Project 026 National Jet Fuels Combustion Program – Area #2: Hybrid Approach to Chemical Kinetics Model Development and Evaluation

Stanford University

Project Lead Investigator

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University Participants

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- P.I.: Hai Wang
- FAA Award Number: 13-C-AJFE-SU-006
- Period of Performance: December 1, 2014 to November 30, 2015
- Task(s):
    1. To develop reduced order reaction models, in close coordination with other areas on conditions and required types of data needed for model development and validation, to capture most important combustion properties of three Category A reference jet fuels and selected category C fuels, including pyrolysis intermediate distributions, ignition delay, flame extinction and flame speed.
    2. To understand the dependency of model parameters on fuel composition and chemical properties (DCN, aromatics, H/C, MW, etc.).

Project Funding Level

Investigation Team

Single PI project

Project Overview

The study is designed to satisfy the objective of Area #2 of National Jet Fuels Combustion Program (NJFCP)– Chemical Kinetics Model Development and Evaluation. The overall objective is to providing validated kinetic models for the combustion of the three reference jet fuels ranging in their performance from the best to the worst case. During the course of the program, it was determined that kinetic models are also needed for two Cat C fuels to meet the overall NJFCP objectives. In all cases, the reaction models are validated to ensure that they can predict combustion phenomena of relevance to extinction and ignition processes controlling lean blowout, cold ignition and high altitude relight.

The work is to be carried out in close coordination with Profs. Ronald K. Hanson and C. Thomas Bowman, also of Stanford University, who carry out research in Area #1 of NJFCP – Chemical Kinetics Combustion Experiments. Coordination with Area #4 is also necessary to reduce the reaction model to a target size of $< \sim 35$ species.

Task 1 – Model Development

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Objective(s)
Develop reduced order reaction models for three category A and two Category C fuels.

Research Approach
Earlier efforts suggest that the pyrolysis of large hydrocarbon fuels leading to smaller molecular fragments precedes the oxidation of the resulting fragments in real fuel combustion. The two reaction processes are separable in time scales. These phenomena have been demonstrated by several experiments in a flow reactor and in shock tubes. In flames, the pyrolysis and oxidation zone are separate spatially. For thermodynamic and chemical kinetic reasons, the pyrolysis of a jet fuel in the flame front or during the induction time of an ignition process yields only a handful of species that may include H_2, CH_4, C_2H_4, C_3H_6, 1-C_4H_8 (1-butene), i-C_4H_8 (isobutene), benzene and toluene. Past studies also suggest that during high-temperature fuel oxidation the rate-limiting steps are largely the oxidation of pyrolysis products. The above considerations led us to take a hybrid approach to chemistry modeling of jet fuel combustion, namely, a lumped approach to jet fuel pyrolysis leading to the production of a handful of molecular fragments, followed by a detailed description of the reaction kinetics for the oxidation of pyrolysis fragments. The kinetic rates and composition of the pyrolysis products are determined experimentally within the range encompassing the gas turbine operating conditions, through a coordinated research effort in collaboration with Prof. Hanson in the area of shock tube measurement and Prof. Bowman using a flow reactor.

