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Simulation of soot formation in turbulent premixed flames

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Abstract

A subgrid model for soot dynamics is developed for large-eddy simulation (LES) that uses a method of moments approach with Lagrangian interpolative closure (MOMIC) so that no a priori knowledge of the particles' distribution is required. The soot model is implemented within a subgrid mixing and combustion model so that reaction–diffusion–MOMIC coupling is possible without requiring ad hoc filtering. The model includes the entire process, from the initial phase, when the soot nucleus diameter is much smaller than the mean free path, to the final phase, after coagulation and aggregation, where it can be considered to be in the continuum regime. A relatively detailed multispecies ethylene–air kinetics for gas phase combustion is used here to study the effect of inflow turbulence, the carbon–oxygen (C/O) ratio, and multicomponent species diffusion coefficients on soot production in turbulent premixed flames. The results show that soot formation occurs when the C/O ratio is above the critical value, in good agreement with past observations. Furthermore, we observe that turbulence increases the collision frequency between the soot particles. As a result, the coagulation rate increases and the total average surface area of the soot particles per unit volume decreases. In addition, the rate of surface growth decreases with the increase in the turbulence intensity. Finally, the inclusion of species transport properties is shown to affect the general structure of the flame in the form of wider curvature probability density function tails and higher turbulent flame speed. In addition, the effect on the relative thermal to molecular diffusivity at the subgrid level (Lewis number effect) changes the surface growth rate and the soot production level.

Keywords: Large eddy simulation; Soot; Method of moments; Turbulent flames

1. Introduction

Emission from propulsion and energy-producing systems is fast becoming a major concern in both the developed and the developing world. Of particular concern is the emission of carbon monoxide (CO), oxides of nitrogen (NO_x), and soot (primarily carbon) particles. NO_x is mainly generated in the high-temperature stoichiometric regions, while CO peaks are due to either local extinction or incomplete combustion. On the other hand, soot results from incomplete combustion and typically occurs only in fuel-rich regions. The soot diameter can range from the order of nanometers (nm) for the primary particles up to 10 μm for soot aggregates [1]. This wide range of particle sizes can coexist at the same time inside the combustor. Although some of these particles are oxidized

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in the flame zone, soot particles that escape oxidation are considered to be serious health concern, since both polycyclic aromatic hydrocarbons (PAHs), which are precursors of soot, and soot-associated organics have been identified as carcinogenic emissions. In addition, the high emissivity of soot particles reduces the chemical energy available for conversion into mechanical energy, which results in a loss in combustion efficiency (estimated to be around 30%) [2]. Moreover, flame visibility and structure are found to be affected by soot formation.

However, the formation of soot particles in flames, and the coupling between the formation processes and the other fluid processes are still poorly understood phenomena, in spite of many seminal studies [3,4]. Measurements [5,6] and modeling studies [7–10] have addressed the physical and dynamical processes of soot formation from the initial gas phase species. Determination of soot inception, the location in the flame zone where it occurs, and the conditions under which it begins is complicated by the fact that many of the PAHs that contribute to the soot formation process, and many of the species (and the reactions) involved in the chemical reactions leading to soot formation, are still unknown [11]. Most measurements are carried out in laminar or low-turbulence atmospheric-pressure flames and only recently have measurements in fully turbulent (but relatively simple) diffusion ethylene and methane/air jet flames been reported [12–18]. However, in high-pressure and in high-turbulence regimes (which occur in real combustors), many new issues can become important. For example, turbulent fluctuation in heat transfer and chemical reactions can directly control and/or modify the locations and the processes of inception, growth, and oxidation of soot. Increase in the combustor pressure can also impact kinetics and hence, soot formation.

Numerical prediction of soot formation and transport in unsteady turbulent flames is very challenging, because both realistic chemical kinetics for gas and soot and flow–chemistry interaction over a wide range of spatial and temporal scales have to be included. In the past, several steady-state approaches have been used to predict soot in realistic turbulent configurations. A good review of soot formation models is summarized in [19]. In general, past soot models can be classified into two general categories. The more popular approach solves two transport equations for the soot volume fraction and the number density in conjunction with other simplified turbulent models. The second category either uses a prescribed soot probability density function (PDF) distribution or solves the transport moment equations for the soot PDF. Syed et al. [20], and Brookes and Moss [21,22] used the laminar flamelet approach combined with the soot mass fraction and the number density transport equations to approximate the soot chemistry to study a low turbulent buoyant fire and an axisymmetric turbulent methane–air jet flame at elevated and atmospheric pressure. These studies were some of the first available numerical studies of turbulent sooting methane–air flames based on the current understanding of the physics of soot formation.

Kronenburg et al. [23] used the same soot transport equations with the conditional moment closure (CMC) approach to study turbulent methane jet flames [22]. They used a detailed hydrocarbon mechanism and obtained good agreement with measurements. Kollmann et al. [24] applied a detailed soot model along with a joint transport PDF equation of the mixture fraction, enthalpy, and soot volume fraction to study an ethylene–air jet flame. They found that most of the soot is formed around 1400 K, and that for such a flame the correlation between the mixture fraction and the soot volume fraction is very weak. The current work also confirms that soot forms around this temperature for premixed flames.

Recently, Aksit and Moss [25] developed a hybrid model that uses a Lagrangian Monte Carlo solution of the joint scalar pdf of the mixture fraction, soot number density, and volume fraction combined with an Eulerian solution of the turbulent flow field. The model used the laminar flamelet-state relationship for the gas phase properties. The model showed good agreement in temperature but an underprediction of the soot volume fraction along the centerline. The results further showed that the radiation effect increases the soot volume fraction. Wen et al. [26] developed a soot model that combines the k–ϵ model for the turbulent flow field with the stretched laminar flamelet approach for a detailed kerosene/air mechanism. They used two soot inception models, one based on acetylene and another based on the formation of aromatic rings. They concluded that the acetylene model significantly underpredicts the soot volume fraction, which indicates the importance of the aromatic species as an intermediate species in such kerosene/air flames.

Another PDF-based transport study was done by Hong et al. [27]. They applied a skeletal n-heptane chemistry model with an assumed lognormal soot size distribution in the KIVA-3V code. Their results show good agreement with experimental results for a high-pressure shock tube. They concluded that correct description of the soot formation, as well as the soot transport processes, is critical for achieving reliable predictions. Lindstedt and Louloudi [28] used the method of moments (MOM) combined with a joint-scalar transport PDF to predict the soot properties for two ethylene turbulent flames with full chemistry.