



Full Length Article

The distillation curve and sooting propensity of a typical jet fuel

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ABSTRACT

Real jet fuels are complex mixtures of many organic components, some of which are aromatic compounds. Towards the high-temperature end of the distillation curve, some of the fuel components are multi-ring compounds. A small amount of these high molecular weight species in the fuel could impact soot nucleation in practical engines especially when the fuel is injected as a spray. This work aims to highlight the variation of the sooting propensity of jet fuels as a function of distillate fractions and to examine the validity of a surrogate fuel in emulating soot production from real fuels. Particle size distribution functions and soot volume fractions are studied in a series of laminar premixed stretch-stabilized ethylene flames doped with Jet A, its various distillate fractions, and the 2nd generation MURI surrogate. Soot formation as a result of doping real jet fuel and its distillate fractions is also investigated in counterflow and coflow diffusion flames. The results show that the higher-boiling distillates mostly influence soot nucleation and produce substantially more soot in nucleation controlled flames than the light molecular fraction and jet fuel as received, while such an effect is seen to be small in flames where soot production is controlled by surface growth. The potential impact of distillate fractions on soot nucleation propensities is discussed.

1. Introduction

Conventional jet fuels are of a distillate origin of crude oils and multicomponent in nature. A typical jet fuel may contain thousands of hydrocarbon compounds [1–3], among which up to ~20% (wt) can be aromatics [1]. The distillation curve of typical jet fuels gives hints about the presence of high molecular weight species in the fuel, some of which are polycyclic in nature [4–6]. For a typical Jet A, the temperature at the 90% distillation volume is around 250 °C [4], which exceeds the boiling point of naphthalene (218 °C) and tetralin (208 °C). The impact of multi-ring species on soot formation is apparent through a range of previous studies of soot formation, most of which were conducted in counterflow or coflow diffusion flames [7–18]. In many of these studies, gaseous-fueled baseline flames were doped with low concentrations of vaporized liquid jet fuels and their surrogates, demonstrating the effects of dopant chemical composition on sooting tendencies while preserving the main properties of the baseline flames

(e.g. temperature, velocity) [11,13–16,18]. With the motivation to identify simple surrogates capable of reliably predicting the sooting behavior of kerosene, Moss and Aksit [7,12] conducted an experimental investigation on the sooting, laminar, and turbulent coflow flames of aviation kerosene and blends of *n*-decane with a range of alkyl-substituted aromatics. The sooting behavior of the surrogates was also compared on the basis of the measured smoke points. They found that a mixture of 30% (mass) mesitylene or propylbenzene and 70% (mass) *n*-decane represents the sooting behavior of an aviation kerosene well in both laminar and turbulent flames. Saffaripour et al. [8] studied coflow diffusion flames of pre-vaporized Jet A-1 and four synthetic jet fuels to compare their sooting characteristics and flame structures. They showed that soot levels along the centerline of coflow diffusion flames are strongly correlated to the aromatic content of the fuel, and soot and acetylene concentrations are not proportional to each other. In more recent studies, Saffaripour and coworkers [9,10] measured soot volume fraction in a Jet A-1 coflow diffusion flame and compared it with the

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volume fraction observed in a corresponding flame burning a surrogate that is comprised of 69% (mol) *n*-decane, 20% *n*-propylbenzene and 11% *n*-propylcyclohexane [19]. They found that such a surrogate underpredicts the soot concentrations of the real Jet A-1 up to a factor of five, and the same trend was observed in the smoke points of these fuels. Consequently, they suggested that the addition of two-ring aromatics is necessary in order for the surrogate to reproduce the sooting propensity of the real Jet A-1. In the work of Witkowski et al. [11], soot volume fraction and morphology measurements were made in a laminar coflow methane-air diffusion flame seeded with approximately 2200 ppm of a real Jet A and the first-generation MURI surrogate [20] in which the aromatic component is represented by 24% by volume of toluene. The surrogate jet fuel was shown to have notably lower soot volume fractions than the real Jet A. In the work of Lemaire et al. [21], soot volume fraction in turbulent diffusion flames burning kerosene and its surrogate was measured and compared. It was shown that a surrogate containing decalin, a two-ring compound, is required to reproduce the sooting behavior of real jet fuels.

The evolution of main oxidation products and soot precursors in methane and ethylene flames doped with small amounts of jet fuel and surrogate mixtures was extensively studied also in counterflow flames [14–16,18]. For example, Honnet et al. [17] measured soot volume fraction in laminar non-premixed flows burning a JP8 and the Aachen surrogate comprised of 80% *n*-decane and 20% 1,2,4-trimethylbenzene by mass. They found that the Aachen surrogate reproduces the sooting tendency of JP-8 well within the range of the flame conditions studied.

