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Study on inversion of morphological parameters of soot aggregates in hydrocarbon flames

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ABSTRACT

This study proposes an effective inversion method to detect the morphological characteristics of soot aggregates in hydrocarbon flames. Firstly, the imaging method is used to measure the distribution of soot aggregates absorption coefficients in flames. Then, the primary particle diameter, primary particle number and volume fraction of soot aggregates are retrieved from the detected absorption coefficients using the particle swarm optimization algorithm. Meanwhile, the thermophoretic sampling particle diagnostic-transmission electron microscopy (TSPD-TEM) technique and the generalized multi-particle Mie-solution theory is employed to verify the absorption coefficients detected by the imaging method and the retrieved morphological parameters of soot aggregates by the proposed inversion technique. The comparison results reveal a deviation below 30% in absorption coefficients between obtained by the imaging method and the TSPD-TEM analysis combined with the generalized multi-particle Mie-solution theory. And the morphological parameters of soot aggregates retrieved using the inversion method are in good agreement with that obtained by the TSPD-TEM technique, which suggests that the inversion method is robust and can accurately retrieve the morphological parameters. Finally the distributions of primary particle diameter, primary particle number and volume fraction in flames for two different cases are presented, and effect of combustion condition and soot formation mechanism on the distribution rules of these morphological parameters is discussed. The proposed inversion method can provide detailed morphological information about soot aggregates for a deeper understanding and control of soot formation.

1. Introduction

A deeper understanding of soot formation in flames is directly motivated by radiative heat transfer accurate analysis, reduction of PM (particulate matter) emission, and combustion efficiency improvement. Flame-generated soot is a complex fractal-like aggregate formed by the aggregation of nearly identical spherical primary soot particles [1–3]. There is a general consensus that soot formation experiences four main processes: soot nucleation (inception), particle surface growth, particle agglomeration, and particle oxidation [4–8]. But a better understanding concerning the primary mechanisms in soot formation, growth, and oxidation is still required [7,9–11]. Detailed information on the morphological characteristics of soot aggregates is one interesting approach to reveal the primary mechanisms in soot formation processes. This requires suitable soot detection techniques.

In recent years, several detection techniques have been developed to identify the morphological characteristics of soot in flames. Optical detection techniques based on flame emission spectrum have been widely used because of their non-intrusiveness and relatively less cost [12–16]. The emission techniques transfer the radiative emission by flames into concentration and morphology information about the flame species such as combustion gases and soot. One of the most typical emission techniques is the imaging method applied to the measurement of soot temperature and concentration distributions in a diffusive flame [14,17]. Recently, researchers have made full use of the wide range of spectrally resolved data of the flame in order to obtain more detailed information on soot. The multi-wavelength emission techniques have been developed by De Iuliis et al. [18] and Snelling et al. [12] to measure the temperature and soot volume fraction in flames and explore the effects of refractive index on the measured results. Ni et al. [16] reconstructed the 3-D distributions of soot temperature and volume fraction using a multi-wavelength method. Since laser-induced incandescence (LII) was suggested by Melton as a soot diagnostics technique, it has been developed into a powerful tool for the measurement of soot volume fraction in flames [19–21].

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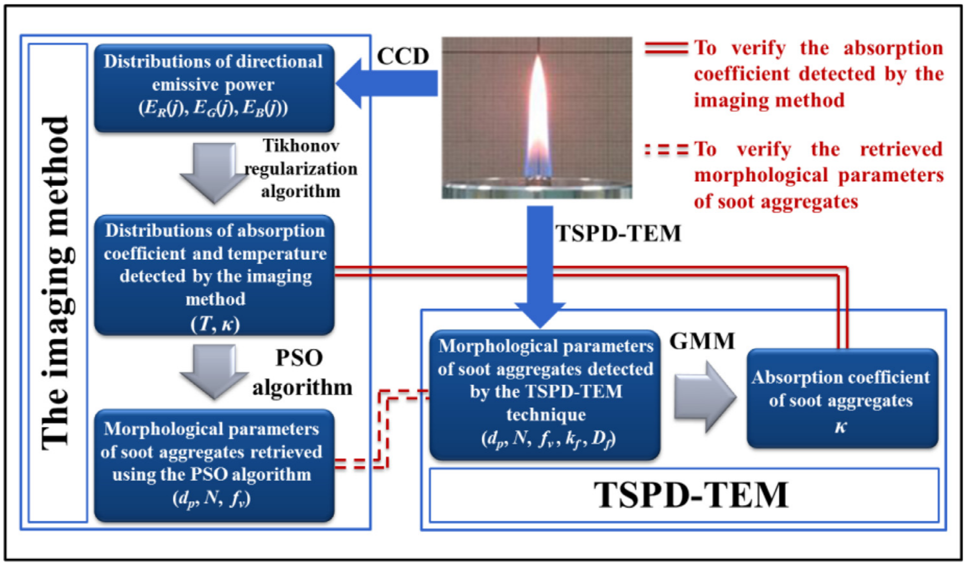

Fig. 1. Research framework of this study.

