Full Length Article

Size evolution of soot particles from gasoline and n-heptane/toluene blend in a burner stabilized stagnation flame

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HIGHLIGHTS

- Soot particle size evolution of gasoline in a premixed flame was investigated.
- Size distribution of gasoline and heptane/toluene blend was qualitatively similar.
- Gasoline's sooting features more persistent nucleation and much faster growth rate.

ARTICLE INFO

ABSTRACT

The evolution of soot particle size distribution function (PSDF) in premixed flames of gasoline (34% aromatics by volume) and a n-heptane/toluene blend (66% n-heptane/34% toluene by volume) was investigated in the burner stabilized stagnation (BSS) flame configuration, using the micro-orifice probe sampling and scanning mobility particle sizer (SMPS). The aim of this study is to illustrate the similarities and differences of sooting propensity between the real fuel and the simple hydrocarbon blend in premixed flame conditions. The mole ratio of carbon to oxygen (C/O) in the unburned gas was kept constant at 0.6 and similar maximum flame temperatures and temperature-time histories were kept between the two cases, so that we could focus on the fuel composition effects on sooting propensity. In addition, the size distribution, the total number density, and the volume fraction of soot were also compared to those previously measured for ethylene and propene flames under comparable conditions. It was observed that the particle size distributions of both gasoline and heptane/toluene flames evolve from the unimodal distribution (nucleation mode only) to the bimodal (both nucleation and coagulation mode) distribution. Compared to the heptane/toluene blend, the soot formation in gasoline flame features more persistent nucleation and much faster growth rate.

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1. Introduction

It is well known that soot emissions from fossil fuel combustion may jeopardize the environment and human health. During the combustion processes, soot formation may be influenced by the flame temperature, carbon/oxygen ratio (or equivalence ratio), fuel molecular structure and so on. Over the past decades, significant progress of the soot formation mechanism has been obtained, and most experimental and modeling work were based on small molecular hydrocarbons such as ethylene [1–9]. Recently, attentions have been shifted to C4 or larger hydrocarbons to explore the fuel effects on soot formation [10–18]. These studies indicated

that the change of fuel molecular structure and composition led to the change in sooting propensity.

Over the past several years, gasoline direct injection (GDI) engines are gaining increased market share due to their improved fuel efficiency. One of the major disadvantages of GDI engines is the high soot emissions. Soot formation from GDI engines originates from the in-cylinder combustion processes, so understanding the soot formation mechanism in gasoline combustion is important.

For the real fuels such as gasoline, it is difficult to study its soot formation mechanism due to the complex fuel composition. With increased understanding in the sooting propensity of C4+ hydrocarbons and their mixtures, it is important to find out the similarities and the differences between the real fuels and simple hydrocarbon mixtures in the matter of sooting process. Witkowski et al. observed in a laminar co-flow methane flame that the soot volume fraction (SVF) of the flame with a toluene reference fuel (TRF) (20% n-heptane/50% iso-octane/30% toluene by volume)

Nomenclature

D_m	particle diameter [nm]
$<D_m>$	median mobility diameter [nm]
F_v	soot volume fraction
H	height above burner surface [cm]
H_p	plate to burner separations [cm]
$H_{p,max}$	largest separation from plate to burner [cm]
i	i = 1, nucleation mode; i = 2, coagulation mode
k_B	Boltzmann constant
N	number density of soot particles [cm^{-3}]
N_g	number density of gas molecules
t	particle residence time [ms]
t′	modified particle residence time [ms]
T	flame temperature [K]
T_m	maximum flame temperature [K]
T_s	stagnation surface temperature [K]
v_0	unburned gas velocity [cm/s]
v_c	convective velocity
v_T	thermophoretic velocity
x_s	defined as (H_p − 0.1) [cm]
x_{T_m}	distance from burner surface to the peak flame temperature position

Greek symbols

Φ	equivalence ratio
λ	thermal conductivity
φ	momentum accommodation factor
σ_g	geometric standard deviation

