolysis yields acquired during the pyrolysis of C4 fuel as a function of temperature and comparison with a preliminary HyChem model. **Figure 2b.** Representative measurements and preliminary modeling of C4 pyrolysis at 1200K, 1.8 atm.

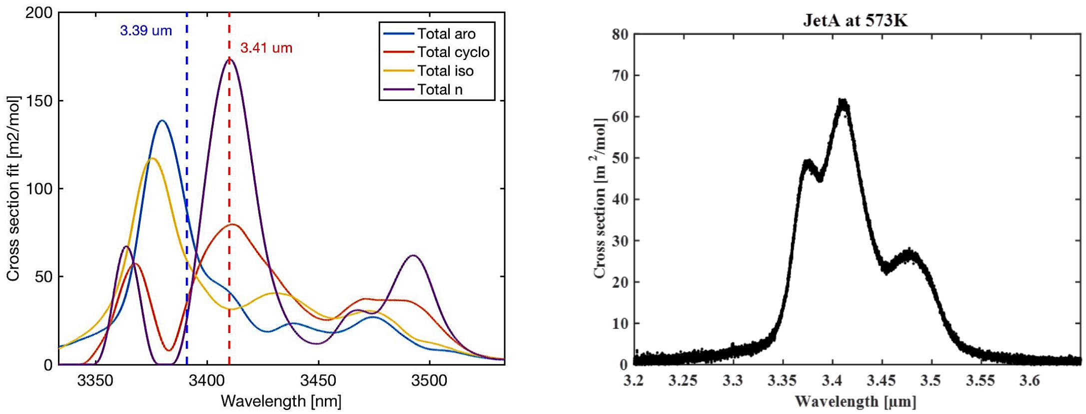


Figure 3a. Average FTIR spectra for alkane (n-, iso-, & cyclo-) and aromatic molecular classes of jet fuel components. Primary wavelengths (3.39 and 3.41 microns) used to measure fuel loading are also indicated. **Figure 3b**. FTIR spectra for Jet A fuel (Cat A2). Strong absorption is seen at the n-alkane peak near 3.41 microns.

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

We have developed or refined infrared laser diagnostics schemes for ethane at 3.35 microns and for aromatics at 3.28 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 the decomposition of the important jet fuel pyrolysis product i-butene and for Cat C4 fuel using a nine-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.

We have acquired FTIR spectra near 3.4 microns for the majority of the FAA Cat A and Cat C fuels as well as verifying the published spectra for single fuel components.

We have developed correlations that relates the measured IR absorption ratio at 3.41 and 3.39 microns to C_2H_4 pyrolysis yield, fuel DCN value, LBO (lean blow out) and IDT (ignition delay times).

We have investigated, and continue to investigate, the link between FTIR spectra measurements and fuel functional groups, combustion properties and HyChem.

Publications

Peer-reviewed journal publications

Archival Publications

S. Wang, T. Parise, S.E. Johnson, D.F. Davidson, R.K. Hanson, "A New Diagnostic for Hydrocarbon Fuels using 3.41-micron Diode Laser Absorption," Combustion and Flame 186 129-139 (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 36 281-288 (2017)

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 193 502-519 (2018)

R. Xu, K. Wang, S. Banerjee, J. Shao, T. Parise, Y. Zhu, S. Wang, A. Movaghar, D.J. Lee, R. Zhao, X. Han, Y. Gao, 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 kinetic models of jet and rocket fuels,” Combustion and Flame 193 520-537 (2018)

J. Shao, Y. Zhu, S. Wang, D. F. Davidson, R. K. Hanson, “A shock tube study of jet fuel pyrolysis and ignition at elevated pressures and temperatures, Fuel 226 338-344 (2018)

N. Pinkowski, T. Parise, Y. Ding, S. Johnson, Y. Wang, D. F. Davidson, R. K. Hanson, “High-temperature infrared absorption cross-sections to facilitate the study of hydrocarbon pyrolysis,” submitted to Journal of Quantitative Spectroscopy and Radiative Transfer, August 2018

Y. Wang, D. F. Davidson, R. K. Hanson, “A new method of predicting derived cetane number for hydrocarbon fuels,” submitted to Fuel, September 2018

N. Pinkowski, “Jet fuel chemical kinetics: shock tubes, laser diagnostics, and machine learning methods,” ASCENT Program Student Paper Competition 2018

Outreach Efforts
FTIR spectral analysis 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.

FTIR spectral analysis 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 successfully defended his Ph.D. thesis that was based on work performed under this contract. Nicolas Pinkowski won an FAA ASCENT Program Student Paper Competition for his paper “Jet fuel chemical kinetics: shock tubes, laser diagnostics, and machine learning methods.”

Plans for Next Period
In the next period we plan to:

1. Acquire IDT & speciation data base for SHELL IH2 fuel and develop a HyChem model for this fuel.
2. Complete the kinetics and HyChem section of the AIAA volume entitled *Fuel Effects on Operability of Aircraft Gas Turbine Combustors.*
3. Finalize HyChem model for Cat C4 fuel.
4. Continue development of correlations between IR fuel absorption, pyrolysis yields & combustion properties.
5. Continue exploration of IR absorption as a fuel screening tool and potential fuel specification.
6. Extend correlations of IR absorption to physical properties (e.g., viscosity, surface tension, etc.).