Fuel 111 (2013) 492–495

Contents lists available at SciVerse ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Analysis of the influences of gas temperature fluctuation on the soot formation and oxidation

Ying Chen, Jian Zhang *

Department of Engineering Mechanics, Tsinghua University, Beijing 100084, China

HIGHLIGHTS

- The instantaneous soot formation is affected by the gas temperature fluctuation.
- The gas temperature fluctuation has influences on the time-averaged soot properties.
- The above effects should be taken into account in the turbulent soot formation model.

ARTICLE INFO

Article history:
Received 3 August 2012
Received in revised form 27 March 2013
Accepted 28 March 2013
Available online 17 April 2013

Keywords:
Gas temperature fluctuation
Soot formation and oxidation
Numerical analysis

ABSTRACT

Numerical analysis is performed to investigate the influences of gas temperature fluctuation on soot formation and oxidation. The gas flow has a time-averaged gas temperature of 1400–1700 K. The instantaneous variations of soot volume fraction with time are obtained under different conditions. Obvious differences are found between the results with and without the gas temperature fluctuation. The time-averaged soot volume fraction decreases with the fluctuation amplitude of the gas temperature. The evident influences of the gas temperature fluctuation on the reaction processes of soot formation and oxidation are thus delineated.

1. Introduction

The combustion of hydrocarbon fuel will usually accompany soot emission. The processes responsible for the generation of soot in hydrocarbon flames include both homogeneous and heterogeneous chemical reactions [1]. The homogeneous reactions involve soot precursor production, while the heterogeneous reactions encompass soot nucleation, surface growth, particle agglomeration, and oxidation. Among them, the heterogeneous reactions play a crucial role in the soot formation. Both detailed reaction mechanisms [2] and reduced multi-step reaction mechanisms [3] have been developed to describe the soot nucleation, growth, and oxidation. The detailed mechanisms account for hundreds of elementary reactions and species. The simplified reaction mechanisms consider several step reactions. The latter have received many applications in soot formation predictions [4–6].

Turbulent combustion is found in most of combustion devices. In turbulent flames, the soot precursor formation is not only influenced by the reaction kinetics, but also affected by the turbulent fluctuations. The interactions between gas turbulence and homogeneous reactions or soot precursor reactions are well recognized. However, the interactions between gas turbulence and soot nucleation and growth reactions need to be further investigated. Some of the models for soot formation in turbulent flames account for these interactions [5], while others ignore these interactions [4]. To explore the turbulence-soot heterogeneous reaction interactions, the commonly used multi-step reaction mechanism of soot nucleation, surface growth, agglomeration, and oxidation is adopted presently. It suggests that the instantaneous rates of these heterogeneous reactions are exponential functions of instantaneous gas temperature. The turbulent fluctuation in gas temperature should have influences on the time-averaged reaction rates of soot nucleation and growth. The effects of gas temperature fluctuation on soot formation and oxidation are thus numerically studied. The gas flow under consideration has a uniform but fluctuating temperature.

2. Model formulation

Based on the simplified reaction mechanism for soot nucleation, surface growth, agglomeration, and oxidation, the two-equation model was proposed [3]. It is utilized presently. Hydrocarbon fuel combustion is considered regardless of specific fuel type. Acetylene

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* Corresponding author. Tel.: +86 10 62772932; fax: +86 10 62781824.
E-mail address: jianzhang@mail.tsinghua.edu.cn (J. Zhang).

0016-2361/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.fuel.2013.03.077

is an intermediate species and is assumed to be the soot precursor in the analysis. The following five-step reaction mechanism is adopted [5]: $C_2H_2 \rightarrow 2C(s)+H_2$, $C_2H_2 + nC(s) \rightarrow (n+2)C(s) + H_2$, $C(s) + 0.5O_2 \rightarrow CO$, $C(s) + OH \rightarrow CO + H$, and $nC(s) \rightarrow C_n(s)$. They are labeled as reaction 1, 2, 3, 4, and 5, respectively. The instantaneous rates for the above five reactions are determined using the expressions given as $R_1 = k_1(T)[C_2H_2]$, $R_2 = k_2(T)A_s^{1/2}[C_2H_2]$, $R_3 = k_3(T)A_s[O_2]$, $R_4 = \varphi_{OH}k_4(T)A_sX_{OH}$, and $R_5 = 2C_\alpha d_p^{1/2}(6\sigma_B T/\rho_s)^{1/2}(\rho N_s)^2$, where $k_1(T) = A_1\exp(-E_1/RT)$, $k_2(T) = A_2\exp(-E_2/RT)$, $k_3(T) = A_3T^{1/2}\exp(-E_3/RT)$ [3], $k_4(T) = A_4T^{-1/2}$ [6], and $A_s = \pi d_p^2(\rho N_s)$. A_s represents the soot surface area per unit volume and d_p is the soot particle diameter. Taking as spherical particles, d_p is related to the soot mass fraction (Y_s) and particle number density (N_s) through $d_p=(6Y_s/\pi\rho_sN_s)^{1/3}$.