Models for Category A fuels
Selected results for the A2 (JP-8) fuel are shown in Figure 1. The left panel shows the time histories of ethylene and methane for a selected experiment, along with model predictions. The fuel pyrolysis model was developed on the basis of this type of data at around 13 atm and over a temperature range of 1100 – 1500 K. Combining the pyrolysis model with a detailed, foundational fuel model for H_2, CO and small hydrocarbon oxidation, the hybrid model is seen to predict very well the ignition delay times and laminar flame speed of the A2 fuel accurately.
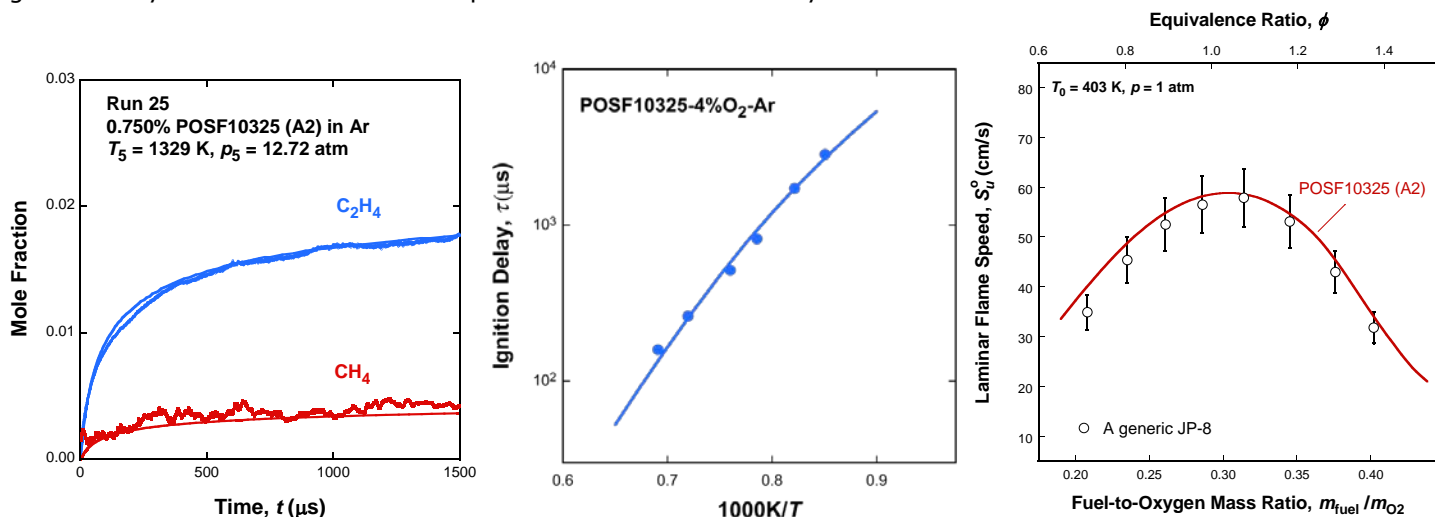

Figure 1. Selected comparisons of the experimental data and predictions for the A2 fuel. Left panel: time histories of ethylene and methane produced during shock tube pyrolysis of A2; middle panel: shock-tube ignition delay time; right panel: laminar flame speeds. The shock tube data were taken from the unpublished work of Hanson and coworkers, and the flame speed data were taken from Egolfopoulos.

