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Predicting the global combustion behaviors of petroleum-derived and alternative jet fuels by simple fuel property measurements

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ABSTRACT

Pre-vaporized global combustion behaviors of a petroleum-derived jet fuel (JP-8), five alternative jet fuels (Shell SPK, Sasol IPK, HRJ Camelina, HRJ Tallow, and Gevo ATJ), and five 50/50 (liquid volume) blends of JP-8/alternative fuels are experimentally examined and compared. Three experiments are performed to investigate the gas-phase combustion behaviors of the tested fuel samples: (1) global oxidative species profiles in a variable pressure flow reactor, (2) diffusion flame extinction in a counterflow burner, and (3) premixed flame initiation in a heated spherical combustion chamber. Multivariate linear regression methods have been applied to investigate the sensitivities of pre-vaporized global combustion behaviors to individual combustion property targets of the fuels, including Derived Cetane Number (DCN), H/C ratio, mean molecular weight, and smoke point. As a proof of concept for fuel screening tool based on the standardized fuel property measurements, a "combustion property target (CPT) index" based upon this regression analysis is found to show promise as a rapid means to evaluate the global pre-vaporized combustion behaviors of the tested fuel samples against each other as well as the spectrum of JP-8 fuels found in use. The present work suggests the applicability of such a methodology not only as an expeditious fuel screening tool for assessing the fully pre-vaporized, kinetically coupled behaviors of emerging alternative jet fuel candidates, but further supports the use of combustion property targets in developing kinetic models that are specific to each real fuel.

1. Introduction

Both global instability of energy security and concerns over environmental issues have driven the transportation sector to explore alternative fuels derived from non-petroleum feedstocks. An integral part of this endeavor is to assure that proposed alternative fuels are compatible with petroleum-derived materials present in fuel blends, as well as with existing devices developed for use with (solely) petroleum-derived jet fuels [1–3]. Fit-for-use petroleum- and alternative feedstock-derived jet fuels can vary significantly in terms of their physical and chemical properties (e.g., Table 1). At present, the impacts of such variations on the performance and emissions of aviation combustion systems remain to be understood fully, and have been principally characterized by empiricism derived from experimental testing [1,4]. Furthermore, it is known that the compositional diversity of alternative jet fuels and their blends with petroleum-derived material can produce fuels with chemical and physical properties that lie outside the historical experience base of petroleum-derived jet fuel application [5,6] that has been the basis for fuel certification standard developments. Considering that the current ASTM standards [3] examine only two combustion properties, the smoke point (SP) and net heat of combustion, which have strong correlation with H/C ratio, the measured H/C ratios and SPs for fuel samples studied here are plotted in Fig. 1 along with the variability of JP-8 reported in PQIS 2013 annual report [7]. Since many of the alternative jet fuels contain no aromatic components, their H/C ratios are typically higher than those of petroleum-derived jet fuels. The absence of aromatic components also consequently yields much higher SPs. Fig. 1 clearly demonstrates the fact that the combustion properties of alternative jet fuels and their blends with petroleum-derived jet fuels cannot be judged by the historical experience with petroleum-derived jet fuels. Evidently, there is a need for fit-for-purpose testing of alternative jet fuels and their blends with conventional fuels and continued evolution of certification standards to reflect their observed combustion properties.

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Table 1
Summary of four combustion property targets, DCN, H/C ratio, MW, and TSI of petroleum-derived and alternative jet fuels studied in this study.

Fuel sample	DCN	MW[g] (g/mol)	H/C ratio	SP (mm)	TSI[c]
Shell SPK POSF 5729 (5172)	58.4	138.3	2.24	84.3[b] (⩾45[a])	1.9
Sasol IPK POSF 7629 (5642)	31.3	148.5	2.195	42.2 (27.5[a])	9.5
HRJ Tallow POSF 6308	58.1	163.7	2.18	61.6[b] (⩾45[a])	6.0
HRJ Camelina POSF 7720	58.9	167.6	2.20	59.1[b] (⩾45[a])	6.7
Gevo ATJ POSF 10151	15.5	175.6	2.17	35 (26[a])	15.6
S-8 POSF 4734 [10]	58.7	154.5[e]	2.14	78.9[b] (⩾45[a])	3.2
Petroleum-derived jet fuels					
Jet-A POSF 4658 [8,9]	47.1	157.5[d]	1.96	22.1	24.2[f]
JP-8 POSF 5699 [42]	49.3	154.5	1.935	23	22.3
JP-8 POSF 6169	47.3	153.6	2.02	24.5 (26[a])	20.7

[a] Measured by Unites States Air Force Research Laboratory.
[b] Determined by virtual smoke point technique described in [59].
[c] Estimated value derived from SP and MW data, using coefficients in [60].
[d] Previously reported at 142 ± 15 [8,9].
[e] Previously reported at 163 ± 15 [10].
[f] Previously reported at 21.0 [8,9], updated based on MW measured in this study.
[g] Overall uncertainty of MW determination is ±6.0 g/mol. The information in this table has been critically updated from the previous conference paper [34].

