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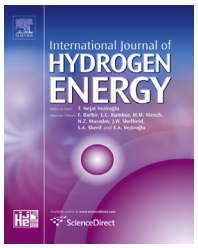

The effects of hydrogen addition on soot particle size distribution functions in laminar premixed flame

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ABSTRACT

The effects of hydrogen addition on soot formation in C_2H_2/air premixed flame was investigated by numerical simulation. In order to clarify the influence of hydrogen addition on soot formation and oxidation, three different contents (0%, 20% and 40%) of hydrogen addition were performed respectively. A Monte-Carlo stochastic method was used to solve the particles dynamical model, which including particle inception, coagulation and surface reaction. Particle size distribution functions (PSDF) in different height above the burner (HAB) were obtained with different amounts of hydrogen addition into C_2H_2/air flame. The results showed that mole concentrations of important soot precursor species, such as C_2H_2 and PAHs, are inhibited by the addition of hydrogen. Thereby, the soot volume fraction was reduced. Meanwhile, the number of maximum particles was reduced when hydrogen added to the flame. Hydrogen is an effectively additive in reducing soot formation.

Introduction

Soot and other gaseous pollutant emissions which result from hydrocarbon fuels have been a big challenge for a long time. Many researchers have been investigating the soot formation process of some practical fuels in the past several years, such as natural gas, gasoline, kerosene and diesel et al. [1–5]. Because of the complexity of soot formation, the development of reliable and effective soot model is still one of the most challenging subjects in combustion science. The addition of H_2, CO and other gases to a hydrocarbon flame is researched by many scientists for a better combustion process [6,7]. It can improve the combustion efficiency and reduce the pollutant emission, such as CO_2, NOx, and soot particles. Zhao H [8] found that gasoline blended with hydrogen can effectively reduce the soot emission in a direct injection spark ignition engine. It revealed that addition of hydrogen results in a significant change in the compressibility of the fuel mixture and could alter the chemical species concentration during the combustion. El-Ghafour [9] experimentally investigated the combustion characteristics of hydrogen blending into natural

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gas fuel in a free jet turbulent diffusion flame when flowing into a slow co-flowing air stream. Results showed that hydrogen addition improved the flame stability and also reduced the flame length. Kumar and Mishra [10] investigated the effect of hydrogen addition to LPG on soot free length fraction (SFLF) in a jet diffusion flame, and found that the SFLF increases as H_2 added to the fuel stream. The addition of H_2 also considered under an experimental method by Shirk MG et al. [11] with diesel as fuel. Fengshan Liu [12] compared the effects of H_2 and helium addition to fuel on soot formation in atmospheric axis symmetric co-flow laminar methane/air diffusion flame. They found that helium addition is more effective than H_2 addition in reducing soot formation through experiment and numerical research. In their research, the different chemical effects by the H_2 addition to ethylene and methane on soot formation are explained. These investigations obtained exciting results that soot emission can be substantially reduced in most engine operating conditions with H_2 addition. It revealed that the addition of H_2 not only affected the gaseous species concentration but also changed some important combustion characteristics, such as flame temperature, swirl strength, and compressibility of the fuel mixture [13,14].

However, most of the previous studies only focus on the effects of H_2 addition on the total amounts of soot particles and give less attention on the particle size distribution functions (PSDF). Recent studies have shown that PSDF is important because particle toxicity, which strongly depends on particle number more than mass concentration, typically increases when particle size decreases [15,16]. Meanwhile, new traffic laws in many countries not only limited the soot mass but also had an limitation on particles quantity and diameter. Therefore, the study of the effects of hydrogen added to fuels on the particle size distribution is necessary.

Soot formation is an extremely complex physical–chemical process and the laminar premixed flames generally served as a reliable platform to study soot evolution. A completed soot formation process includes soot precursor formation, particle inception, coagulation and surface growth. As an effective additive to reduce soot formation in hydrocarbon fuels, H_2, gained more and more attentions by many researchers. However, the effects of H_2 as an additive to hydrocarbon fuels on soot particles size distribution functions (PSDF) have been researched less by scientists; especially the H_2 addition on important sub-process of soot formation has less discussed in previous works. Therefore, further investigation on the effects of H_2 addition to C_2H_2/air flame on PSDF is necessary to be conducted.

Mathematical model

The evolution of PSDF in the present work was simulated in two steps. Firstly, the gas species concentration and moments of the soot size distribution [17] were simulated using detailed chemical reaction mechanism for gas phase chemistry [18] and soot formation [19]. Secondly, the soot size distribution was calculated with a Monte Carlo stochastic approach using some gas species from the first step as inputs. Gaseous species were calculated by the PREMIX flame code, which is a subroutine of the CHEMKIN II package [20]. The PREMIX code used in the present study was modified [21] to include transport equations for the soot moments [22]. The processes of soot particles formation were described on the basis of the detailed kinetic soot model developed by Frenklach and coworkers [18] and the method of moments [22].

Governing equations

The equations governing of one-dimensional flame propagation can be written as follows [23]:

Continuity equation:

$$\dot{M} = \rho u A$$

Energy equation:

$$\dot{M}\frac{dT}{dx} - \frac{1}{c_p}\frac{d}{dx}\lambda A\frac{dT}{dx} + \frac{A}{c_p}\sum_{K=1}^{K}\rho Y_k V_k c_{pk}\frac{dT}{dx} + \frac{A}{c_p}\sum_{K=1}^{K}\dot{\omega}_k h_k W_k = 0$$

Species equation:

$$\dot{M}\frac{dY_k}{dx} + \frac{d}{dx}(\rho A Y_k V_k) - A\dot{\omega}_k W_k = 0$$

$$(k = 1, \ldots, K)$$

In these equations, x denotes the spatial coordinate; $\dot{M}$ the mass flow rate; T the temperature; Y_k the mass fraction of the kth species (there are K species); p the pressure; u the velocity of the fluid mixture; ρ the mass density; W_k the molecular weight of the kth species; λ the thermal conductivity of the mixture; c_p the constant-pressure heat capacity of the mixture; $\dot{\omega}_k$ the molar rate of production by chemical reaction of the kth species per unit volume; h_k the specific enthalpy of the kth species; V_k the diffusion velocity of the kth species; and A the cross-sectional area of the stream tube encompassing the flame.

Chemical reaction kinetics model

The detailed chemical kinetic mechanism used in this work is known as the ABF mechanism, which can be divided into four main components: (1) C1 and C2 chemistry; (2) benzene (A_1) and phenyl (A_{1^-}) formation; (3) PAHs growth; (4) PAHs oxidation. Details of the ABF mechanism are well documented in Ref. [18]. The mechanism includes 101 species and 544 reactions with the growth and oxidation of aromatic rings up to A_4. The first aromatic ring (A_1) formation has three main pathways, respectively the C_4H_x and C_2H_2 reactions, two C_3H_3 radicals combination reaction, and cyclization reactions of C_6Hx.

The PAHs growth (A_2–A_4 formation in this study) was described by an H-abstraction C_2H_2 addition (HACA) mechanism after the first ring has formed

$$PAH_i + H \rightarrow PAH_{i^-} + H_2 \quad \text{(R1)}$$

$$PAH_{i^-} + C_2H_2 \rightarrow PAH_{i+1} + H \quad \text{(R2)}$$

PAHs oxidation was described as the following reactions

$$PAH_{i^-} + O_2 \rightarrow PAH_{i-1} + products \quad \text{(R3)}$$