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An LES-PBE-PDF approach for predicting the soot particle size distribution in turbulent flames

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ABSTRACT

In this article, we combine the large eddy simulation (LES) concept with the population balance equation (PBE) for predicting, in a Eulerian fashion, the evolution of the soot particle size distribution in a turbulent non-premixed hydrocarbon flame. In order to resolve the interaction between turbulence and chemical reactions/soot formation, the transport equations for the gas phase scalars and the PBE are combined into a joint evolution equation for the filtered *pdf* associated with a single realization of the gas phase composition and the soot number density distribution. With view towards an efficient numerical solution procedure, we formulate Eulerian stochastic field equations that are statistically equivalent to the joint scalar-number density *pdf*. By discretizing the stochastic field equation for the particle number density using an explicit adaptive grid technique, we are able to accurately resolve sharp features of evolving particle size distributions, while keeping the number of grid points in particle size space small. Compared to existing models, the main advantage of our approach is that the LES-filtered particle size distribution is predicted at each location in the flow domain and every instant in time and that arbitrary chemical reaction mechanisms and soot formation kinetics can be accommodated without approximation. The combined LES-PBE-PDF model is applied to investigate soot formation in the turbulent non-premixed Delft III flame. Here, the soot kinetics encompass acetylene-based rate expressions for nucleation and growth that were previously employed in the context of laminar diffusion flames. In addition, both species consumption by soot formation and radiation based on the assumption of optical thinness are accounted for. While the agreement of our model predictions with experimental measurements is not perfect, we indicate the benefits of the LES-PBE-PDF model and demonstrate its computational viability.

1. Introduction

Soot particles form in hydrocarbon combustion devices and are typically created in fuel-rich regions of high temperature. From an engineering perspective, soot particles contribute a heat sink through thermal radiation, but may also pollute a combustor if deposited on its walls. On the other hand, soot particles are known to be harmful to the environment, acting as greenhouse agents, and to the human body as they may cause respiratory diseases [1] or act as carcinogens. By consequence, many of the recent modeling efforts in the combustion community have targeted the prediction of soot formation in hydrocarbon combustion, taking into account the effect of soot on the flame structure.

Typically, soot is considered as a particulate phase that is polydispersed with respect to particle size and behaves non-inertially, that is, the individual soot particles are assumed to be small enough such that they respond instantaneously to changes in the carrier flow field. From a Eulerian perspective, the soot phase can be described by the population balance equation (PBE) which governs the evolution of the soot particle size distribution throughout the flow domain and is formulated in terms of the number density of soot particles per unit volume of mixture and unit of length in particle size space.

In this article, we present a comprehensive LES-PBE-PDF approach for predicting the evolution of the soot particle size distribution in a turbulent flame. The main ingredient of our model is an evolution equation for the LES-filtered one-point, one-time joint probability density function (*pdf*) associated with a single realization of the reactive gas phase scalars and the particle number density. Here, the physical processes related to chemical reactions, soot particle inception, soot growth and coagulation appear in closed form, while velocity and two-point correlations require modeling. For these, we adopt a standard gradient diffusion hypothesis as well as an IEM-based (interaction by exchange with the mean) micromixing model.

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Originally, the PBE–PDF concept was introduced by Rigopoulos [2] who showed that, upon discretization in particle size space, the PBE reduces to a collection of particle phase scalars which may be incorporated into a transported *pdf* approach in the same way as the reactive scalars describing the gas phase [3]. This leads to a transport equation for the so-called joint scalar-discrete number density *pdf* which naturally accounts for all one-point, one-time correlations of the gas phase composition and the discrete number densities. In the context of RANS, Di Veroli and Rigopoulos [4,5] showed that a numerical solution of this transport equation based on a stochastic particle method is computationally feasible for practical flow configurations and realistic nucleation/growth kinetics, albeit expensive. Subsequently, Akridis and Rigopoulos [6] and Akridis [7] applied the RANS–PBE–PDF methodology to investigate soot formation in two turbulent diffusion flames.

More recently, the PBE–PDF concept has also been combined with LES and, coincidentally, different strategies have emerged for reducing the computational expense associated with conventional solution schemes of the *pdf* transport equation. Neuber et al. [8], for instance, devised a sparse stochastic particle solution scheme by invoking the generalized multiple mapping conditioning (MMC) method. From a physical perspective, the MMC–LES approach is based on shifting micromixing locality from physical space to the space spanned by the reactive scalars and discrete number densities. Sewerin and Rigopoulos [9], on the other hand, revisited the PBE–PDF rationale and formulated a joint scalar-number density *pdf* transport equation that is independent of a specific particle size discretization. An important consequence is that particle size persists as an independent coordinate in a statistically equivalent stochastic particle or field reformulation and that these stochastic systems may hence be discretized with respect to particle size using both fixed and adaptive grid schemes.