The same approach was applied to the A1 and A3 fuels. It was found that the two fuels do not differ from the A1 fuel in their properties of pyrolysis, ignition and flame propagation. Figures 2 and 3 present comparison between experiment and model for selected cases. Again, the model predictions are shown to be in close agreement with the experimental data.
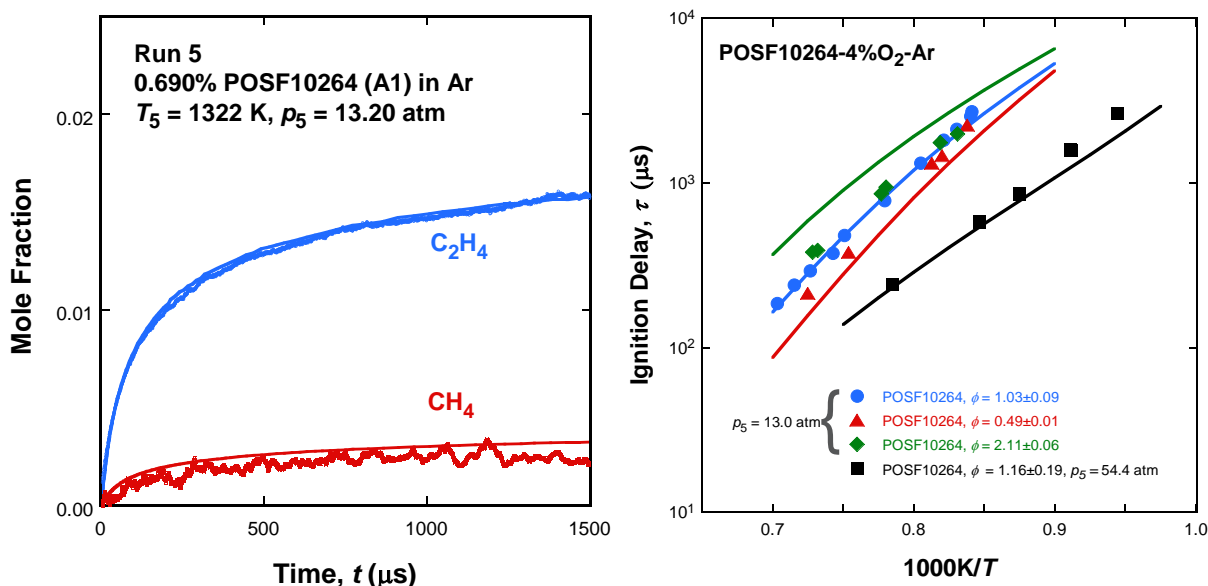
Figure 2. Selected comparisons of the experimental data and predictions for the A1 fuel. Left panel: time histories of ethylene and methane produced during shock tube pyrolysis; right panel: ignition delay time for several equivalence ratio and under two different pressures. The experimental data were taken from the unpublished work of Hanson and coworkers.
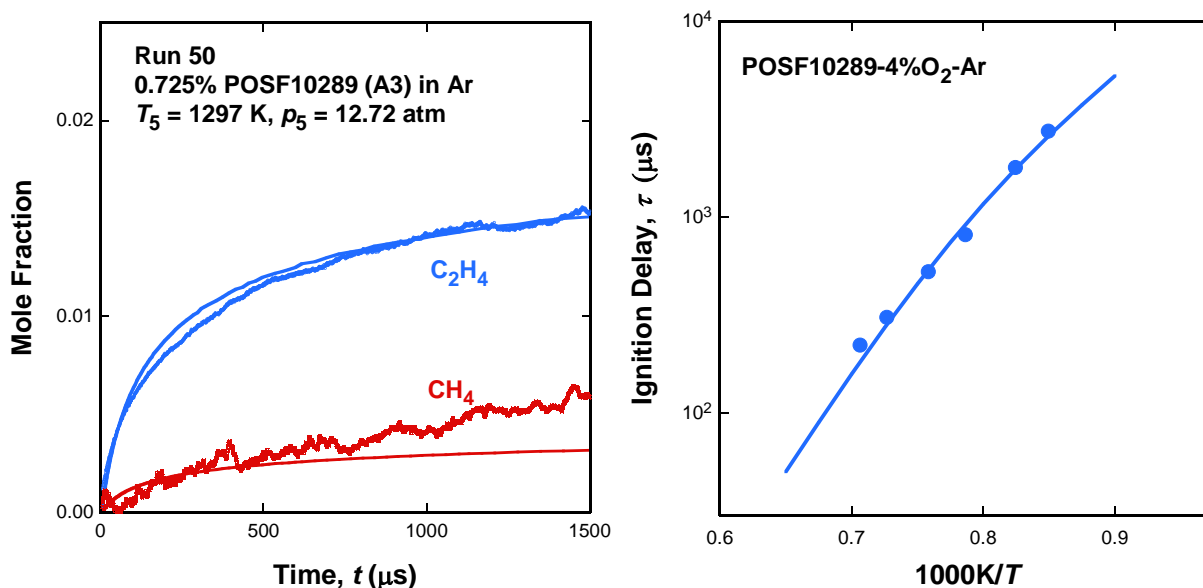

Figure 3. Selected comparisons of the experimental data and predictions for the A1 fuel. Left panel: time histories of ethylene and methane produced during shock tube pyrolysis; right panel: ignition delay time for several equivalence ratio and under two different pressures. The experimental data were taken from the unpublished work of Hanson and coworkers.

