Shock Tube Ignition Delay Studies of Hydrocarbon Components Found in Jet Fuels

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ABSTRACT

The autoignition of several representative hydrocarbon compounds found in jet fuels and proposed as jet fuel surrogate mixture components (iso-octane, toluene, m-xylene, o-xylene, p-xylene, ethylbenzene, n-heptane, n-decane, n-dodecane, n-tetradecane, and decalin) were studied in a newly constructed high-pressure heated shock tube at Rensselaer Polytechnic Institute. Measurements were made at conditions relevant to combustion in aero-propulsion devices: temperatures of 780-1400 K and pressures of 7-60 atm for fuel/air mixtures with equivalence ratios of 0.25, 0.5, and 1.0. Ignition times were determined using electronically excited OH emission and pressure measurements made at or near the shock tube driven section endwall. The measured ignition times provide kinetic modeling targets for large hydrocarbon compounds for which little to no data previously existed, particularly at engine relevant conditions. The measurements also illustrate the differences in reactivity of hydrocarbon compounds of different molecular structure under the practical combustion conditions. In addition, kinetic modeling predictions, where available, are compared to the experimental data and sensitivity analysis is performed to determine the significance of reactions and identify potential areas for model improvement.

Measured iso-octane/air ignition times agreed well with previously published results for Φ = 1.0 and 0.5, providing a validation of the shock tube facility and experimental techniques; the results at Φ = 0.25 and for iso-octane/O_2/argon mixtures provide an extension of the iso-octane ignition database. Mixtures with argon as the diluent exhibited ignition times 20% shorter, for most conditions, than those with nitrogen as the diluent (iso-octane/air mixtures). The difference in measured ignition times for mixtures

containing argon and nitrogen as the diluent gas can be attributed to the differing heat capacities of the two diluent species and the level of induction period heat release prior to ignition.

The aromatics varied in reactivity depending on the length and position of alkyl side chains. Ethylbenzene was by far the most reactive C_8H_{10} aromatic with ignition times a factor of two to three shorter than the xylenes and toluene. The xylene isomers exhibited ignition times that were similar, with o-xylene the most reactive, p-xylene the least reactive, and m-xylene just slightly more reactive than p-xylene. The p-xylene ignition times are almost identical to measurements for toluene at the same conditions. These results represent the first ignition measurements for C_8H_{10} aromatics at the elevated-pressure moderate-temperature conditions studied, providing needed targets for kinetic modeling at engine-relevant conditions. Additionally, the toluene ignition measurements illustrate the influence shock tube contamination can have on measured ignition times.

For larger alkanes, the combination of the current data with previous shock tube and rapid compression machine measurements show that any differences in reactivity for C_7 and larger n-alkanes is slight, within the experimental uncertainties, for n-alkane/air mixtures with common carbon content at a large range of temperatures (650-1400 K) and elevated pressures. This allows for the conclusion that the oxidation pathways and rates are similar, irrespective of n-alkane chain length. To our knowledge, the n-tetradecane measurements presented here are the first ignition measurements to be reported for this compound.

Finally, shock tube experiments for decalin/air ignition at elevated pressures relevant to jet fuel combustion in aero-propulsion engines are presented. These measurements are, to our knowledge, the first ignition measurements for decalin at conditions relevant to practical combustion devices. A kinetic mechanism has been developed by collaborators at Politecnico di Milano (Ranzi and co-workers) which describes with satisfactory agreement the experimental measurements.