



Physicochemical properties of soot generated from toluene diffusion flames: Effects of fuel flow rate



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ABSTRACT

Aromatic hydrocarbons are commonly found in fossil-derived transportation fuels, and their combustion in engines produce most of the observed soot particles. Toluene is an important component of gasoline (about 6 wt%), diesel (1–2 wt%), and jet fuels (1–2 wt%), and forms a part of their surrogates. This paper reports the nanostructures and chemical constituents of soot, formed in toluene diffusion flames at different fuel flow rates. High resolution transmission electron microscopy (HRTEM) and X-ray diffraction (XRD) are employed to study the physical properties of soot, while Fourier transform infrared spectroscopy (FTIR), electron energy loss spectroscopy (EELS), and elemental analysis are used to investigate its chemical properties. With increasing fuel flow rate, HRTEM and XRD analyses showed that the lateral size of aromatic layers in soot reduced, while the FTIR analysis revealed that the concentration of aliphatic and oxygenated groups decreased, and that of aromatic group increased. The elemental analysis showed that soot from lower fuel flow rates had more hydrogen and oxygen content than those from higher flow rates. The experimental observations indicate that both physical and chemical characteristics of soot derived from toluene flame are dependent on the fuel flow rate used for its production.

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1. Introduction

Aromatic hydrocarbons are important constituents of fossil-derived transportation fuels, representing about 20–50% by weight in gasoline, 10–25% in diesel, and 5–16% in jet fuels [1–6]. They are frequently used as a fuel additive to improve the anti-knock index and oxidative stability of fuels [7]. A major disadvantage of their presence in fossil fuels is that they are responsible for the generation of soot particles when the fuel is burnt, as their aromatic structure provides a base for the formation of polycyclic aromatic hydrocarbons (PAH) and soot [8]. Due to the harmful effects of soot, the environment protection agencies in various countries have strictly implemented emission standards on soot to improve air quality and to avoid possible threats to human health and environment [9,10]. To develop the emission standards and to come up with innovative routes to minimize soot formation, it is imperative to understand the pathways of its formation, and the effects of feed conditions on soot emissions from fuels.

Several studies in the literature are focused on understanding the pathways of soot formation during fuel combustion, and their dependence on the type of fuel and the process conditions for combustion [11,12]. Soot formation consists of several steps, including the growth of small aromatics to PAHs, which are known as soot precursors, soot nucleation from PAHs, and its growth through agglomeration and chemical reactions including gas-phase species [13]. Soot can also undergo oxidation and fragmentation in flames [14,15]. Its formation during the combustion of aromatic fuels is important, as the fuel molecules provide some species such as cyclopentadienyl (C_5H_5) [16–18] and benzyl ($C_6H_5CH_2$) [17–19] that promote the formation and growth of PAHs in flames [20,21], and thus, support soot formation. Out of all the aromatic fuels, toluene has gathered significant attention in the literature [18,22–27] due to its presence in an appreciable quantity in transportation fuels (about 6 wt% in gasoline [28], 1–2 wt% in diesel [29] and 1–2 wt% in jet fuels [29]). It also forms an important part of their surrogates [3,30,31], and contributes to soot emissions from these transportation fuels. Some works related to the characterization of soot emitted from toluene flames are highlighted below.

In [32], soot particles collected from the flames of *n*-heptane, toluene, their mixture, and gasoline were analyzed. While soots from these fuels exhibited onion-like arrangements of fringes in

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their HRTEM images, the degree of order within each soot sample varied. Toluene soot appeared to be the most graphitic with large concentric shell of parallel PAHs and less disordered core. It is shown in earlier studies as well that soot characteristics such as its chemical constituents and the relative composition of crystalline and amorphous-like phases in soot are highly dependent on fuel type and the experimental conditions (e.g., temperature, fuel flow rate, pressure, equivalent ratio, and retention time) [33–37]. In general, the combustion of aliphatic fuels generates soot particles with a lower degree of graphitization than those from the combustion of aromatic fuels [38,39] due to faster carbonization in the post fuel-oxidation zone of aromatic flames [40,41]. In [42], the chemical characterization of soot particles emitted from hexane and diesel surrogate containing toluene was presented. It was found that the surrogate fuel produced much higher quantity of soot as compared to hexane due to its aromatic content, though the particles in hexane flame, on an average, were found to be larger than that from the surrogate fuel, possibly due to high temperatures that allowed soot particles to grow at a fast rate in hexane flame. In [43], the sooting properties of real fuels and their surrogates (such as toluene and *n*-heptane) were studied, and it was reported that, in order to meet the sooting tendencies of real fuels, surrogate fuels were required to have the appropriate amount of aromatics in them, as they have a good impact on amount of soot formed from real fuels. In [44], the sooting tendency of the surrogates for the aromatic fractions of diesel and gasoline (toluene, tetralin, trimethylbenzene, and butylbenzene) was studied. Though toluene was the smallest aromatic species among the fuels studied, it produced soot particles that were larger than those from butylbenzene and similar to those from trimethylbenzene (but, smaller than the particles from tetralin that is a two-ring species). In [45], the sooting tendencies of heptane and *n*-heptane/*n*-propylbenzene premixed flames were studied. It was shown that *n*-heptane/*n*-propylbenzene flame led to more condensed species on soot at lower flame heights that were responsible for higher soot mass in it as compared to heptane flame. Thus, even among aromatics, fuel structure plays an important role in their sooting tendencies. The physical properties of in-cylinder soot produced from the combustion of *n*-heptane and toluene/*n*-heptane mixture in a diesel engine were studied in [46]. Toluene/*n*-heptane soot exhibited more number of primary particles with larger size as compared to *n*-heptane soot. The differences in soot nanostructures such as the fringe length and interlayer spacing were also observed. In [47], the structures of soot formed from hexane and benzene flames were determined using UV spectroscopy. It was found that the fringes in benzene soot were more organized and curved than those present in hexane soot. Along with the type of fuel, the variation in soot properties with operating conditions such as fuel flow rate has also been discussed in the literature, as highlighted below.