Models for C1 and C5 fuels

Experimentally, the C1 fuel shows different pyrolysis behaviors. The dominant pyrolysis products are isobutene and propene, and the rate of pyrolysis of the C1 fuel was measured to be greater than that of the Cat A fuels. The C5 fuel, on the other hand, is very similar to the Cat A fuel in its pyrolysis and oxidation kinetic behaviors. The hybrid modeling approach yields satisfactory results. These are summarized in Figures 4 through 7. Improvements can be made for the prediction of the

laminar flame speed of the C1 fuel in the fuel-rich stoichiometry. Analysis shows that the cause for the discrepancy lies in the chemistry of isobutene oxidation, which is quite uncertain presently.
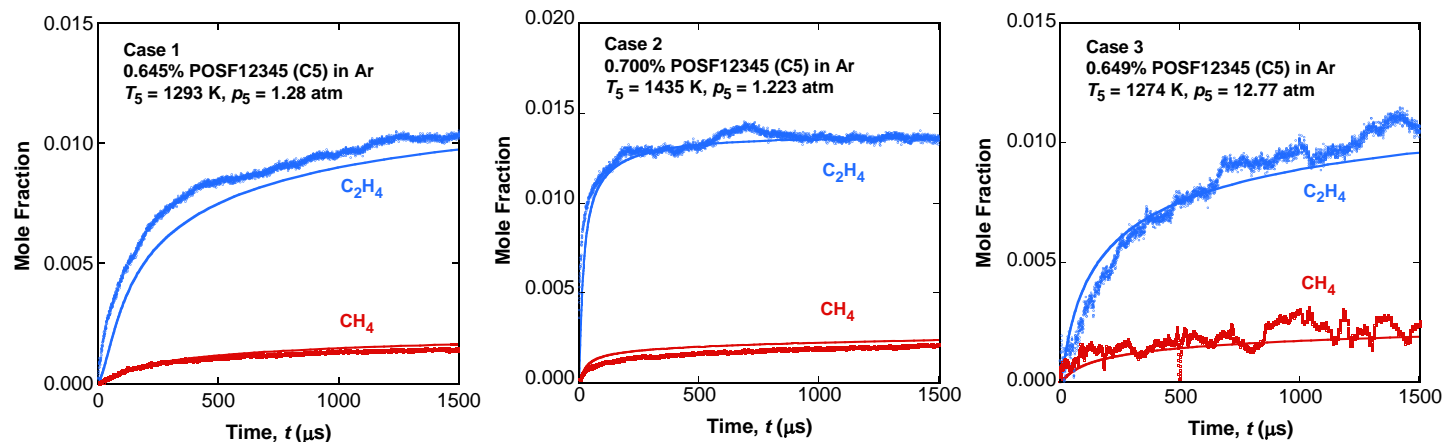

