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Comparison of one-dimensional turbulence and direct numerical simulations of soot formation and transport in a nonpremixed ethylene jet flame

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Abstract

Accurate models of soot formation in turbulent flames are important for correctly predicting and simulating flames and fires. Modeling soot formation and transport is challenging due to the complex chemical formation processes, and differential diffusion of soot relative to a flame. Direct numerical simulations (DNS) have highlighted the importance of such transport on soot concentrations, however DNS is computationally expensive. The one-dimensional turbulence (ODT) model is able resolve a full range of length and timescales and solves the evolution of diffusive and reactive scalars in the natural physical coordinate. We present results of soot formation in ODT and compare the model to simulation results from DNS in a temporally-evolving planar ethylene jet flame where the same transport, thermodynamic, and kinetic models are applied. Good agreement is found for the jet evolution in terms of the mixture fraction profiles. Conditional soot statistics (mean and fluctuations) are presented, along with joint soot-mixture fraction PDFs that illustrate the location and motion of soot in the mixture fraction coordinate. Good qualitative agreement between the models is found and the soot behavior is similar. While the ODT cannot capture three-dimensional flow structures, the ODT simulations are less computationally expensive than the DNS suggesting its use in conjunction with DNS for parametric study, model validation, and investigation at parameter ranges not currently available to DNS.

Keywords: Soot; ODT; DNS; Turbulent; Nonpremixed flame

1. Introduction

Soot is an important component of most non-premixed flames and fires. Soot radiation affects flame temperatures, impacting, for instance, flame spread and industrial radiative heat transfer. Large fires exhibit increases in radiative intensity with size, but when smoke breaks through the fire, smoke shielding can reduce this intensity. Emission of soot from flames results in fine carbonaceous particles that contribute to air pollution, and are a known health hazard contributing to lung diseases, such as asthma, bronchitis, and other problems [1].

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Modeling soot formation and transport is a challenging problem. Soot formation involves complex formation chemistry based on large aromatic hydrocarbons. Soot is a particle phase with an evolving size and composition distribution, which grows to form primary particles that aggregate into chain-like structures [2]. The low diffusivity of soot results in very fine soot filaments due to turbulent stretching and folding. This increases computational costs of direct numerical simulations (DNS) that resolve all turbulent scales. Similarly, the low diffusivity implies differential diffusion between soot and gaseous species so that soot is transported relative to flame surfaces largely by the relative velocity difference between convection and the stoichiometric (flame) isosurface [3]. The transport of soot relative to a flame will affect the temperature and composition environment of the soot, impacting soot formation, and radiation. The differential diffusion complicates LES modeling since subgrid differential diffusion should be accounted for in combustion models (but is often neglected). The differential diffusion coupled with longer formation timescales results in the well-known lack of a state relationship between soot and the mixture fraction [4].

These challenges, among others, motivate detailed study of soot formation in turbulent combustion. DNS is a useful tool for such investigation. A few recent DNS have been performed of soot formation in turbulent flames. These include a two-dimensional study with one-step ethylene chemistry in an opposed jet configuration by Yoo et al. [5]. Lignell et al. [3] simulated a two-dimensional flame with detailed chemistry and a semi-empirical soot model. See also Bisetti et al. [6] who used a detailed soot model. Lignell et al. [7] simulated a three-dimensional DNS with soot formation using a similar model in a turbulent ethylene jet flame. Attili et al. [8] performed DNS of soot formation in nonpremixed n-heptane flames.

While DNS provides detailed spatial and temporal information on composition, temperature, velocity, and soot fields, the simulations are limited to relatively short run times and lower Reynolds numbers compared to practical flames and fires. The high computational cost of DNS also increases processing time and limits the number of parametric simulations that can be performed.

The one-dimensional turbulence (ODT) model [9] solves unsteady transport equations for mass, momentum, energy, and reacting scalars in one dimension. ODT resolves diffusive mixing and flame interactions in the natural physical coordinate, but models turbulent advection through stochastic mapping processes that occur concurrently with the scalar evolution equations and reproduce key aspects of turbulent mixing. ODT is limited to geometrically simple flows and is best suited boundary-layer flows, such as jets, with a dominant direction of mean shear. Boundary layer flows are commonly studied and practically important. Three-dimensional simulations have been performed with ODT by constructing grids of interacting ODT lines that could permit study of more complex flows [10]. The model has been successfully applied to a wide range of reacting and nonreacting flows [11]. ODT is computationally efficient compared to DNS because it is one-dimensional. Several ODT simulations have been performed of combustion including comparison to experiments of jet flames [12], and investigation of flame extinction and reignition [13]. ODT has been compared directly to DNS data for application to flame extinction and reignition in syngas flames [14], and ethylene flames [15]. Ricks et al. [16] simulated soot evolution in buoyant pool fires, and Zimberg et al. [27] simulated soot formation using the linear eddy model (LEM) [17], which is a precursor to ODT.

Here, we compare the ODT model directly to three-dimensional DNS [7] of soot formation in a turbulent, planar, temporal ethylene jet flame. This comparison has the advantage of using the same combustion, transport, and soot models in a compatible configuration. Hence, the accuracy of the ODT model may be assessed without complicating uncertainties that often arise in comparing ODT to experimental data, such as consistency of boundary conditions, spatial versus temporal evolution, planar versus cylindrical geometry, and limited data for comparison. Successful comparisons of ODT and DNS will lend confidence to, and quantify limitations of, using ODT directly to study turbulent soot formation, preferably in conjunction with DNS, LES, and experiments to develop and validate more accurate models of soot formation in turbulent flames. We emphasize however, that ODT is a model and cannot replace DNS. In addition, we note that turbulent soot formation is a complex process; and while the ODT and DNS are compared using the same models, the model used in the DNS is not a *true* solution. Continued investigation is needed (including experimental validation) with more detailed soot models in a variety of turbulent flow environments that exercise a wide range of time and length scales, soot-temperature-mixture fraction histories, and radiative effects.

2. Numerical methods

The flow configuration and DNS were described in Lignell et al. [7]. Here a summary description is given, along with a description of the ODT model and simulations.