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Interactive transient flamelet modeling for soot formation and oxidation processes in laminar non-premixed jet flames

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ABSTRACT

The Interactive Transient Flamelet (ITF) model has been devised to realistically simulate slow processes such as soot formation and radiation in a laminar non-premixed flame with a relatively long residence time. In context with the ITF model, soot formation in the laminar non-premixed jet flame is modeled by the two-equation soot model to simulate physical processes such as nucleation, surface growth, oxidation and agglomeration. In the present ITF approach, gaseous chemistry is effectively coupled with soot chemistry. The present ITF model accounts for radiative cooling induced by gaseous species and soot particles in the same mixture fraction space simultaneously while it treats the unphysical diffusion of soot to be practically zero. Moreover, the present ITF procedure can maintain consistency to extend the present transient flamelet model to the simulation of turbulent non-premixed sooting flames. To validate the present ITF approach together with the two-equation soot model, in terms of soot volume fraction, number density, temperature, OH and C_2H_2 mass fractions, as well as reaction rates for nucleation, surface growth, and oxidation, numerical results are compared with those obtained by the full transport equation approach. Furthermore, to assess the applicability of the present ITF approach and to evaluate the effects of gaseous differential diffusion on the soot formation processes, numerical results obtained by the present ITF model with equal and differential diffusion are also compared with experimental data in terms of temperature; CH_4, OH, H_2O, CO_2 and C_2H_2 mole fractions; and soot volume fraction. Based on these numerical results, the detailed discussion has been made for the capability and limitations of the present ITF approach to predict the precise flame structure and soot formation characteristics in the laminar non-premixed methane/air jet flames.

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1. Introduction

To comply with strict environmental regulations, considerable research has been performed regarding the development of combustion systems with low pollutant emissions. Among the combustion pollutants, soot emission is considered crucial because of the well-known impacts of particulate matter on human health and environment pollution. Both computational modeling and experimental investigations have been performed to understand the formation and evolution of soot particles in combustion processes. It has long been recognized that numerical and physical modeling of soot formation and oxidation is a challenging task due to the significant nonlinearities and the strong coupling involved in the physically complex reaction processes that occur at widely separated characteristic time and length scales. Research efforts for reliable and robust soot formation model are mainly motivated to gain better understanding of the soot formation mechanism as well as to identify the optimum design and operating conditions of combustion devices with the higher engine performance and the lower pollutant emission.

The soot formation mostly caused by the incomplete oxidation of fuel results in the production of aromatic compounds which grow to Polycyclic Aromatic Hydrocarbons (PAHs). These PAHs are considered important compounds in the reactions involved in the first stages of the soot formation process [1]. The soot precursor species such as PAH and C_2H_2 eventually contribute to formation of soot particles. Especially in a non-premixed flame, the flame structure and pollutant emission characteristics are substantially influenced by soot size distribution, number density and particulate radiation. Through a sequence of comprehensive studies for the soot formation process, important progress has been achieved in understanding soot formation pathways. Detailed reviews of soot

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Nomenclature

Roman symbols

C_a	agglomeration rate
k_b	Boltzmann constant
N_s	soot number density [#/kg]
h, h_k	total enthalpy of mixture and species k
Y	mass fraction
A_S	soot surface area per unit volume
k	reaction constant
q_{rad}	radiative heat loss
N_A	Avogadro's number
t	time
T	temperature
x	physical domain
Z	mixture fraction
$\dot{r}$	reaction rate for soot

Greek symbols

$\dot{\omega}_k$	chemical reaction rate of species k
ϕ	scalar
ρ	density
χ	scalar dissipation rate

Subscripts

s	soot
n	soot nucleation
st	stoichiometry
g	soot surface growth

formation researches were made by Kennedy [2], Frenklach [3] and Karatas and Gülder [4].

According to Kennedy [2], soot formation models are largely classified into empirical, semi-empirical and detailed models. Empirical soot models were developed by experimentally phenomenological correlations of soot formation rates for specific combustion conditions in terms of pressure, temperature, and species concentration. These intuitive empirical models find useful applications for analyzing the soot emission characteristics of large practical combustion systems due to their ease of numerical implementation and high computational efficiency. However, these empirical models are unable to provide global information on soot formation processes.

