



Full Length Article

A shock tube study of jet fuel pyrolysis and ignition at elevated pressures and temperatures



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ABSTRACT

The development of compact HyChem hybrid models for jet fuels requires datasets of pyrolysis product yields to constrain the model and of kinetic targets to evaluate the model. To this end, we have measured selected species time-histories during fuel pyrolysis using laser absorption, and ignition delay times using multiple methods behind reflected shock waves in a heated shock tube. Measurements were performed for three different jet fuels diluted in air or argon over a temperature range of 1000–1400 K, a pressure range of 12–40 atm, and equivalence ratios of 0.5–1. Fuel loading was measured using an IR He-Ne laser at 3391 nm; ethylene with a CO₂ gas laser at wavelengths of 10532 nm and 10674 nm; and methane with a tunable diode laser at wavelengths of 3175 nm and 3177 nm. Ignition delay times were measured in three ways: by monitoring fuel removal with laser absorption, by sidewall pressure, and by OH* emission. Particular care was taken in mixture preparation and efficient transfer of the gaseous fuel mixture to the shock tube. The current HyChem model by Wang et al. shows good agreement with these data.

1. Introduction

In support of the development and deployment of alternative engine fuels, recent efforts have been focused on the development of accurate and reliable chemical kinetics models for these fuels. Traditionally, a surrogate approach has been employed to facilitate the development of these models; by selecting representative hydrocarbons to mimic the real fuels; for example, primary reference fuel (PRF) and toluene reference fuel (TRF) have been used as surrogates for gasoline [1–5] and different hydrocarbon blends were used as surrogates for Jet fuel [6–9]. However, many of the proposed new alternative fuels contain species with large molecular weight and diverse compounds such as oxygenates and naphthenes whose combustion kinetics are less well known, and as such the surrogate and/or detailed reaction mechanisms for many of these alternative fuels are still in their infancy or do not exist. To exacerbate the situation, the surrogate model approach often uses a large number of fuel-related intermediate species and reactions that significantly increase the size of the surrogate mechanisms. To produce a more compact chemical kinetics model for jet fuel that accurately reproduces the pyrolysis and oxidation behavior of real jet fuel, a new approach entitled HyChem has been suggested by Wang and coworkers [10,11]. In this approach, an experimentally constrained fuel-pyrolysis model is combined with a detailed foundational chemistry model to provide both a compact reaction mechanism and a direct link to real

fuels.

In this model for large hydrocarbon oxidation, fuel molecules undergo thermal or oxidative thermal decomposition followed by oxidation of these decomposition products. At sufficiently high temperatures, the two processes are effectively separable in time or spatial scales. The model proposes that the number of significant fuel decomposition products or intermediates is small, typically six to ten in all. The composition distribution of these rapidly-formed thermal decomposition products determines the combustion properties of the original, multi-component real fuel. At engine pyrolysis conditions, the dominant thermal decomposition product in many distillate fuels is ethylene (C₂H₄), while the smaller, but important, methane (CH₄) yields are related to the aromatic content of the original fuel [10–12]. The development of HyChem hybrid models to describe the combustion behavior of conventional and alternative fuels requires a set of kinetic targets or constraints (including methane and ethylene species time-histories) to constrain the parameters of the reaction mechanisms. These types of species time-history data for distillate fuels are scarce.

Shock tube/laser absorption methods can furnish reliable, economical and accurate kinetic targets/tests of ignition, pyrolysis and oxidation that are needed both to validate the reaction mechanisms and characterize the chemical and physical fit-for-purpose properties for these fuels. In this study, species concentration time-histories during pyrolysis using laser absorption methods provide the necessary

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Table 1
Properties of A1, A2, A3 fuels.

Fuel	Average Formula	H/C ratio	MW (g/mol)	LHV (MJ/kg)	Composition (Mass %)			
					n-paraffin	iso-paraffin	cyclo-paraffin	aromatics
A1	C _{10.8} H _{21.6}	2.00	151.9	43.2	26.8	39.7	20.1	13.4
A2	C _{11.4} H _{21.7}	1.90	158.6	43.1	20.0	29.4	31.9	18.7
A3	C _{12.0} H _{22.3}	1.86	166.1	42.9	13.9	18.1	47.4	20.6

