Project 026 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: October 1, 2015 to November 30, 2015
- Overall 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

Funding from FAA: $200,000
Matching funding: $140,000 (Stanford University), $60,000 (United Technologies Research Center, in-kind)

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 our 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 < ~ 35 species. During the current reporting period, we have partially address questions surrounding Task 2. Results of Task 1 has been reported in the 2015 report.

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 1, 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.

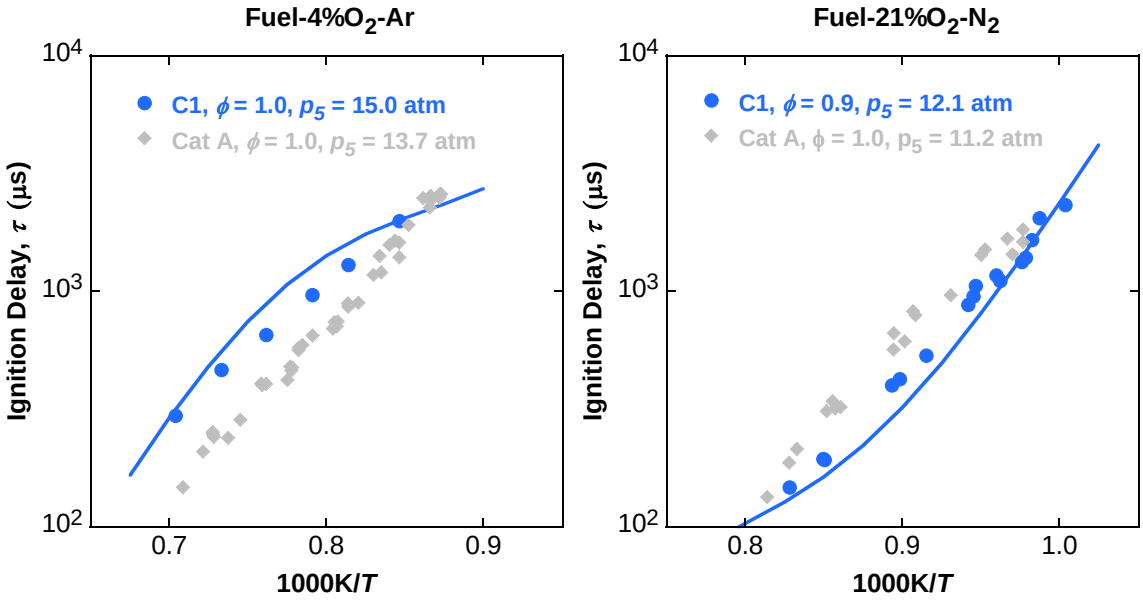

Figure 1. Comparison of the ignition delay times of the C1 and Cat A fuels in 4%O_2-Ar (left panel) and in air (right panel). The symbols are experimental data and the lines are computed results.

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 and an understanding of the fuel effects on intermediate formation and its effect on basic combustion properties of different jet 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. The models also help us to understand the causes for the different combustion behaviors of different fuels.

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.