As discussed above, surrogate fuels have become a widely used approach for dealing with the challenges of modeling real fuels. Most of the studies on jet fuels aimed at formulating surrogate mixtures capable of reliably predicting chemical and physical properties of common aviation fuels, such as volatility, boiling point curves, smoke point, advanced distillation curves, average molecular weight, H/C ratio, the derived cetane number, and the threshold sooting index (TSI) [22]. Dooley et al. [23] utilized the TSI, along with the average fuel molecular weight, H/C ratio, and derived cetane number, as targets to match a 4-component surrogate to a target Jet A fuel (POSF 4658). The components of the surrogate were blended in proportions, which minimizes the difference in the aforementioned targets between the fuel and its surrogate. The performance of the surrogate was compared to the real fuel in several controlled combustion experiments, including a wick-fed laminar diffusion flame, which was used to measure the smoke points of the fuel and surrogate. Additionally, soot volume fractions in the flame were quantified using laser light extinction; the peak of volume fraction values was found to be comparable for the Jet A fuel and the surrogate at their respective smoke points.

The aromatic content of a fuel is an important practical indicator of its sooting tendency [24]. This has motivated attempts to match the proportion and distribution of aromatics between a real fuel and its surrogate as a way to ensure a wide range of applicability of the fuel surrogate. Importantly, it has been noted that the sooting tendency of real fuels correlates well with their aromatic content as long as the ratio of polyaromatics/monoaromatics is similar between the real fuel and the surrogate. In a recent work [25], sooting tendencies of several jet fuels and their surrogates were experimentally measured in terms of the Yield Sooting Indices (YSIs). It was found that while the sooting behavior of a fuel is largely dependent on the aromatics present in the fuel, a lumped parameter such as the aromatics volume percent can be inadequate for predicting the fuel sooting tendency. To develop surrogates with fidelity to mimic the sooting behavior of real fuels, it is important to characterize the nature of their aromatic content.

We wish to point out here a simple fact that has not received sufficient attention in earlier studies, namely the role of the real-fuel distillation curve in soot formation. As observed in the work of Bruno and coworkers [4], there is a continuous drop in the content of one-ring aromatics and a simultaneous increase in the content of the two-ring aromatic compounds towards the high boiling-point fractions. The very

tail end of the distillation curve can reach a temperature as high as 350 °C, which is in the range of the boiling points of high-molecular weight, three to four-ring aromatics (e.g., 340 °C for phenanthrene and 378 °C for pyrene). Obviously, these multi-ring compounds within the fuel are trace species but they still could shortcut the growth process of polycyclic aromatic hydrocarbons (PAHs) and in this way, induce soot nucleation in engines especially in non-premixed spray combustion. Currently, the composition of the tail end of the distillation curve is not well known, as available distillation curve studies typically stop at 90% volume fraction. A range of questions thus arise:

- 1) What is the nature of the fuel compounds in the tail end of the distillation curve and what role do they play in soot formation?
- 2) Jet fuels are utilized in practical systems as a spray, and the distillation curve must impact, at least in some cases, the local concentrations of the different constituents of the multicomponent fuels. Hence, can the sequential evaporation of the fuel components, from low to high boiling points, produce transient, spatial enrichment of multi-ring fuel components, thus impacting soot nucleation and growth?

The current work aims to address a range of related questions surrounding the effect of the likely existence of multi-ring species on soot formation from real jet fuels. We carry out our studies across three laboratory flame platforms, from laminar premixed stretch-stabilized flames to the counterflow and coflow diffusion flames. One of our emphases was to examine the sooting properties of different distillate fractions of a typical Jet A. A comparison of the sooting properties of the Jet A and the 2nd generation MURI surrogate (40% *n*-dodecane, 29% *iso*-octane, 7% 1,3,5-trimethylbenzene and 23% *n*-propyl benzene by mole) [23] is also presented and discussed to shed light on the above questions.

2. Methodology

2.1. Distillation setup

The fuel investigated in this study is an average commercial Jet A, designated as POSF 10325 [1], which is basically POSF 4658 [4,6]. In order to understand the impact of the different distillation fractions on the sooting property, a range of the distillate fractions was obtained by distillation. The setup and procedure follow that of Bruno and coworkers [4–6] with small modifications to ensure reliable output in the volume fraction range of 90–100%. As depicted in Fig. 1, a round-bottom flask was filled initially with 400 ml of Jet A. The liquid was

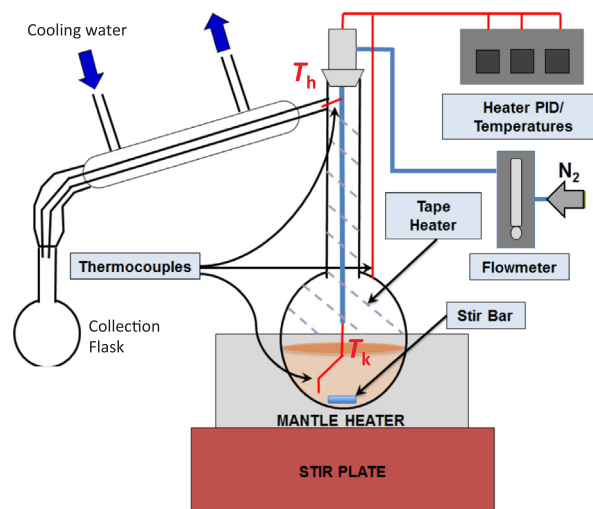


Fig. 1. Schematic diagram of the distillation setup.

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