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Multi-environment probability density function approach for turbulent partially-premixed methane/air flame with inhomogeneous inlets

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ABSTRACT

The present study aims to systematically evaluate the capability of a multi-environment PDF approach using non-premixed and premixed tabulated chemistry to predict the fundamental characteristics of turbulent partially-premixed piloted flames with near-homogeneous and inhomogeneous inlets. For the near-homogeneous case, the non-premixed manifold yields better agreement with measurements in terms of conditional mean, unconditional mean, and rms scalars; however, the premixed manifold generates a narrower hot flame zone, which is mainly attributed to its inability to account for diffusion in the mixture fraction space. For the inhomogeneous flame, the premixed and non-premixed manifolds are limited in their ability to reproduce the measured flame at upstream locations with multiple combustion modes, while the non-premixed manifold is reasonably good at predicting the unconditional and conditional profiles of all scalars in the downstream regions with dominant non-premixed combustion. In terms of the predicted environment-conditioned scalar profiles, the present multi-environment PDF approach demonstrated the ability to realistically predict the near-vertical transition from the fuel-rich flammable mixture condition to the stoichiometric pilot condition. Unlike the near-homogeneous case, the inhomogeneous case generates a distinctly different distribution of CO conditional means, where the peak conditional CO level is leaning to the richer side along the downstream region. This tendency is a clear indication of the flame transition from a premixed-dominated flame to a diffusion-dominated flame. Based on our numerical results, detailed discussions about the essential features of turbulent partially-premixed flames with multiple combustion modes are presented, as well as the limitations of the proposed approach.

1. Introduction

In order to comply with stricter environmental regulations, the gas turbine and automobile industries have devised low-emission combustion systems with complex flame modes such as lean premixed prevaporized gas turbine engines, low-temperature diesels, direct injection stratified charge engines, and homogenous charge compression ignition engines [1,2]. Moreover, lean premixed gas turbine combustors usually adopt pilots with an inhomogeneous mixture distribution to enhance the flame stability. Recently, Meares et al. [3,4] and Barlow et al. [5] experimentally investigated the stability and structure of turbulent partially-premixed flames with a broad range of mixture inhomogeneity in a jet piloted burner. Their results indicated that flame stabilization is sensitively influenced by the degree of inhomogeneity in the mixture. Thus, it is desirable to fully understand the essential features of partially-premixed flames with an inhomogeneous mixture. In this regard, turbulent combustion models must have the ability to predict the turbulence–chemistry interactions in turbulent premixed and non-premixed flames as well as partially-premixed flames with multiple combustion modes.

Among the state-of-the-art turbulent combustion models, the transported PDF model could be the most reliable approach for modeling the complex turbulent reacting flows that accompany auto-ignition, local extinction, reignition, and pollutant formation [6–10]. The transported PDF model has the inherent capability to directly treat a non-linear chemical source term without additional assumptions. However, the stochastic Lagrangian PDF (SLPDF) model based on the Monte Carlo method is computationally expensive when used to simulate turbulent flames, particularly in large-scale practical combustors. To circumvent the computational burden of the SLPDF model, the transported PDF equation is solved by two alternative Eulerian approaches: the deterministic multi-environment probability density function (MEPDF) approach [11–15] and the stochastic Eulerian PDF (SEPDF) method [16–19]. To obtain the transported PDF information, these two Eulerian approaches use fewer environments or stochastic fields compared to the composition particles in the SLPDF. In the SEPDF

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method, the joint composition PDF transport equation is solved using sets of Eulerian stochastic fields that are defined over the entire spatial domain. The SEPDF method specifies equal-weighted fields, which evolve according to a stochastic partial differential equation by remaining statistically equivalent to a one-point joint composition PDF. Alternatively, in the MEPDF approach, the joint composition PDF transport equation is approximated using a weighted discretization in the composition space, and the evolution of the PDF is expressed as sets of deterministic equations of weights and weighted abscissas.

Comparisons between the MEPDF and SLPDF methods have been reported for simulations of reactive precipitation in a plug-flow reactor [19], turbulent scalar mixing, and reacting flows [13]. Akroyd et al. [20,21] systematically compared the MEPDF and SEPDF methods in terms of the formulations and computational performance. For three non-premixed, piloted, methane–air turbulent jet flames [22] with distinctly different levels of local extinction and turbulence-chemistry interactions, Jaishree and Haworth [23] made an extensive comparison of three composition PDF transport models (i.e., SLPDF, SEPDF, and MEPDF) in terms of numerical accuracy and computational efficiency. The RANS- or LES-based multi-environment PDF methods [12–15] successfully predicted the structure of the turbulent non-premixed flames. Recently, in the context of the RANS-based MEPDF approach, Lee et al. [24,25] realistically simulated a turbulent partially-premixed H_2/N_2 lifted jet flame with vitiated co-flow [26] and turbulent CH_4/H_2 flames under moderate or intense low-oxygen dilution (MILD) conditions [27].

