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Effects of turbulent combustion modeling errors on soot evolution in a turbulent nonpremixed jet flame

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ABSTRACT

Due to the long time scales associated with soot evolution and its sensitivity to the background thermochemical state, even small errors in a turbulent combustion model have the potential to lead to large errors in soot evolution. For example, in turbulent jet flames, small upstream errors in the temperature and species concentrations could lead to large errors in soot volume fraction downstream. In this work, an algorithm is developed for propagating upstream errors in the thermochemical state, specifically, the temperature, into soot predictions downstream. The algorithm is based on a stochastic collocation approach that perturbs the reaction progress variable in the flamelet model at an upstream location and lets this error passively propagate downstream in the soot and combustion models (i.e., the hydrodynamic field is unaffected). The approach is applied to the simulation of Delft Flame III, a natural gas turbulent nonpremixed piloted jet flame for which both upstream temperature measurements and downstream soot volume fraction measurements are available. The results indicate that upstream errors in temperature, which are within the experimental uncertainty, can lead to errors in the soot volume fraction downstream up to 30%; the downstream error in the temperature is comparable in magnitude to the upstream perturbation. Further analysis reveals that the primary source of the downstream error in soot volume fraction is the accumulation of errors in the soot precursor mass fraction with downstream distance.

1. Introduction

Soot particles are formed from the incomplete combustion of hydrocarbon fuels under fuel-rich conditions. In propulsion and power generation applications, these particles are undesirable byproducts of combustion due to their adverse effects on both human health and the environment as well as being indirect indicators of more severe combustion inefficiencies such as excessive CO and UHC emissions. The ability to predict soot emissions in practical devices is of immense value in combustion system design but is complicated by the complex interaction between the turbulent flow that is present in these systems, gas-phase chemical reactions, and soot particles dynamics. Stated differently, the modeling challenges arise from the broad range of physical and chemical phenomena that must be represented accurately in order to make reliable predictions of soot evolution.

In the recent past, the use of Large Eddy Simulation (LES) [1–4] and Direct Numerical Simulation (DNS) [5–7] along with detailed descriptions of soot and chemical processes has provided some interesting insights. First, turbulent transport plays an important role in determining the dominant soot growth mechanism. In turbulent jet flames [2,7], soot growth is dominated by Polycyclic Aromatic Hydrocarbon (PAH) pathways at very fuel-rich conditions. On the contrary, acetylene pathways are important in flames that contain large recirculation zones, such as a bluff-body stabilized flame [3]. Such recirculation zones with long residence times are typical of Rich-Quench-Lean (RQL) aircraft combustors [8]. Second, turbulence leads to a characteristic intermittent soot formation process. In both experiments [9] and DNS [7], localized regions of high soot volume fraction appear very infrequently in the flow. Analysis of DNS data [7] revealed that this intermittency is due to the confinement of Polycyclic Aromatic Hydrocarbons (PAH), the immediate gas-phase precursors of soot, to regions of low scalar dissipation rate and the negligible diffusivity of large soot particles.

Despite these qualitative insights observed from models, quantitative predictions of soot evolution in a wide variety of turbulent reacting flows have been more elusive. Consider the two laboratory-scale LES calculations performed by Mueller and Pitsch [2,3]. In the former study [2], a LES of a natural gas turbulent nonpremixed piloted jet flame (Delft Flame III [10]), the soot volume

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fraction was overpredicted by about a factor of two compared to the experimental measurements with a significant upstream shift of the maximum; Fig. 11a from Mueller and Pitsch [2] is reproduced here as Fig. 1a (with only the nominal results). The authors, after performing some sensitivity analysis, attributed this shift to the chemical mechanism and its inability to accurately predict PAH formation in methane flames. In a follow-up study [3], the authors used the same LES model to simulate an ethylene turbulent nonpremixed bluff body flame. Despite the increased complexity of the fluid mechanics, agreement was improved relative to the jet flame, attributed in large part to the use of ethylene rather than natural gas as a fuel; a portion of Fig. 8 from Mueller et al. [3] is reproduced here as Fig. 1b (with only the nominal results).

One major problem with the validation of LES models for soot evolution in turbulent reacting flows against experimental measurements is the relative sparsity of joint data, which these authors define as spatially co-located measurements of multiple quantities (but not necessarily simultaneous measurements, which are often substantially more difficult). In other words, measurements in sooting flames consist predominantly of soot volume fraction but do not contain information about other quantities such as temperature, gas-phase species concentrations, etc. While recent and forthcoming techniques and datasets of simultaneous measurements of soot volume fraction with velocity [11,12], temperature [13,14], and mixture fraction [15] will help to alleviate this issue, even such data are not as reliable as the experimental measurements that exist in gas-phase nonsooting flames. Of course, the main issue is that measurement techniques used for gas-phase flames are either not applicable in sooting flames or introduce unacceptably large errors. In addition to the physical modeling challenges discussed above, sparse datasets introduce an equally challenging model validation issue.