In [48], the effect of the variation in fuel flow rate, temperature, and residence time on soot nanostructures was studied. For high fuel flow rate, low temperature, and low residence time, the presence of fullerenic nanostructures or curved PAHs were observed, whereas a low fuel flow rate, high temperature, and high residence time resulted in graphitic soot. In [49], the effect of fuel flow rate and temperature on the evolution of soot particles in diffusion flames was investigated. A higher fuel flow rate resulted in higher temperature in the soot inception region near the burner, but a lower temperature in the sooting zone due to radiative heat loss from soot. With increase in fuel flow rate, the amount of generated soot increased. The changes in temperature, diameter, and the number density of particles with increasing fuel flow rate were studied in [44], where it was observed that increasing flow rate gradually decreased the soot number density and increased the average soot aggregate size. Similar trends in soot parameters were observed in [50,51]. The effect of fuel flow rate on soot growth

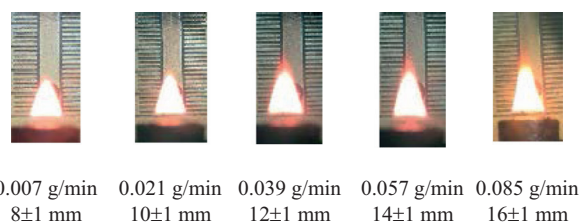


Fig. 1. Images of toluene flames with different flame vertical extents (mm) and fuel flow rates (g/min) that were used for soot collection.

and oxidation was studied in [52], where, at low flow rates, flames were non-sooting due to rampant soot oxidation. However, at high fuel flow rates, soot oxidation rate was greatly diminished due to the low concentration of O_2 molecules, and hence, soot particles were released from the flame tip.

While several investigations prove the dependence of experimental condition and fuel properties on soot emissions [48,53], the data related to the physico-chemical properties of soot from smoking aromatic flames remains limited in the literature. Along with fuel sooting tendencies, it is necessary to study the characteristics of soot particles generated from them, since the harmful effects and the reactivity towards oxygen of soot particles depend highly on their nanostructures and the elemental composition [54].

The aim of this study is to evaluate the effect of fuel flow rate on the nanostructures and the chemical constituents of soot formed from toluene in a diffusion flame. Toluene is selected for this study due to its presence in appreciable quantities in real fuels (specially, gasoline), and its high tendency to produce soot. A wick-fed burner will be used to collect soot particles from toluene flames at different fuel flow rates. The collected particles will be characterized using different techniques to understand the reasons behind the observed variation in the chemical composition and the nanostructural parameters of soot with varying fuel flow rate.

2. Experimental details

Soot particles were collected from the tip of diffusion flames of toluene at atmospheric pressure, using the smoke point apparatus. A description of this apparatus and soot collection technique are provided in [55]. This apparatus consists of a cylindrical fuel reservoir with a circular nozzle encompassing the wick, which is used to supply the fuel and to generate a diffusion flame. The fuel flow rate to the flame is varied by raising the wick exposure height above the nozzle through a screw mechanism (as a result, the vertical extent or height of the flame also increases). In the rest of the paper, the height of the flame has been referred to as the vertical extent of the flame, since the experimental data at different flame heights in the literature usually refer to the results from different vertical locations in a flame. However, in this paper, the results have been reported for flames of different heights produced with different fuel flow rates.

For soot collection from the tip of toluene flames, a filtration system consisting of a particulate filter holder (from Sierra Instruments, USA), a 70-mm borosilicate microfiber filter (TX40H120-WW, United Filtration Systems, USA), and a vacuum pump was used to allow the exhaust gas exiting the chimney of the smoke point apparatus to pass through the filter, where soot particles would be entrapped. This apparatus was chosen for this study on soot characteristics due to its capability of generating a stable flame that allows the collection of soot particles at various flame vertical extents above the smoke point of 7.5 mm by varying the fuel flow rate. Figure 1 provides the photographs of the flames with vertical extents of 8, 10, 12, 14 and 16 mm (with an uncertainty of 1 mm). The fuel flow rates are also provided. A higher fuel

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