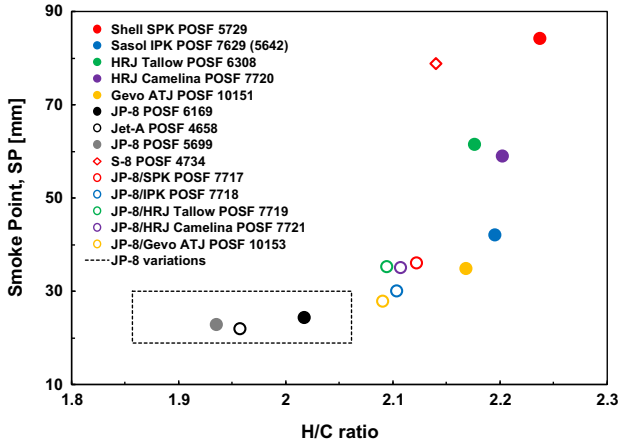

Fig. 1. Comparison of measured smoke points (SP) and H/C ratios of fuel samples tested in this study. The rectangle with black dashed lines indicates the variations of H/C ratio and SP found in JP-8 [7]. Data for alternative and JP-8 mixtures are for 50/50 (by volume) mixtures, see Table 2.

Currently, the alternative fuel certification process is limited to fit-for-purpose verification that inevitably requires extensive and resource-intensive rig and full-scale tests [3,6]. To overcome this significant limitation, an *a priori* fuel screening technique is desirable. The ideal fuel pre-certification screening approach would test emerging alternative fuel candidates with (a) a minimal fuel sample volume requirement and (b) standardized, commercially-available test equipment/methods. Moreover, it would (c) provide quantitative relationships between test metrics and the combustion performance (and emission characteristics) of the fuels/fuel blends to be tested, as they relate to fuel properties. When one considers that there is a broad spectrum of possible gas turbine configurations that may respond differently to fuel properties, the advantages of pre-screening are obvious, particularly for ruling out non-viable fuel candidates or suggesting acceptable fuel blending fractions to be further investigated. Though much is speculated qualitatively from empirical larger scale testing results, and despite the utility of such tools, *there presently appears to be no quantitatively predictive relationships among the physical and chemical kinetic properties of jet fuels and their global combustion behaviors*. To address this issue, the present work demonstrates a simple screening methodology for pre-vaporized fuel combustion that considers all of points (a)–(c). Elements of this methodology also address (d), developing kinetic models to describe combustion of both petroleum- and alternative-derived fuels and their blends through combustion property target → fuel surrogate formulation techniques described elsewhere [8–11].

Identification and characterization of those fuel properties that control global combustion behaviors have been a challenging problem for the experimental and computational study of gas turbine combustion. Some progress has been made through formulation of "surrogate fuel mixtures", which are designed to emulate the combustion behaviors of a targeted jet fuel. Petroleum-derived jet fuels consist of a few hundred hydrocarbon components, which can be categorized either by molecular size or carbon number and molecular class distribution over classes including paraffins, naphthenes, and aromatics [12]. Physical properties of fuels are strongly affected by molecular weight and organic class structure. But even multi-dimensional gas chromatography that can discriminate the molecular weight and organic class structure of a real fuel cannot today distinguish the isomeric composition of the weakly branched alkanes, cyclo alkanes and aromatics, which affects chemical kinetic behavior. Due to the lack of a comprehensive understanding of the complicated, highly coupled physico-chemical processes involved in applied multiphase combustion environments, fuel fit-for-purpose characterization presently relies on experimental measurement of engineering performance indicators rather than on fundamental scientific metrics [2].

The concept of a surrogate aims to reduce the high dimensional complexity of real fuel by formulating the mixture with a few chemical components by matching either the composition fractions of all molecular classes measured in the target jet fuels [13–27] or implicit correlations of fuel physical properties [28–33]. Consequently, depending on the purpose of the surrogate mixtures, they can be either overly-simplified, for example, binary mixtures [21,23] typical for reflecting a limited number of kinetically controlled combustion properties, or composed of considerably larger numbers of molecules typical of attempting to reflect primarily distillation and vapor dome properties, surface tension, viscosity, and sound speed [28–33]. Developing means to reflect both kinetic and physical properties have typically required some approximations in the manner in which these property emulations are incorporated in multi-phase combustion. This is especially so if one wishes to reflect the molecular organic class distribution over the distillation curve. We set aside these questions here as there are at present many ASTM laboratory tests to assess those properties of new fuel candidates that characterize physical properties known to be significant to atomization, vaporization, and related