Furthermore, Will et al. [22–24] and Roth et al. [25–28] made significant advances in establishing relations between time-resolved signals and soot particle diameter, which was usually referred to as time-resolved LII (TiRe-LII) in numerous studies to determine the primary particle sizes of soot aggregates [28–31]. Additionally, the coupling of LII with laser light scattering allows for more detailed information about aggregate properties (such as particle volume fraction, particle and aggregate sizes, and fractal properties) [31–34]. Sorensen provided a recipe of how aggregate morphological distribution information in flame can be derived from relative multi-angle scattering intensities [35]. Nevertheless, Link et al. [36] investigated the capability of the multi-angle light scattering method, suggested the combination of the absolute multi-angle scattering method and LII as a future powerful technique to evaluate the morphological and fractal parameters of nanoparticle. In comparison, the contact soot detection techniques such as the thermocouple particle densitometry (TPD) technique [37] and the thermophoretic sampling particle diagnostic (TSPD) technique [38] have generally been treated as a useful supplement or calibration tool for other soot diagnostic techniques. Because they can simultaneously characterize the local concentration and morphology of soot, and can be applied to a wide range of conditions with relatively less restrictions, but cannot achieve high temporal and spatial resolutions. Several efforts have been devoted to providing detailed information on the morphological characteristics of soot aggregates in flames, however, little attention has been paid to the promotion of flame emission technique for the morphological distribution detection of soot aggregate. In this study, we try to develop a flame emission technique, which has the promise of being simpler and cheaper than laser based techniques, to detect the distributions of primary particle diameter, primary particle number and volume fraction of soot aggregates in flames.

In the present study, an inversion of soot aggregates morphological parameters in C_2H_4/air flames from absorption coefficients detected by the imaging method using the particle swarm optimization (PSO) algorithm is experimentally studied. Figure 1 shows the research framework of this study. Firstly, the absorption coefficients distribution of soot aggregates in flames will be detected by the imaging method. To verify the reliability of the absorption coefficients detected by the imaging method, the TSPD-TEM technique is employed to obtain the morphological parameters (primary particle diameter, primary particle number, and volume fraction) of soot aggregates at different axial heights above the burner, and then the absorption coefficients are calculated by the generalized multi-particle Mie-solution (GMM) theory. The comparison of the absorption coefficients retrieved by the imaging method and obtained by the TSPD-TEM analysis combined with the GMM theory is carried out. After the validation of the accuracy of absorption coefficients, the PSO algorithm is utilized to inverse the primary particle diameter, primary particle number and volume fraction of soot aggregates. And the inversion method is validated to be feasible by comparing the results of morphological parameters inversed using the PSO algorithm and obtained by the TSPD-TEM technique. Finally, the distributions of the morphological parameters of soot aggregates in flames can be obtained, moreover, the effect of combustion condition and soot formation mechanism on the distribution rules of these parameters is discussed.

2. Experiment

2.1. Ethylene diffusion flame

The axisymmetric laminar C_2H_4/air diffusion flame was generated on a flame burner manufactured by National Research Council (Canada) [12]. Its fuel nozzle is a stainless steel pipe of 10.9 mm inner diameter, and the air flows through 100-mm-inner-diameter packed beds of glass beads and porous metal foam to maintain the stability of the flame. The fuel (ethylene) and oxidizer (air and oxygen) flow rates were 194 mL/min and 120 L/min, respectively. The oxidizer was composed of air and oxygen, 30% and 40% of oxygen concentrations in the oxidizer were used to illustrate the versatility of the present inversion method, additionally, investigate the effect of oxygen addition to the air on the morphological characteristics of soot. The detailed experimental conditions are summarized in Table 1. The flames were imaged by a Manta G-504 camera with a Sony ICX655 Charge Coupled Device (CCD) sensor

Table 1
Experimental condition of axisymmetric laminar C_2H_4/air diffusion flames.

Case	C_2H_4 flow rate (mL/min)	Air flow rate (L/min)	O_2 flow rate (L/min)
30% O_2–air	194.0	106.3	13.7
40% O_2–air	194.0	91.1	28.9