Abbreviation

BSS	burner stabilized stagnation
C/O	mole ratio of carbon to oxygen
CPC	Condensation Particle Counter
DMA	Differential Mobility Analyzer
EC	Electrostatic Classifier
G	gasoline
GDI	gasoline direct injection
HT	heptane/toluene blend
PSDF	particle size distribution function
SMPS	scanning mobility particle sizer
SVF	soot volume fraction

was almost the same as that with simpler fuel mixture (70% n-heptane/30% toluene, by volume), and both soot volume fraction were just slightly lower than that of the flame of gasoline (28% aromatics by volume) [19]. Lemaire et al. [20] observed in turbulent diffusion flames that SVF measured using the laser-induced incandescence was in a very good agreement between the commercial gasoline and the surrogate proposed by Lenhert et al. [21] (a fuel mixture of 1-pentene, toluene, n-heptane and iso-octane). Botero et al. compared the soot formation of a commercial gasoline (44% aromatics by mass) with the binary mixtures of n-heptane and toluene in a wick-fed diffusion flame. They found that both the smoke point and the particle size distribution function (PSDF) of gasoline were similar with those of the mixture with 50% n-heptane/50% toluene by volume, but the mean aggregate mobility size, the number of particles and the primary particle size formed by the gasoline were smaller [22].

The above mentioned research progresses regarding the sooting propensity of different fuels are in the non-premixed flames. In premixed flames, Abid et al. observed that the PSDF of n-dodecane premixed flame was similar with that in the ethylene flame under comparable conditions, but the nucleation mode was stronger [10]. Ciajolo et al. detected an earlier soot inception in the sooting premixed cyclohexane flame with respect to that in the n-hexane flame [11]. Echavarria et al. doped benzene into premixed ethylene flame and found that the growth of nucleation and agglomeration-sized particles was faster than that in the pure ethylene flame [15]. Camacho et al. measured the PSDF of n-butane, i-butane, n-butanol, and i-butanol in premixed flames and the results showed that the onset of soot nucleation of branched fuels was faster compared with the straight-chain counterparts [16]. Although some progresses have been made, studies on real fuel sooting propensity were still scarce in premixed flame conditions, and this study filled this gap.

In this study, soot formation characteristics of gasoline and a blend of n-heptane and toluene were measured and compared in laminar premixed flames, in which carbon to oxygen ratio (C/O) and flame temperature were well controlled to explore the similarities and differences of sooting behaviors between the real fuel and simple hydrocarbon blend. N-heptane and toluene were selected because they form the simplest binary mixture for sooting propen-sity comparison with gasoline. Also, the combustion properties of both fuels have been widely studied in the literature. A burner stabilized stagnation (BSS) flame configuration coupling with micro-orifice probe sampling technique was applied. To a large extent, this method could avoid intrusiveness to flame as in the traditional probe sampling methods [23].

2. Experimental and computational method

The experimental and computational methods are similar to the authors' previous studies [8,24], except for those related to the change of fuel. Since the test fuels in this study are in liquid phase at room temperature, the fuel injection and vaporization systems were added. Besides, the reaction kinetic model used was extended. Detailed experimental and computational methods are as followed.

Fig. 1 schematically shows the experimental setup. The flame burner was composed of a bronze porous plug of 5 cm in diameter, and a concentric porous ring. Premixed atmospheric fuel/oxygen/nitrogen flowed into the plug, and a shroud nitrogen flowed through the ring to isolate the flame from the ambient air. A water-cooled aluminum alloy plate served as a surface for flow stagnation and sampling, and the BSS flame formed between the burner and the stagnation plate. More details about the BSS flame configuration could be found in [23,25]. Liquid fuel flow rate was controlled by a syringe pump (Harvard PHD 2000 Series, syringe pumps of this series have ±0.35% relative accuracy). The liquid fuel broke up into droplets through a nebulizer (Precision Glassblowing, Glass Concentric Nebs). The upstream gauge pressure for the carrier gas of nebulizer was 199.26 kPa (28.9 PSI), corresponding to nitrogen flow of 0.68 L/min (STP condition, 298 K and 1 atm) at the outlet of the nebulizer. The fuel droplets were mixed with the preheated oxygen/nitrogen flow and were vaporized in the heated gas tubes. The burner was not cooled as in previous studies [8,24]. Temperature of the reactant gas tubes and the burner was maintained at 190 °C to prevent fuel vapor condensation. No residual fuel was observed inside the reactant delivery system. The volume flow rate of oxygen and nitrogen used was metered by the critical orifices and the relative error is below 1%.