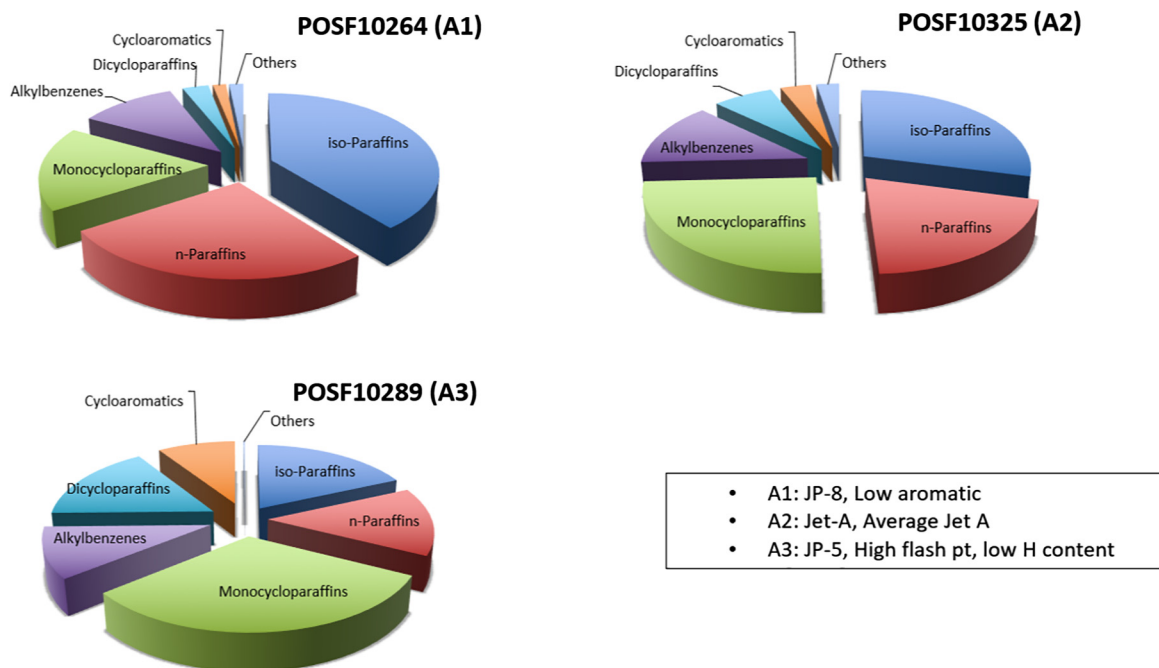


Fig. 1. Components of the tested jet fuels [11].

Table 2
Wavelengths and laser types for some chemical kinetics target species.

Wavelength (μm)	Laser Type	Usage
3.175	Interband Cascade Laser	Methane on-line
3.177	Interband Cascade Laser	Methane off-line
3.391	He-Ne	Fuel in Region 1
10.532	CO ₂	Ethylene on-line
10.675	CO ₂	Ethylene off-line

constraint data for HyChem model generation. Ignition delay time (IDT) measurements provide separate HyChem model validation targets.

Here, three jet fuels were investigated: A1, POSF10264, a low aromatic JP-8; A2, POSF10325, an average Jet A; and A3, POSF10289, a high flash point JP-5. The U.S. Air Force POSF number identifies each particular batch of fuel. GCxGC analyses and physical properties of the fuels are given in tables in the [Supplementary Material](#). A summary of these properties is given in [Table 1](#) and graphic representations of the fuel composition are shown in [Fig. 1](#).

In this paper, experimental methods are first discussed. This is followed by experimental results and discussion for these three jet fuels. Finally, some conclusions are given. This ignition delay time and pyrolysis datasets were used in the development of the HyChem model described by Wang and coworkers [11]. The purpose of this paper is to fully describe the measurement strategy and fully report the dataset.

2. Experimental method

2.1. High pressure shock tube

Current pyrolysis and ignition delay time experiments for all fuel mixtures were performed using the Stanford high-purity, high-pressure shock tube (HPST). Typical uniform test times behind reflected shock waves are of the order of 2 ms when helium is used as the driver gas. The stainless steel driven section has an internal diameter of 5 cm and was heated to 110 C to prevent condensation of the test gas mixture. Diaphragms were made of 1.27–2.0 mm thick aluminum (with cross-scribing) to allow measurements over a broad range of pressure

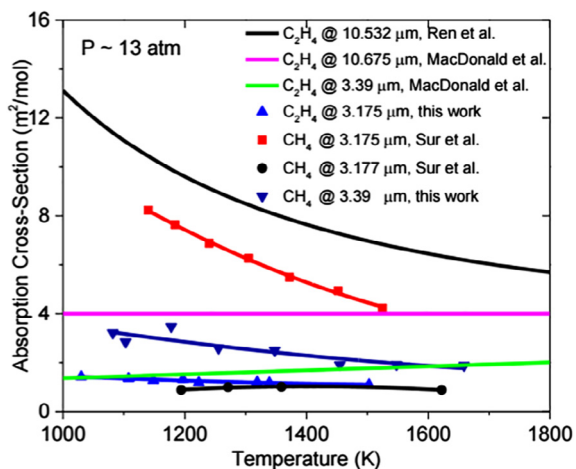


Fig. 2. Representative IR absorption cross-section data.

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