Sooting characteristics of surrogates for jet fuels

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Currently, modeling the combustion of aviation fuels, such as JP-8 and JetA, is not feasible due to the complexity and compositional variation of these practical fuels. Surrogate fuel mixtures, composed of a few pure hydrocarbon compounds, are a key step toward modeling the combustion of practical aviation fuels. For the surrogate to simulate the practical fuel, the composition must be designed to reproduce certain pre-designated chemical parameters such as sooting tendency, H/C ratio, autoignition, as well as physical parameters such as boiling range and density. In this study, we focused only on the sooting characteristics based on the Threshold Soot Index (TSI). New measurements of TSI values derived from the smoke point along with other sooting tendency data from the literature have been combined to develop a set of recommended TSI values for pure compounds used to make surrogate mixtures. When formulating the surrogate fuel mixtures, the TSI values of the components are used to predict the TSI of the mixture. To verify the empirical mixture rule for TSI, the TSI values of several binary mixtures of candidate surrogate components were measured. Binary mixtures were also used to derive a TSI for iso-cetane, which had not previously been measured, and to verify the TSI for 1-methylnaphthalene, which had a low smoke point and large relative uncertainty as a pure compound. Lastly, surrogate mixtures containing three components were tested to see how well the measured TSI values matched the predicted values, and to demonstrate that a target value for TSI can be maintained using various components, while also holding the H/C ratio constant.

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1. Introduction

The development of efficient and accurate computational design methodologies for aircraft gas turbine engines requires the capability to model the combustion of practical aviation jet fuels such as JP-8. The multi-component nature of practical fuels, however, introduces an enormous complexity to the modeling task. The use of surrogate fuels composed of only a small number of components (e.g., 3–5 components) of varying chemical structure can significantly reduce the complexity of the chemical kinetic model. To be useful, however, the surrogate fuel must meet important combustion-related specifications of the practical fuel so that key combustion processes of the two fuels match with reasonable fidelity. Publications on the status of jet fuel surrogates [1,2] help to refine the set of target parameters from a long list of chemical kinetically limited processes within a gas turbine engine. The authors were part of a jet fuel surrogate working group whose goal was to create a consensus on the status and direction of the development of surrogate fuels [1,2]. Three key combustion related properties of the practical fuel were chosen to be reproduced by the surrogate. These are H/C ratio, autoignition characteristics, and sooting tendency. The selection of surrogate components for JP-8 reflects the type of molecular structures in the practical fuel, as well as the availability of chemical kinetic models for which validation data already exist, or are recently under investigation as part of collaborative projects or elsewhere. It should be noted that work by other groups has also explored surrogates with the goal of matching physical properties of JP-8 such as boiling range and density, in addition to matching chemical composition see, e.g., Refs. [3,4].

As an initial approach, the composition of JP-8 was simulated using hydrocarbons from the three main classes of compounds present in the fuel: n-alkanes, iso-alkanes, and aromatics. Higher carbon number n-alkanes and iso-alkanes were selected in order to match typical H/C ratio and autoignition properties of JP-8. Aromatic compounds, which have the most influence on sooting characteristics, make up the remaining fraction.

The sooting characteristics of JP-8 are important because radiation from soot formed in the combustor heats and stresses the combustor liner [5]. In addition, soot particles that escape from the combustor may deposit in the turbine section or leave with the exhaust. The particles that exit from the engine are typically below 2.5 μm, which are known to cause serious health effects [6]. The surrogate fuel should be able to accurately simulate in-combustor soot formation as well as soot emissions of JP-8. With regard to sooting tendency, specifications for JP-8 require the following [7]:...