Mobility size distributions of soot in premixed propene flames

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ABSTRACT

The evolution of mobility particle size distribution function (PSDF) for premixed propene flame soot was investigated in the burner stabilized stagnation (BSS) flame configuration. The measurements were carried out for two series of flames with the equivalence ratio equal to 1.8 and 2.07, as a function of the burner-to-stagnation surface separation distance. The flame temperature was varied from 1820 to 1940 K in each series to examine flame temperature effects on the measured PSDF in a systematic manner. Measurements were compared to those determined previously for ethylene flames. Qualitatively, bimodal PSDFs were observed in all propene flames. Like the ethylene flames studied previously, the mobility diameter at the trough of the bimodal distribution and the median mobility diameter of the large size lognormal mode both shift towards smaller particle size as the flame temperature increases. Quantitatively, soot nucleates and grows in propene flames earlier and faster than in ethylene flames under comparable conditions. In particular, the propene flames produce a substantially higher number of soot nuclei than in the ethylene flames. The observations made for the propene flames and the comparison with ethylene flames strongly indicate that detailed soot formation processes, such as the PSDF, can be extremely sensitive to parent fuel structure in premixed flames.

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1. Introduction

It is traditionally understood that under comparable conditions the parent fuel structure has a weak influence on soot production in laminar, premixed flames [1–3]. Comparable conditions mean that the initial C/H/O ratio is the same and temperature-time history during growth is similar. Under the fuel-rich condition, the fuel decomposes and/or is oxidized in the main flame zone and the composition of the dominant species in the post-flame region is largely governed by chemical equilibrium. The amount of soot produced should be dependent largely on the post-flame temperature and only weakly impacted by the fuel structure since soot nucleates and grows in the post-flame region of the premixed flame. Indeed, a previous study [4] showed that the evolution of PSDF and mobility volume fraction are not drastically different in premixed *n*-dodecane and ethylene flames with the same equivalence ratio and similar flame temperature. More recent studies suggest

that this lack of sensitivity to fuel structure is not a universal phenomenon. For example, *n*-butane and *i*-butane were reported to have different rates of soot nucleation and mass/size growth; and similar observations have been made comparing soot production in *n*-butanol and *i*-butanol flames [5]. Meanwhile, abundant observations have been made for the sensitivity of soot production to fuel structure in counterflow and coflow diffusion flames and shock tubes (see, e.g., [2, 6–18]).

In the present work, measurements for the evolution of detailed soot particle size distribution function (PSDF) in two series of propene flames were carried out in the burner-stabilized stagnation flame (BSSF) configuration. Measurements were made under conditions that overlap with those of ethylene flames reported earlier [19,20] thus enabling direct comparisons of the detailed properties and kinetics of soot during its nucleation and growth processes. The primary focus of the work is to demonstrate the strong sensitivity of detailed sooting processes to the parent fuel structure in premixed flame.

Ethylene has been used as a model fuel for soot formation studies not only because it is relatively easy to handle, but also because ethylene is a key intermediate of fuel decomposition in flames for a wide range of hydrocarbon molecules. The evolution of soot PSDF in premixed ethylene flames has been studied quite extensively through probe sampling coupled with mobility sizing in the BSSF
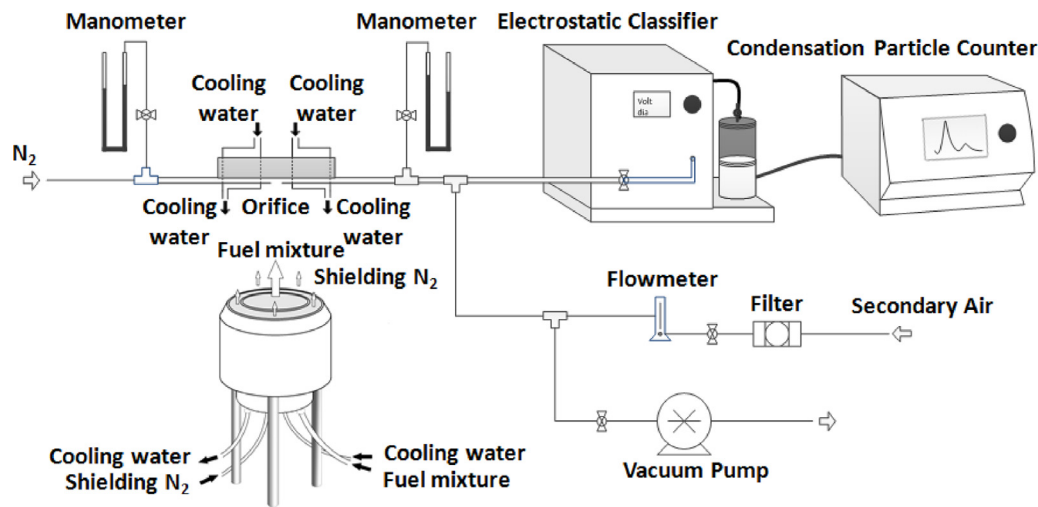

Fig. 1. Schematic of experimental setup.