Figure 4. Selected comparisons of the time histories of ethylene and methane during shock-tube pyrolysis of the C5 fuel. The experimental data were taken from the unpublished work of Hanson and coworkers.
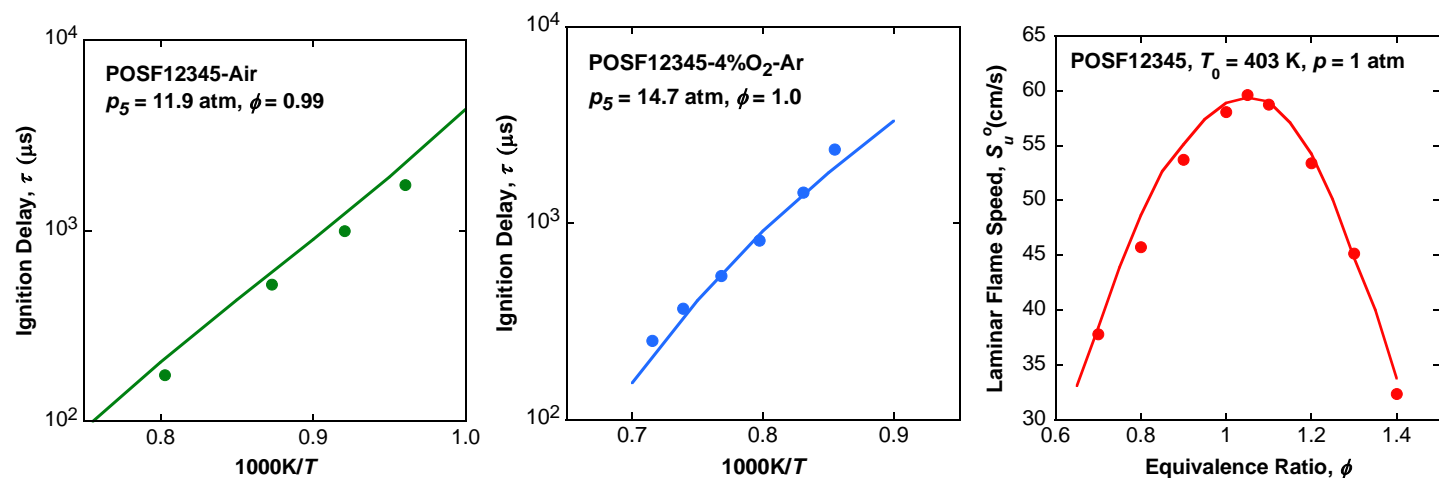

Figure 5. Comparisons of experimental (symbols) and computed (lines) ignition delay times (left and middle panel) and laminar flame speed of the C5 fuel. The shock tube data were taken from the unpublished work of Hanson and coworkers, and the flame speed data were taken from the unpublished work of Egolfopoulos and coworkers.