In this study, due to the inherent advantages of computational efficiency and compatibility with conventional Eulerian PDF formulation, the MEPDF approach was adopted to systematically analyze combustion processes and precise structures in turbulent partially-premixed flames. Since the MEPDF uses only two or three environments to represent the composition PDF, it requires much less CPU time than stochastic PDF transport approaches that utilize a much larger number of Lagrangian particles or Eulerian fields. Moreover, the present MEPDF approach adopted tabulated chemistry to effectively reduce the numerical burden for the large number of transported scalars involved in the detailed chemistry.

Owing to its robustness and applicability, the present study employed the flamelet-generated manifold (FGM) method [28]. Although the FGM method is capable of drastically reducing the CPU time, it has its own limitations because the manifold is a projection of the whole composition space. Therefore, the reaction pathway in low-dimensional manifolds could be different from that represented by the detailed chemistry. This situation occurs when the real flame is not compatible with the assumptions made during manifold construction or if the definition of the control parameter is inappropriate. It is also uncertain whether these reduced-order manifolds properly represent the flame configuration with multiple combustion regimes. Thus, it is necessary to systematically assess the capability of these manifold-based turbulent combustion models for the prediction of complex partially-premixed flames, including both non-premixed and premixed combustion modes.

Due to modeling difficulties with an inhomogeneous inlet, few computational studies have been conducted for these turbulent partially-premixed flames [3–5] with multiple combustion modes. According to Meares et al. [4], the LES-based Eulerian stochastic field method shows qualitative agreement with the measured instantaneous OH fields, conditional temperature scatters, and flame stabilization characteristics for an inhomogeneous-inlet flame. To precisely identify the reaction regime in turbulent partially-premixed flames, Wu et al. [29] have systematically analyzed the characteristics of the drift term for a partially-premixed turbulent pilot flame with nearly homogeneous and inhomogeneous inlets using the non-premixed flamelet/progress-variable (FPV) model and the premixed filtered tabulated chemistry LES (F-TACLES) formulation. Their numerical results suggest that the drift term is capable of identifying the chemically-sensitive reaction regions. Additionally, the conventional flame index based on major species and flame topology is inadequate to represent the complex physical processes in multi-regime combustion. Perry et al. [30] have proposed a modified FPV model with two mixture fraction formulations to analyze three-stream turbulent partially-premixed jet flames with nearly homogeneous and inhomogeneous inlets. Their numerical results indicate that the predictions of the two-mixture fraction FPV model conform better to the measured structure of the turbulent partially-premixed pilot flame with inhomogeneous inlets compared to the single-mixture fraction approach. Galindo et al. [31] have applied LES-based sparse-Lagrangian multiple mapping conditioning (MMC) to simulate the piloted turbulent flames where the compositional inlet conditions varied from homogeneous to inhomogeneous. This MMC-LES model showed very good agreement with the experimental results for the homogeneous-inlet case with a prevalence of non-premixed combustion; however, it was not able to correctly predict the multi-mode combustion structure of a turbulent stratified premixed flame with an inhomogeneous inlet. Kleinheinz et al. [32] have employed a multi-regime flamelet model to numerically analyze the structure of piloted turbulent partially-premixed flames with an inhomogeneous inlet. In terms of the velocity, mixture fraction, and temperature fields, the numerical results agreed reasonably well with the experimental data [5]. However, in the region further downstream, the conformity with measurements was worse due to underestimation of the local extinction. They also analyzed the effects of mixture heterogeneities on the location of heat release and the combustion modes. By splitting the progress variable source term into the individual contributions of the combustion regimes, they precisely investigated the contributions of premixed and non-premixed combustion as well as the essential mechanism of flame stabilization in partially-premixed jet flames.

However, the state-of-the-art turbulent combustion models have not been extensively explored to assess the prediction capabilities for turbulent partially-premixed flames with a broad range of inhomogeneities and stratification. For these reasons, the present study aims to systematically evaluate the capability of premixed and non-premixed FGM manifolds to predict the fundamental characteristics of turbulent partially-premixed piloted flames with multiple combustion regimes with a RANS-based MEPDF approach. Herein, a novel combustion model that combines the MEPDF approach with an FGM was developed to predict turbulent partially-premixed flames with inhomogeneous inlets. Moreover, the three-environment PDF approach was applied to realistically analyze three-stream turbulent partially-premixed jet flames [5]. Based on our numerical results, detailed discussions are made about the essential features of turbulent partially-premixed flames with multiple combustion modes as well as the limitations of the manifold-based MEPDF approach.

The rest of this paper is organized as follows: in Section 2, we describe the three-environment MEPDF approach and the FGM procedures used in this study. Simulation details are presented in Section 3. The numerical results are presented, and detailed discussions about the essential features of the turbulent partially-premixed flames are presented in Section 4. Finally, in Section 5, we draw conclusions from the present numerical results.

2. Physical and numerical models

2.1. Multi-environment probability density function

MEPDF equations can be derived from a density-weighted transport equation for a one-point one-time joint composition PDF,