The next-class approaches based on a semi-empirical concept are modeled by integrating several essential features of physics and chemistry phenomenologically. The two-equation soot model proposed by Fairweather et al. [5] is a typical semi-empirical soot model. Unlike empirical models, the semi-empirical approach is able to incorporate general physical sub-modeling of soot formation processes including particle inception, surface growth, and particle oxidation. Even though this two-equation soot model realistically describes the soot formation mechanism in terms of soot volume fraction and particle number density, it is incapable of providing detailed soot properties such as soot aggregate structure and size distribution. However, this soot model is straightforward to couple the soot formation with gaseous chemistry and also has the prediction capability to address the interaction of flame structure with soot formation at a low computational cost.

On the other hand, the detailed soot models incorporate the fundamental combustion chemistry and aerosol dynamics theory. These models are based on detailed chemical kinetics and physical models to describe the interphase processes between gases and solid particles, as well as thermophysical processes on the surface of soot particles. These detailed models describe precise information about soot formation processes such as soot particle inception, condensation, surface growth, particle oxidation, and coagulation. Particle inception is represented by the detailed chemical kinetics to account for the precise gaseous chemistry and the formation and growth of PAHs up to larger aromatics. It is assumed that the transition from gaseous species to solid soot particles occurs through collisions of pyrene and larger aromatics. The soot chemical mechanisms describing PAH formation in hydrocarbon fuels flames are precisely described by Frenklach et al. [3,6], Appel et al. [7], Ranzi et al. [8], Chernov et al. [9], and sophisticated soot oxidation models [10–12] with detailed PAH chemistry have been proposed. The surface growth and particle oxidation are modeled by chemical analogies to the reaction process of aromatics. The coagulation of soot particles is described utilizing methodologies from aerosol particle dynamics. Compared to the semi-empirical soot models based on the mono-dispersed particle distribution, these detailed soot models using advanced aerosol dynamics can address the poly-dispersed particle distribution in terms of soot aggregate structure and particle size distribution. The soot particle dynamics are modeled by various approaches including the sectional method [13–16], the Method of Moment [6,17,18], the Direct Quadrature Method of Moments [19,20], the Hybrid Method of Moments [21,22], and the stochastic method [23,24]. These detailed soot models have the potential capability to apply to wide-range combustion conditions. However, many elementary reactions involved in the chemical analogy and reaction rates are modeled by simple estimation. Due to these shortcomings, application of the detailed soot models is still limited even if the prediction capability has been continuously improved.

In systematically assessing the prediction capability of state-of-art soot models, steady laminar non-premixed jet flames have been generally regarded as excellent benchmark cases among various flame conditions. These laminar non-premixed jet flames also include regions from the soot nucleation to the oxidation and therefore provide opportunities to gain better understanding about the complex soot formation processes. Numerical simulations of laminar non-premixed sooting jet flames are mostly performed using full transport equation approaches [25,26] together with semi-empirical models or detailed soot models. However, the full transport equation approaches with detailed physical sub-models including PAH chemistry and a particle dynamics model require excessive CPU time, especially for heavier hydrocarbon fuels. For instance, reaction mechanisms describing the precise PAH chemistry usually contain several hundreds of reactions, and this results in a huge computational burden. On the other hand, to evaluate the sooting tendencies of various fuels, there has been a practical research need to predict yield sooting indices (YSI) [27], which are linear functions of the maximum soot volume fraction measured on the centerline of an axisymmetric co-flow diffusion flame with the fuel stream doped with a reference hydrocarbon fuel. Even if the full transport equation approach [15] with a detailed soot model is the most reliable tool to predict YSI, the required CPU time is quite long, especially for a flame doped with a reference fuel.

In these aspects, to predict the characteristics of laminar non-premixed sooting flames, it is quite desirable to develop computationally efficient and accurate procedures such as laminar flamelet

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