The spatial distributions of gas temperature and species mass fractions are assumed to be uniform in a hot gas flow. The instantaneous governing equations for soot mass fraction and particle number density are deduced as

$$\frac{dY_s}{dt} = 2k_1(T)M_s\frac{Y_{C_2H_2}}{M_{C_2H_2}} + 2k_2(T)A_s^{1/2}M_s\frac{Y_{C_2H_2}}{M_{C_2H_2}} - k_3(T)A_sM_s\frac{Y_{O_2}}{M_{O_2}} - \varphi_{OH}k_4(T)A_s\frac{RTY_{OH}}{pM_{OH}} \tag{1}$$

$$\frac{dN_s}{dt} = \frac{2}{C_{\min}}N_Ak_1(T)\frac{Y_{C_2H_2}}{M_{C_2H_2}} - 2C_ad_p^{1/2}\left(\frac{6\sigma_BT}{\rho_s}\right)^{1/2}\rho N_s^2 \tag{2}$$

where $N_A = 6.022 \times 10^{23}$ mol^{-1} is the Avogadro number, $\sigma_B = 1.38 \times 10^{-23}$ J/K is the Boltzmann constant, $M_s = 12.011 \times 10^{-3}$ kg/mol is the molecular weight of soot, and $C_{\min}$ is the number of carbon atoms in the incipient soot particle.

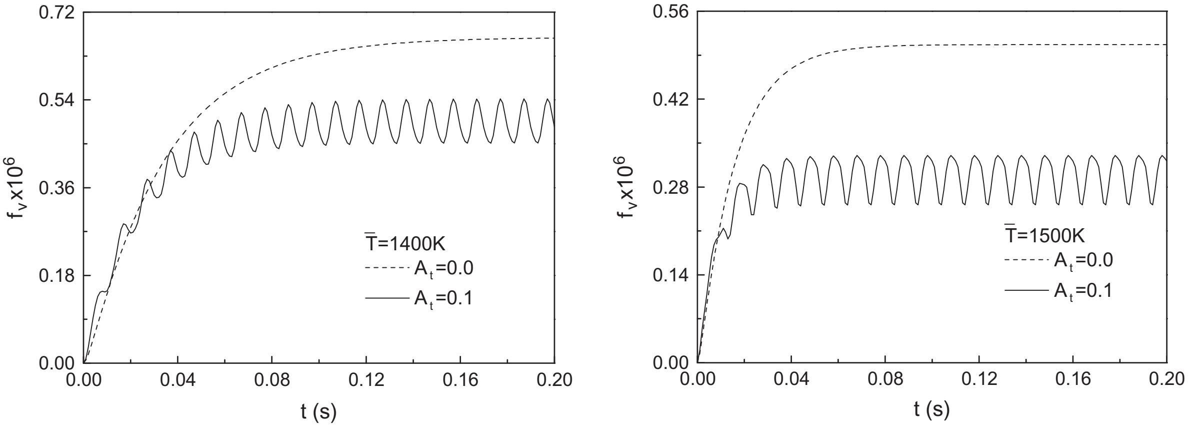
The above reaction mechanism indicates that the instantaneous rates of soot inception, surface growth, and oxidation are exponential functions of instantaneous gas temperature and linear functions of instantaneous gas species concentrations. The instantaneous gas temperature is thus a dominant factor affecting the soot heterogeneous reaction rates. To reveal the influences of gas temperature fluctuation on the soot formation and oxidation processes, the instantaneous temperature of the gas flow is further assumed to vary with time in a simple harmonic way as

$$T = \bar{T}[1 + A_t\sin(2\pi ft)] \tag{3}$$

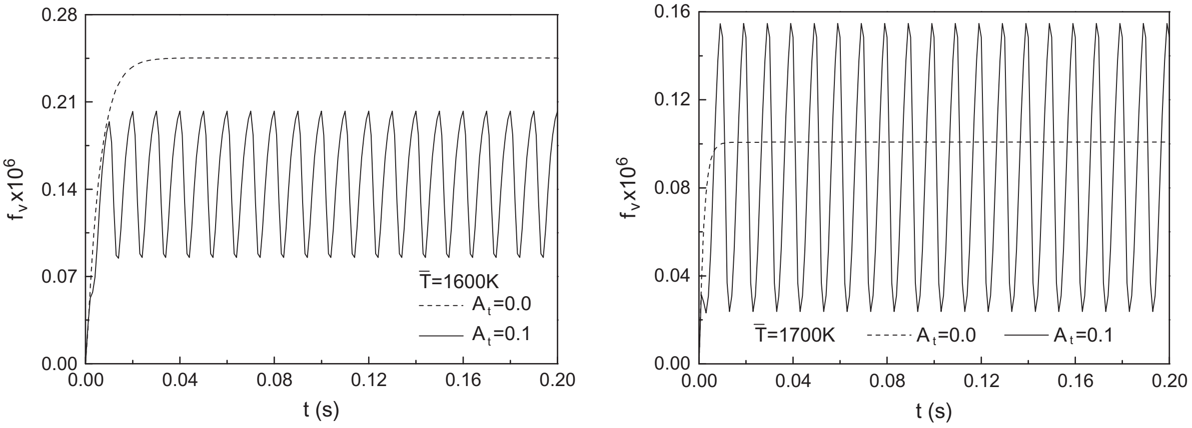
where $\bar{T}$ is the time-averaged gas temperature, A_t is the fluctuation amplitude of the gas temperature, and f stands for the fluctuation frequency of the gas temperature. f is determined by $f = 1/\tau_T$. Here τ_T represents the turbulent time scale of gas flow.

3. Calculation conditions

The instantaneous governing equations for soot mass fraction and particle number density are numerically solved. The instantaneous gas temperature is given by Eq. (3) and the instantaneous gas energy equation needs not to be solved. Solving Eqs. (1) and (2) provides the instantaneous variations of soot mass fraction and particle number density with time. The instantaneous soot volume fraction is obtained as $f_v = \rho Y_s/\rho_s$. The time-averaged soot volume fraction and particle number density are further calculated



(a) $\overline{T}$=1400K (b) $\overline{T}$=1500K



(c) $\overline{T}$=1600K (d) $\overline{T}$=1700K

Fig. 1. Effect of gas temperature fluctuation on the instantaneous variations of soot volume fraction.