Table 1
Summary of the two series of propene flames studied.

Flame	Cold gas velocity, v_0 (cm/s)[a]	Maximum temperature, T_m (K)[b]	Sheath velocity, (cm/s)[a]	Burner surface temperature, T_0 (K)[b]	Stagnation surface temperature, T_s (K)[b]	Largest separation, $H_{p,\max}$ (cm)
		M-Series: 11.4 mol% C_3H_6–28.6 mol% O_2–N_2 ($\phi = 1.8$)				
M1	3.2	1829 ± 79	13.3	439 ± 20	404 ± 10	1.4
M2	3.9	1887 ± 84	14.4	450 ± 20	400 ± 10	1.4
M3	4.7	1939 ± 89	15.5	447 ± 20	400 ± 10	1.4
		N-Series: 12.6 mol% C_3H_6–27.4 mol% O_2–Ar ($\phi = 2.07$)				
N1	3.75	1856 ± 88	13.3	450 ± 35	403 ± 10	1.0
N2	4.0	1888 ± 91	14.4	448 ± 20	405 ± 10	1.0
N3	4.5	1908 ± 92	15.5	480 ± 20	405 ± 10	1.0
N4	5.0	1945 ± 96	17.7	515 ± 20	402 ± 10	1.0

[a] STP condition (298 K and 1 atm).
[b] Measured for the largest separation of the burner-to-stagnation surface ($H_{p,\max}$) for each series of flames.

[19–31]. The experimental studies have shown that PSDF bimodality and persistent nucleation are ubiquitous features of soot size distributions. The onset of nucleation, nucleation rate, size/mass growth rate and mobility volume fraction are heavily dependent on the flame temperature and equivalence ratio (C/H/O). Models of soot formation have also undergone intense development which has been facilitated by these measurements [32–37].

Propene is another important intermediate in flames burning liquid hydrocarbons (see, e.g., [38–40]) but experimental observations of soot PSDF are scarce. Here, detailed PSDF measurements made for two series of propene flames fill this gap. Each series of the flame span a range of maximum flame temperature. The measurements were made with well-defined boundary conditions so as to enable numerical simulations with well-defined flame boundary conditions. This constitutes the second objective of the present study as the data to be reported here is expected to be useful for testing models of soot formation.

2. Experimental and computational method

The experimental setup, shown schematically in Fig. 1, has been described in detail elsewhere [19,20]. Measurements of mobility PSDF of soot were carried out within the BSSF configuration, wherein the probe may be treated as the downstream boundary condition. Soot models assume a non-slip downstream boundary condition and this introduces the need to shift the computed PSDF slightly upstream to account for the finite flow into the probe during sampling [20,41]. As discussed previously [20], the method used herein is highly reproducible across different facilities utiliz-

ing McKenna-type burners and sampling probes if a set of standard flame characterization and calibration procedures are employed.

Flames were isolated from the ambient air by a flow of sheath nitrogen. A soot sample was drawn into the sampling orifice 130 μm in diameter and immediately diluted by a flow of cold nitrogen (30 L/min, STP) to minimize coagulation and diffusion losses in the sampling lines. A fraction of the diluted sample (1.5 L/min, STP) was analyzed by a TSI Scanning Mobility Particle Sizer (SMPS) consisting of a 3085 nano-Differential Mobility Analyzer (DMA), a Kr-85 Neutralizer and a 3776 ultrafine Condensation Particle Counter (CPC). Similar to previous studies [4,5,19–29, 32], the mobility diameter was corrected based on the nanoparticle transport theory because particle size smaller than 10 nm can be overestimated by the Cunningham slip correction [42–44].

Previous studies have shown that the evolution of PSDF of soot is highly sensitive to the flame temperature [19,20,27]. As such, it is essential that the temperature profile be made available for model comparison. In the current study, temperature was measured by a type-S fine wire thermocouple coated with an Y/Be/O ceramic mixture to prevent catalytic reactions on its surface [45]. Radiation correction was carried out using the Shaddix procedure [46]. In making the radiation correction, the local transport and flow property values were calculated by a modified OPPDIF code [47] with USC Mech II [48]. The burner surface temperature, T_0, was extrapolated from the linear region of the temperature profile measured close to the burner surface [19,20]. The stagnation surface temperature, T_s, was directly measured by a K-type thermocouple embedded in the stagnation plate. As in previous studies [5,19,20,26], the radiation corrected temperature was assumed to be the average of the two temperature values corresponding to the