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Full Length Article

Predicting the soot emission tendency of real fuels – A relative assessment based on an empirical formula

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ABSTRACT

Significant progress is going on in the development of non-fossil based alternative fuels which are designed to be sustainable, have potential to substitute (fully or partially) the fossil-based fuels and importantly are targeted to reduce emissions. Though soot emission characteristics has not been focus of fuel certification process yet, due to growing environmental concerns it is important to consider this aspect in the fuel design and understand its emission patterns.

It is known that soot formation in combustion is linked to the degree of branching, degree of unsaturation or the degree of cyclization of a fuel molecule. This information is used to extract soot emission properties of complex real fuel mixtures. To do so, we use the definition of hydrogen deficiency (HD) which gives information on the number of double bonds or cyclic structures present in a fuel. With the help of one measured emission property, the same property of different fuels is predicted using HD. This way, we obtain a relative assessment of fuels' sooting tendency compared to other known fuels. In this work, soot emission pattern of six jet fuels (reference fuels and synthetic fuels) is predicted based on HD and compared them with the recent ground-test measurements of V2527-A5 engine of an Airbus A320. In addition, two more test cases are provided: aviation fuels and diesel fuels, to predict sooting tendency using HD to support our concept. The prediction of the sooting propensity based on HD was found in excellent agreement with the measurements.

1. Introduction

Aviation kerosene is a multi-component complex mixture of hundreds of different hydrocarbons of varying molecular classes mainly categorized by four major classes namely n-paraffins, iso-paraffins, cy-paraffins, and aromatics [1]. The amount of n- and iso-paraffins dominates the fuel composition of most of the conventional fossil-based fuels [2]. Not only the composition varies among the different kerosenes (Jet A, Jet A-1, JP4, JP8), they also vary among the region, feedstock used, and variability in production processes [3]. This leads to a fuel of diverse chemical composition which is furthermore complicated by the new variety of alternative fuels being synthesized. The most notable impact of fuel composition variation is anticipated on the soot emissions where new fuels are paraffinic (Fischer-Tropsch FT-fuels) or are derived through hydro-processed esters and fatty acid (HEFA) [4–11]. See ASTM7566 [12] for a complete list of certified production paths.

Worldwide efforts are being undertaken to replace energy sources based on crude oil to fuels from alternative sources owing to the growing concerns about the security of supply, as well as negative effects on the environment and climate [13]. Alternative fuels have been of great interest due to their potential for reduction in net emissions. These fuels are synthesized from various alternative sources with an aim to produce fuel that emits lower emissions. The alternative fuels are still primarily hydrocarbons obtained from natural gas, coal or biomass as feedstock and their compositions can be typically dependent on the production process and the feedstock used. Since they are synthesized from different production technologies, they differ in their chemical composition. Synthetic fuels from FT-processes are mainly paraffinic in nature [14]. Due to the absence of aromatics, the density of synthetic fuels is lower compared to the existing jet fuels. In order to comply with specification limits one would require addition of components of higher densities such as cyclo-paraffins or aromatics [3]. Thus, alternative fuels may contain hydrocarbons of different molecular nature not present in conventional fuel. Therefore, an understanding of not only the physical and chemical process occurring during combustion but also the molecular structural effect on emissions is important. This can help to understand how the particular chemical structure of the fuel influences emission patterns. Understanding this influence can help us to better understand and design the fuels of future.

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In this context, in the present work we aim to understand how the fuels' molecular structure influences the particulate emissions irrespective of the conditions they are burned. To this end, we present a simple correlation to predict the soot emissions of fuels at a given combustion condition. For this reason, we exploit the fact that soot emissions are linked to the unsaturation and cyclization of fuel molecules. Through this we can assess relatively the fuel emission pattern based on the fuels' molecular structure.

2. Background – fuel property effects on soot emission

The presence of different molecular classes in different fuels has an influence on various physical and chemical processes occurring inside the combustor. Such differences may influence the ignition, spray characteristics such as atomization of droplets, fuel vaporization which may subsequently affect the combustion and soot emissions. Several reports are available in literature showing strong link between fuel properties and measured particulate matter (PM) emission from engines and gas turbines [4–7,15–23], also supported by theoretical correlations [15,19,21–23]. The correlations on fuel effects are empirical in nature and links sooting tendency of fuel such as smoke point, smoke number, and particle emissions with fuels' chemical or physical properties such as the amount of aromatics or hydrogen, H/C ratio, viscosity, volatility, vapor pressure, distillation parameters or boiling range etc. [24].

There are numerous studies on the soot emissions involving varying scales of experiments and models starting from simple laboratory flames to complex engine tests. Based on the type of fuels studied, i.e. aviation fuels (conventional and alternative fuels), road transportation fuels (diesel and gasoline) and depending on the focus of these studies one can categorize these studies into: (a) relationship of fuel parameters to the emissions based on experimental observations, (b) theoretical fuel-property correlations to estimate the emissions, and (c) fundamental studies on sooting tendencies of individual fuel components in laminar flames. In this work, we focus on the second aspect using knowledge gained from aspect one and three.