In this context, Delft Flame III is a prototype for developing relatively well-characterized datasets. Due to the low sooting tendency of methane, the upstream region (up to roughly 40 jet diameters) in this piloted jet flame is relatively soot free, and all diagnostic tools for nonsooting flames are applicable. Further downstream, soot volume fractions are sufficiently large to be accurately measured by Laser Induced Incandescence (LII) but prohibits other measurements. This unique data set has also been chosen as a target flame for the International Sooting Flames (ISF) Workshop [16] predominantly due the availability of such measurements (even though they are not joint measurements as defined by these authors). A recent study by Mueller and Pitsch [2] showed that LES predicted the upstream radial temperature profiles to within 100 K at the centerline, which is comparable to the experimental uncertainty [17]. However, as shown above in Fig. 1a, the downstream soot volume fraction is overpredicted and its maximum shifted upstream. Given the available measurements, the source of this discrepancy is difficult to elucidate.

Soot evolution is highly sensitive to temperature and gas-phase composition. Therefore, considering the disparity in location between the available temperature measurements and soot volume fraction measurements, given even a small disparity between the predictions and the experimental measurements of temperature within the uncertainty of the latter upstream, what is the effect on soot volume fraction downstream? In other words, how does an error in the upstream temperature contribute to the error in the downstream soot volume fraction? This is a particularly relevant question for these jet flames due to the large axial distances at which soot is present. Two outcomes are possible. If the small error in the upstream temperature results induces no error in the downstream soot volume fraction, then the lack of experimental measurements of temperature, etc. is not actually a major impediment to validating the soot model, only a sanity check on the combustion model (with the significant assumption that the combustion model does then not degrade downstream). More likely, if the small error in the temperature results in a large error in the soot volume fraction, then joint data consisting of both soot volume fraction and temperature (or other quantities) are absolutely necessary to fully validate the model; without these measurements, agreement with soot volume fraction measurements alone cannot be claimed to be more than coincidental.

Therefore, the objective of this work is to develop an algorithm for propagating upstream errors in the combustion model (i.e., errors in the temperature) through the soot model. Specifically, using the same Delft Flame III considered by Mueller and Pitsch [2], a temperature perturbation, consistent with both the experimental uncertainty and the discrepancy between LES and experiment, will be introduced upstream relatively close to the burner, and its effect on the far downstream evolution of soot will be quantified. In the next two sections, a brief description of the modeling framework is provided followed by a detailed description of the error propagation algorithm, which will take advantage of the mechanics of the model framework. Next, the configuration and numerical simulation are described including a justification of the shape, magnitude, and location of the temperature perturbation. Then, the results are presented with an analysis of the error propagation including the effect on the different soot processes. Finally, the work is summarized with a few concluding remarks.

2. Modeling overview

Before presenting the algorithm for the propagation of upstream errors, the integrated LES model for turbulent sooting flames developed by Mueller and Pitsch [2] is first briefly

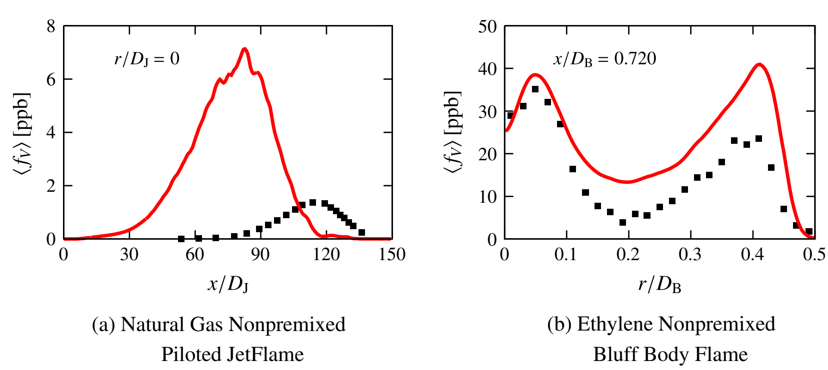

Fig. 1. Profiles of soot volume fraction from a natural gas turbulent nonpremixed piloted jet flame (Delft Flame III) LES reproduced from Mueller and Pitsch [2] (left, centerline profile) and from an ethylene turbulent nonpremixed bluff body flame LES reproduced from Mueller et al. [3] (right, representative radial profile in the recirculation zone).