



# Effect of fuel flow rate on the characteristics of soot generated from unsubstituted and disubstituted aromatic hydrocarbon flames: Experimental and numerical study

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## ARTICLE INFO

### Article history:

Received 16 August 2017

Revised 18 September 2017

Accepted 11 December 2017

### Keywords:

Soot  
Nanostructures  
Benzene  
*m*-Xylene  
HRTEM  
XRD  
EELS

## ABSTRACT

Aromatic hydrocarbons in liquid transportation fuels help in suppressing auto-ignition and knocking tendency in engines, but are toxic and can generate polycyclic aromatic hydrocarbons (PAHs) and soot during combustion that are harmful for human health and the environment. Benzene, toluene, and xylenes are present in noticeable quantities in liquid fuels. This paper reports the sooting propensity of benzene and *m*-xylene, and the role of substituted aliphatic chains on soot emissions at different fuel flow rates along with their effects on soot characteristics. Soot particles collected from the aromatic diffusion flames at different fuel flow rates are characterized using high resolution transmission electron microscopy and X-ray diffraction to examine their nanostructural changes, and using, electron energy loss spectroscopy, Raman spectroscopy, and elemental analysis to determine their chemical properties. With increasing fuel flow rates in benzene and *m*-xylene flames, the size of the primary particles in soot increased, but that of PAHs reduced. The chemical changes introduced by increasing fuel flow rates in both the diffusion flames were the reduction in the concentrations of oxygen and hydrogen content. Though aliphatics are less sooting than aromatics, the presence of methyl groups on the aromatic ring in *m*-xylene not only increased the soot production rate, but also led to soot particles with less hydrogen content than those from benzene flames. Soot modeling studies are conducted to study the sooting behaviors of benzene and *m*-xylene fuels. The results from benzene and *m*-xylene flames suggest that increasing the rate of fuel consumption (which happens while increasing engine load) can significantly affect the physicochemical properties of soot from the same fuel.

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## 1. Introduction

Aromatic hydrocarbons are present in conventional liquid fuels such as diesel [1,2], gasoline [3], and jet fuels [4–6]. They are often used as fuel additives due to their advantageous properties such as suppressing auto-ignition to reduce the tendency of engine knock [7–10]. A drawback of their presence in the transportation fuels is the emission of harmful polycyclic aromatic hydrocarbons (PAHs) and soot particles to the atmosphere, when the fuel is burnt [11–13]. Several studies have focused on aromatic fuel combustion to explore their effects on soot emission and find ways to reduce soot formation from them [11,14–16]. These studies indicate that the high sooting tendency of aromatic hydrocarbons is mainly be-

cause of the mono-aromatic rings that may stay intact during fuel oxidation, and provide a base to form PAHs and soot [14,16–18].

The fuel molecular structure plays an important role in soot production, and the changes in the molecular structure around an aromatic ring in a fuel lead to changes in their sooting tendency [19]. In a methane flame doped with 400 ppm of mono alkyl aromatic hydrocarbons, McEnally and Pfeifferle [20] observed that increasing the length of the alkyl chain increased the fuel sooting tendency. The same trend was found in [11]. In [21], the addition of up to 5% *m*-xylene to an ethylene flame led to a significant increase in soot volume fraction and the amount of aromatics in flames. Some recent studies have also focused on the effect of the position of methyl groups bonded to a mono aromatic ring on the sooting tendency [11,22,23]. The neighboring methyl groups on the aromatic ring make the formation of soot precursors easier, which favor soot formation [24]. When the methyl groups are not adjacent, the mono aromatic ring is more stable, and the

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formation of PAHs and soot is slightly reduced [11]. Recently, the effects of methyl group on the fuel sooting propensity and on the nanostructure of combustion-generated soot were explored in aromatic diffusion flames of benzene, toluene, and *m*-xylene in our previous study [25]. Soot particles generated from the flames of these fuels at the same fuel flow rate in a smoke point apparatus were collected. It was found that, while the smoke point of benzene, toluene and *m*-xylene appeared close to each other, the remarkable differences in their threshold sooting indices (TSI) were observed. The TSI values increased with increasing number of methyl group on the monoaromatic ring, indicating that the presence of methyl group enhances soot formation. The primary particle size and the PAH length were found to reduce, while the randomness in the orientations of their PAHs increased with increasing number of methyl group on the aromatic ring. In general, soots from the flames of fuels with methyl groups had lower oxidative reactivity and less amount of oxygenated groups as compared to benzene soot. For the further insight on soot formation from aromatic fuels, the effects of flame temperature, residence time, equivalent ratio, fuel flow rate, and fuel structures are also studied in the literature [26–31]. Some works on the sooting tendency and the characterization of soot produced during aromatic fuel combustion are emphasized below.