Model Reduction

Model reduction was carried out by Prof. Tianfeng Lu of UConn. The results show that the hybrid model can be reduced to about 30 species for each fuel to capture a wide range of combustion phenomena over a wide range of thermodynamic conditions.
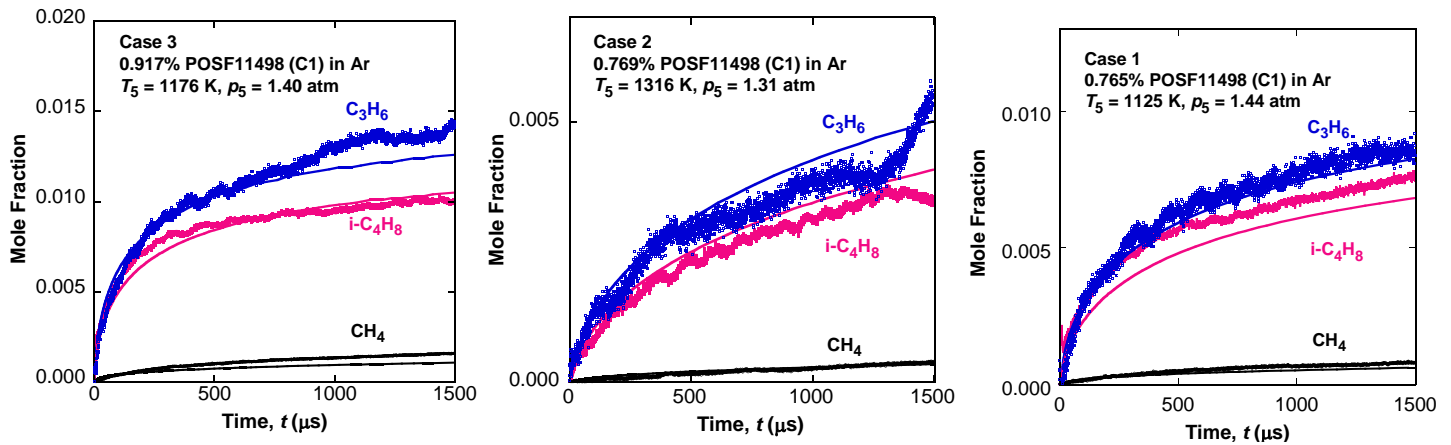
Figure 6. Selected comparisons of the time histories of ethylene and methane during shock-tube pyrolysis of the C1 fuel. The experimental data were taken from the unpublished work of Hanson and coworkers.
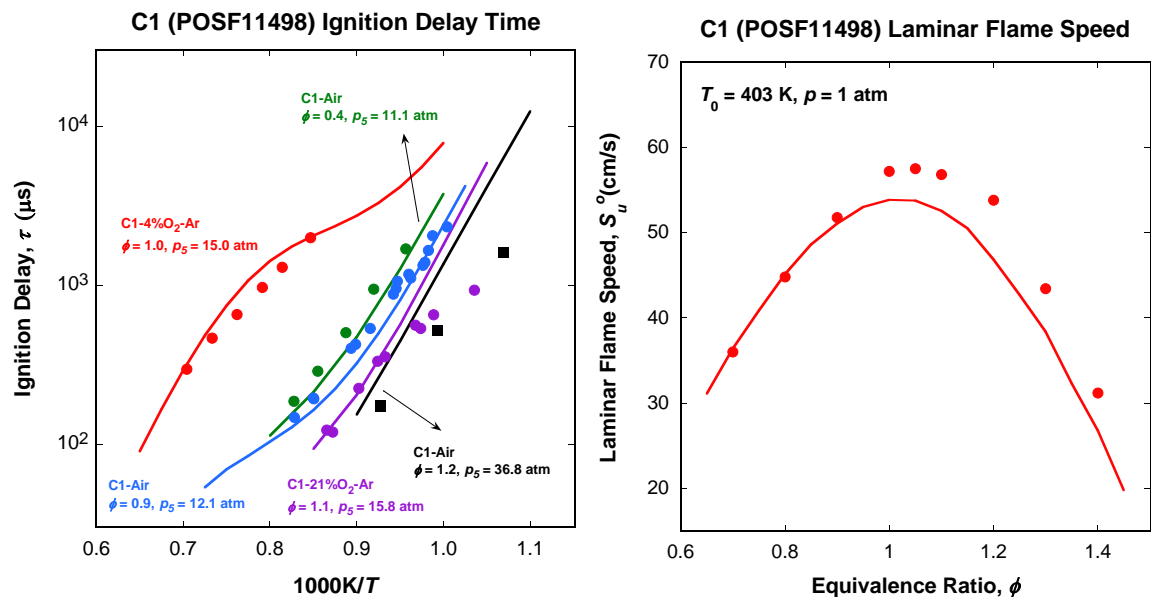

Figure 7. Comparisons of experimental (symbols) and computed (lines) ignition delay times (left and middle panel) and laminar flame speed of the C1 fuel. The shock tube data were taken from the unpublished work of Hanson and coworkers, and the flame speed data were taken from the unpublished work of Egolfopoulos and coworkers.

Task 2 – Dependency of Model Parameters on Fuel Properties
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Objective(s)
Understand the dependency of model parameters on fuel composition and chemical properties (DCN, aromatics, H/C, MW, etc.).

Research Approach
The dependency of model parameters on fuel composition and chemical properties is understood primarily through experimentation, aided with interpretation by kinetic modeling.

