2D03: EXPERIMENTAL AND MODELING STUDY ON THE PYROLYSIS AND OXIDATION OF *ISO*-OCTANE

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High pressure iso-octane shock tube experiments were conducted to assist in the development of a Jet-A surrogate kinetic model. Jet A is a kerosene based jet fuel composed of hundreds of hydrocarbons consisting of paraffins, olefins, aromatics and naphthenes. In the formulation of the surrogate mixture, *iso*-octane represents the branched paraffin class of hydrocarbons present in aviation fuels like Jet A. The experimental work on *iso*-octane was performed in a heated high pressure single pulse shock tube. The mole fractions of the stable species were determined using gas chromatography and mass spectroscopy. Experimental data on *iso*-octane oxidation and pyrolysis were obtained for temperatures from 835–1757 K, pressures from 21–65 atm, reactions times from 1.11–3.66 ms, and equivalence ratios from 0.52 to 1.68, and ∞. *Iso*-octane oxidation showed that the fuel decays through thermally driven oxygen free decomposition at conditions studied. This observation prompted an experimental and modeling study of *iso*-octane pyrolysis using an *iso*-octane sub-model taken from a recently published *n*-decane/*iso*-octane/toluene surrogate model. The revised *iso*-octane sub-model showed improvements in predicting intermediate species profiles from pyrolytic experiments and oxidation experiments. The modifications to the *iso*-octane sub-model also contributed to better agreement in predicting the formation of carbon monoxide and carbon dioxide when compared to the recently published 1st Generation Surrogate model and a recently published *iso*-octane oxidation model. Model improvements were also seen in predicting species profiles from flow reactor oxidation experiments and ignition delay times at temperatures above 1000 K at both 10 and 50 atm.

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