In [28], the effect of temperature in benzene flames was studied. It was found that the low temperatures increased the amount of condensates on soot that increased their mass. In [32], the effect of residence time on soot formation in aromatic flames was investigated. Increasing the residence time in a flame enhanced soot nucleation and growth rates to form large-sized particles. In [33], an increase in the equivalence ratio in a benzene flame enhanced soot precursor formation to lead to high soot emissions [34,35]. A similar result of accelerated soot nucleation and growth was observed in Echavarria et al. [36], when an ethylene flame was doped with benzene. Botero et al. investigated the sooting tendency of aliphatic and aromatic hydrocarbons including paraffinic hydrocarbons and their isomers in [37], mono-, di-, and tri-substituted aromatic hydrocarbon constituents of diesel and gasoline in [31], and different heptane/toluene blends in [38]. The results revealed that the combustion of cyclic hydrocarbons produced particles with larger diameters as compared to straight-chain alkanes [37]. The mono-substituted aromatic hydrocarbons with large aliphatic chains produced particles of lower size as compared to toluene and 1,2,4-trimethylbenzene, while the mono- and di-substituted aromatic flames generated soots of similar particle size. In [39], by studying soot formation in the diffusion flames of ethylene with alkyl aromatics, it was found that the aromatics with branched chains containing one carbon atom only (toluene, xylenes, and trimethylbenzene) had similar sooting tendencies, but the aromatics with aliphatic chains having two or more carbons had significantly high sooting tendency.

Along with the effect of aromatic fuels on the size of soot particles, their chemical and nanostructural properties have also been studied widely. For example, Velásquez et al. [12] conducted the chemical characterization of soot particles emitted from hexane and diesel-surrogate (containing aromatics) flames. The aliphatic flame supported the formation of tar on soot surface, but the soots from the surrogate flame did not have much of such material. The carbonization (dehydrogenation) of soot particles during the combustion of the fuel containing aromatics was also observed, which was also proposed in [40]. In [41], the effect of increasing oxygen content in a benzene flame on soot nanostructure was investigated using HRTEM images. The flame with high oxygen content produced soot with shorter fringe lengths (indicative of PAHs in soot) and with higher tortuosity than the particles from the flame with low oxygen content. In [42], with increasing aromatic content in

the fuel, soot production increased, but the fringe lengths in them decreased.

For a given fuel, the change in the fuel flow rate in a flame can also affect soot properties. In [31,37,38], the effect of varying fuel flow rate on flame temperature and on soot formation was studied. With increasing fuel flow rate, the temperature near the flame tip and soot particle number density reduced, while the amount of soot produced and the soot aggregate size increased. The increase in the amount of soot with increasing fuel flow rate was due to the lack of oxygen in the flame to oxidize soot particles before they escape from the flame tip [43]. The increased aggregate size and reduced number density were a result of increased coagulation of particles at low temperatures. The change in the fuel flow rate may also affect the physicochemical features of soot particles, which was studied in our previous investigation [44] for a toluene diffusion flame. In that study, a smoke point apparatus was used to generate a diffusion flame of toluene, and the flow rate of the fuel to the flame was increased by adjusting the exposed length of the wick. It was shown that, with increasing fuel flow rate in a toluene flame, the larger soot aggregates and primary particles were formed due to the lack of oxygen in the sooting zone to oxidize soot particles. Moreover, the PAH length reduced and the randomness in the orientations of their PAHs slightly increased due to the temperature drop in the sooting zone that are not sufficiently high to allow the rearrangement of PAHs in soot and due to a longer residence time of soot particles in the flame to allow PAH condensation. Interestingly, the concentration of aliphatic and oxygenated groups on soot decreased and aromatic content increased with increasing fuel flow rate indicating that for a given fuel, its flow rate can affect the chemical properties of the generated soot particles. However, such studies need to be conducted for different fuels to ascertain that fuel flow rates can substantially affect their characteristics.

As pointed out above, several investigations report the dependence of the amount of soot produced and the particle size on the experimental conditions and the fuel properties [26,45,46] using aliphatic-aromatic mixtures as fuels. However, the information associated with the physicochemical properties of soots from the flames of unsubstituted/substituted aromatics, which are responsible for most of soot produced from transportation fuels, is scarce. It is important to study the characteristics of soot particles along with the sooting tendency of fuels, since the oxidative reactivity of soot particles strongly depend upon their morphology and the chemical composition [47,48], which, in turn, affect the regeneration rate of particulate filters that are used to collect them from engine exhaust. Moreover, the nanostructural properties of soot particles can also reveal some information about their formation process that is less-understood.

The aim of this investigation is to examine the effect of fuel flow rate on the variation in the nanostructures and the chemical characteristics of soot particles from benzene and *m*-xylene diffusion flames. These aromatic hydrocarbons have been selected in this study as model fuels to represent unsubstituted and disubstituted aromatics due to their presence in appreciable concentrations in liquid transportation fuels [49–51] along with toluene, which is studied in [44]. Moreover, xylenes form an important part of the jet fuel surrogate [52,53]. Due to these reasons, different properties of benzene and xylene flames (e.g., flame propagation and extinction, determination of species profiles, and reaction mechanism and model development) have been explored in the literature [23,33,54–58]. Though three isomers of xylene (*o*-, *m*-, and *p*-xylenes) are present in fossil fuels, *m*-xylene was chosen for this study due to its high concentration in fossil fuels [59] and the longest ignition delay time [7,60] among the three isomers that lets it survive during fuel oxidation to contribute to PAH and soot formation [61,62].

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