2.1. Emission measurements

With increasing use, the performance of alternative fuels with respect to the soot emission has received considerable attention [25–27]. The particles emitted from aircraft engine are influenced by the fuel composition, fuel flows, as well as engine design/operating conditions and altitude [28]. The effect of fuel composition on emissions has been part of many studies. Compared to the aromatics present in fuel that has been identified as compounds that primarily influence the tendency to form soot [29–32,4,5,17,2,23] the fuel hydrogen content has been considered a more fundamental parameter that is independent of molecular structure [33–35,23]. Most of the studies identify the aromatic content of the fuel to be correlated to the emissions [4,5,8,19,18,36]. However, many of these earlier studies are done on conventional kerosene or existing jet fuels [6,18,19,22,23]. With emerging demand of alternative fuels, it is important to expand our current knowledge/database on aircraft emission and increase knowledge towards influence of other fuel components on soot emissions [37,18]. Recent measurements of soot emissions in aircraft engines using alternative fuels [11,23] have shown that the aromatic content of fuel does not always explain the trends measured. The data presented by [23] who studied various blends of various conventional and alternative fuels could not differentiate the impact of aromatics and H/C ratio as both were varied simultaneously. They demonstrated that non-volatile particulate emission showed strong function of fuel composition, consistent with other similar studies [20,19]. Other criteria that showed relationship to emissions are hydrogen content or H/C ratio of fuel [33–35,4,20,11]. The H/C ratio criterion is disputed in the literature: It has been found to correlate in some studies [33–35] whereas the trend of PM emissions to H/C ratio was found to be inconsistent by others [38,23]. This is not surprising as complexity of fuel composition also implies complexity in assessing their influence on the emissions.

However, these relationships are not widely applicable and are often valid only for specific fuel and the specific conditions investigated. For example, a few fuels present in this study showed no linear relation to the aromatics content mainly due to the presence of a significant amount of cy-paraffins. The soot emissions can be linearly related to the H/C ratio but this relationship is non-predictive, i.e. cannot be extended to predict soot emissions directly. Christie et al. [23] also reported that the correlation between H/C ratio and aromatics content is poor and insufficient to define the fuel. Similarly, correlation based on hydrogen content can be influenced by molecular structure especially when large aromatics are present in fuel [30].

2.2. Theoretical correlations

Regarding aviation fuels, there are many scientific reports addressing the issue of emissions involving both conventional and synthetic fuels [4–7,15–20,39,40,22,23]. Among them there are examples where fuel properties effects have been emphasized to correlate with the soot emissions of aviation fuels [15,19]. Similar studies are also available for fuels used in road transport. Relevant to this work, among these fuel composition-property relationships, are the ones which emphasized the correlation of the fuel's chemical composition to the emission. These studies include correlations obtained from studies on jet and diesel fuels [15,19,21] as well as relations obtained in gasoline engines [41–45].

Cookson and Smith [15] provided a simple linear relationship of the fuel composition to the smoke point, aromatics content, H-content, and other physical properties. Their model requires the amount of n-alkane, branched plus cyclic saturates and aromatics content of fuel as well as three respective fitting coefficients determined from multiple linear regression analysis to predict the property of blends in question. They demonstrated their model validation through blends of verified jet and diesel fuel. Recently Brem et al. [19] obtained a correlation for emission indexes of conventional kerosenes using the hydrogen content of fuel as well as information on engine thrust whereas Speth et al. [21] predicted black carbon emissions as a function of the aromatic content and engine thrust. Both studies reported that the validity limit of their correlations is mainly restricted to similar technology or similar fuels respectively.

The influence of fuel composition on particulate emission in gasoline engines are also demonstrated in literature [41–45] using physical properties along with the chemical composition of the fuel to obtain particle number (PN) indexes. Aikawa et al. [41] obtained the PN index based on the vapor pressure and double bond equivalent (alias hydrogen deficiency) of each fuel component. Subsequent studies [42–45] have also presented correlations based on the fuel composition and fuel properties to predict the particulate emissions. All of these correlations use, along with fuel compositions, at least one physical property; like vapor pressure [41,45] or distillation range parameter [43] and may employ up to fourteen properties [44] of each fuel component. Such correlations are cost intensive as they require specialized laboratory tests which also multiply with number of components present in a fuel.

2.3. Fundamental soot investigations

On the fundamental level, a detailed description of soot formation and growth process is in itself a wide field of research originating from pioneering work of K.H. Homann, H.G. Wagner, B. Haynes, H. Bockhorn, M. Frenklach and a detailed discussion is beyond the scope of this work. In addition, a large body of work in terms of sooting tendencies of fuel components and their relation to the fuels' molecular structure has been reported in literature [46–51]. It has been demonstrated that the sooting tendencies of hydrocarbons are governed by the structure of the molecules [49,31,51]. Among them, aromatics are found to be most prolific sooters whereas fused aromatic-aliphatic