In the present article, we generalize this approach to polydispersed particle formation in variable density flows of gases at low Mach numbers. The joint scalar-number density *pdf* transport equation which we obtain is solved numerically by the method of Eulerian stochastic fields [10–12] and, for the discretization in particle size space of the stochastic field equation associated with the particle size distribution, an explicit adaptive grid technique is applied [13].

By construction, the PBE–PDF approach achieves a direct resolution of the particle size distribution. This is different from moment-based approaches [14] in which the particle size distribution is described in terms of a small number of low order statistical moments such as the particle number or volume density. Moment-based methods are well-established by now and are not only computationally very economical, but also readily generalize to situations in which the particulate phase is characterized by more than one characteristic property. However, the main challenge associated with these formulations is that the moment equations are closed only for particular functional forms of the particle growth rate and the coagulation kernel. Common closure schemes such as the quadrature method of moments involve an assumption on the shape of the particle size distribution which allows for truncated moments to be expressed in terms of the first few resolved moments.

The scientific contribution of our work is threefold: First, we develop an LES-based model for predicting the evolution of the soot particle size distribution in a turbulent combusting flow at low Mach number. An integral part of our approach is the PBE–PDF closure of the interaction between turbulence and chemical reactions/particle formation which allows for the incorporation of arbitrary gas phase and soot kinetics without approximation. Second, we present a stochastic field formulation that reproduces, in a statistical sense, the evolution of the joint scalar-number density *pdf* and can be combined with both fixed and adaptive grid discretization schemes along the particle size coordinate. Finally, the computational viability and predictive capabilities of the combined LES-PBE-PDF approach are demonstrated in the context of the Delft III turbulent diffusion flame. In particular, we show that a detailed resolution of the soot particle size distribution hardly increases the computational cost and that the overall model is computationally feasible on modern computing devices. Furthermore, to our awareness, the present modeling effort constitutes the first attempt to directly predict soot particle size distributions within the scope of LES.

This article is organized as follows: In Section 2, we first review existing modeling strategies for predicting soot formation in turbulent non-premixed flames. Subsequently, in Section 3, the PBE and the LES concept are formally introduced and an evolution equation for the joint scalar-number density *pdf* is obtained. Here, we also discuss the micromixing closure and formulate the stochastic field equations. This is followed by Section 4, where the gas phase and soot kinetics and the radiation model are detailed. In Sections 5 and 6, we summarize details on the Delft III flame as well as the computer implementation used in this work. Model predictions are compared with experimental measurements from the Delft III database in Section 7 and discussed in the light of previous modeling attempts. Finally, we offer conclusions in Section 8 and provide a view towards further model enhancements.

2. Approaches for modeling soot formation in turbulent non-premixed flames

In the present section, we briefly review existing approaches for modeling soot formation in turbulent non-premixed flames. As an aid to the reader, the references discussed here are classified in Table 1.

From a modeling perspective, incorporating the formation of soot into models for turbulent reacting flows has been challenging for several main reasons. On the one hand, soot particles contribute significantly to radiative heat emission and, potentially, reabsorption, thus influencing the distribution of temperature and density in the carrier gas. On the other hand, the synthesis of soot precursors, the inception of soot and soot surface growth (both by PAH condensation and surface reactions) are characterized by much longer time scales than the mixing of reactants [15–17]. Attili et al. [16] argued that, as a consequence, the soot formation kinetics react only slowly to changes in the local turbulent mixing (scalar dissipation) rate. Furthermore, soot particles are characterized by a very low mass diffusivity and, contrary to light gas phase species, are mainly convected along by the ambient velocity field without significant dispersion [17].

Since RANS-based conserved scalar/presumed *pdf* approaches are computationally very economical, an early idea for accommodating the first challenge mentioned above was to introduce an indicator for radiative heat losses into such a model. Following Gore et al. [18], Young and Moss [15] augmented a steady-state flamelet representation of the gas composition by a heat loss parameter such that the reactive scalars could formally be parameterized by a mixture fraction, the scalar dissipation rate and a heat loss coefficient. As a criterion for determining the heat loss coefficient, Young and Moss [15] proposed the condition that, locally, the Favre-averaged enthalpy computed from the extended flamelet library and the presumed mixture fraction *pdf* coincides with the value obtained by solving a transport equation for the Favre-averaged mixture enthalpy with radiative heat losses. For the description of the soot particulate phase, Young and Moss [15] adopted the semi-empirical model of Moss et al. [19] based on two evolution equations for the Favre-averaged soot number density and volume fraction.