Comparisons

Experimental and modeling results show very little dependency of the reaction model parameters on the fuel composition or properties among all Cat A fuels and the C5 fuel. The C1 fuel, on the other hand, exhibits notably different pyrolysis behaviors. Rather than ethylene and methane being the dominant pyrolysis products, the C1 fuel produces predominantly propene and isobutene, both of which tend to have smaller reactivity towards oxidation than ethylene. Indeed, the laminar flame speed of the C1 fuel was computed to be about a few cm/s smaller than those of the Cat A fuels. The ignition delay time shows mixed behaviors. As shown in Figure 8, the ignition delay time of the C1 fuel is larger than that of the three Cat A fuels in a dilute, 4%O_2-Ar mixture, but the trend is seen to be opposite in the air mixture. Analysis of the computational results shows that the ignition delay time is impacted by two factors. The production of isobutene and propene from the pyrolysis of the C1 fuel leads to a longer induction time of radical buildup and thermal runaway, whereas the pyrolysis rate of the C1 fuel is larger than those of the Cat A fuels. It is the competition of these two processes that lead to the behaviors of switched overall reactivity, as seen in Figure 8.
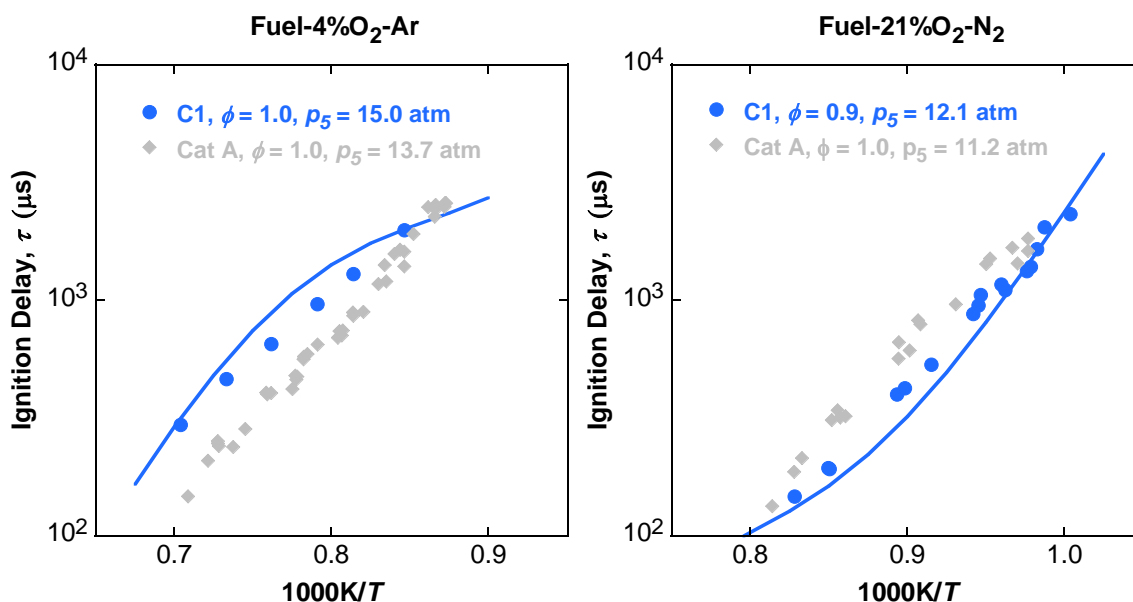

Figure 8. Comparison of the ignition delay times of the C1 and Cat A fuels in 4%O_2-Ar (left panel) and in air (right panel). The symbols are experimental data and the lines are computed results.

Milestone(s)

All milestones have been accomplished. These include the reaction models that can be reduced to less than 35 species for all three Cat A reference fuels and two Cat C fuels.

Major Accomplishments

The hybrid modeling approach is shown to be critical to obtaining the predictive capability for five multicomponent real fuels. The resulting models have shown to yield satisfactory results when reduced to about 30 species (by T.-F. Lu). They are used by modelers in Area #4 in their CFD simulations.

Publications

Nothing to report.

Outreach Efforts

Nothing to report.

Awards

Nothing to report.

Student Involvement
One student (Ray Xu) and one postdoctoral fellow (Dongping Chen) worked on the project. They gained useful experience through the project effort.

Plans for Next Period
- Develop and implement a strategy for and approach to modeling jet fuels of arbitrary composition from the knowledge of fuel composition.
- Refine the reaction models for cat A and C fuels.
- Test NO_x chemistry in these models.
- Explore an approach to address the NTC chemistry.