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Compliance of combustion models for turbulent reacting flow simulations

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ABSTRACT

The utilization of low-dimensional manifold combustion models for large-eddy simulation (LES) of turbulent reactive flows introduces model simplifications that represent sources of uncertainties in addition to those arising from turbulent closure models and numerical discretization. The ability to quantitatively assess these uncertainties in the absence of measurements or reference results is vital for reliable and predictive simulations of practical combustion devices. This paper is concerned with the extension of the *manifold drift term* to LES to examine the compliance of a particular combustion model in describing a quantity of interest (QoI) with respect to the underlying flow-field representation. This drift term was previously introduced as a key component of the Pareto-efficient combustion (PEC) framework. The behavior of the drift term is examined in a series of test cases. To this end, large-eddy simulations of a partially-premixed turbulent pilot flame with inhomogeneous inlet streams are performed, in which the non-premixed flamelet/progress-variable (FPV) model and the premixed filtered tabulated chemistry LES (F-TACLES) formulation are employed. The drift term is shown to be capable of identifying chemically sensitive regions with respect to user-specific QoIs. With this, a species-specific combustion regime indicator is derived by computing the relative magnitude of the drift terms for different combustion models. Comparisons with commonly employed flame indicators suggests that the flame index and other indicators that are solely based on major species and flame topology are insufficient in describing complex physical processes in multi-regime combustion.

1. Introduction

The modeling of turbulent combustion is complex and requires the consideration of different physico-chemical processes involving a vast range of time and length scales as well as a large number of scalar quantities. Consequently, requirements for computational resources to perform detailed simulations that directly capture the oxidation of realistic fuels remains intractable in practical applications. To reduce the computational complexity, various combustion models are developed. Many of them can be abstracted using a lower-dimensional manifold representation [1]. Common to these techniques is the representation of the thermo-chemical state space in terms of a reduced set of scalars, whose evolution can be computed at a reduced cost. One class of such manifold models, often referred to as flamelet-like or topology-based models, exploits the topological structure of the flame. The solution of representative flame configurations, such as laminar counterflow diffusion flames, freely propagating premixed flames, or unsteady flame elements are often used to construct the reaction-transport manifolds. Examples of topology-based combustion models are the steady laminar flamelet (SLF) formulation [2], the flame prolongation of intrinsic low-dimensional manifold (FPI) [3], the flamelet-generated manifold (FGM) method [4], and the flamelet/progress variable (FPV) formulation [5,6].

A key issue in using such reduced-order models, however, is the assessment as to whether a particular combustion model is adequate in representing a required flame configuration. In this work, we introduce the notion of "model adequacy" as the model's ability of representing a user-specific quantity of interest (QoI), ϕ, within a user-define accuracy and computational cost. This metric is essential in conducting combustion simulations as it determines the user's selection of a combustion model – and with this the necessary computational resources. However, providing a viable answer to the question of an optimal model selection is non-trivial. Consider for instance the case of topology-based manifold models: although the complexity of the combustion process is greatly reduced by this approach, the construction of the manifold introduces assumptions that are specific to the presumed flame

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topology. Models of this type are commonly perceived as being vulnerable to conditions where no single combustion regime dominates or the flow of interest is not represented by a canonical flame configuration. One plausible type of approach to this problem is to assess the applicability of a lower-dimensional manifold model by verifying the basic assumptions that are invoked in the construction of the manifolds. One of the most fundamental assumptions is the reaction–diffusion topology, i.e., the distinction whether the local combustion process occurs in the premixed regime or the non-premixed regime. Several regime indicators have been proposed, including the Yamashita-Takeno flame index that examines the alignment between the fuel and oxidizer gradient [7,8], the flame index that examines the alignment between the mixture fraction and progress variable gradient [9], and a time scale index comparing the relative contributions in the diffusion–reaction balance [10]. Besides the distinction of the reaction–diffusion topology, other modeling assumptions have also been examined by considering flame curvature effects [11,12], non-unity Lewis-number effects [13], pressure effects [14], flame-orthogonal transport effects [15], among others.

Despite previous efforts, two issues remain in the discussion of regime indicators, namely the lack of universality and the indifference to quantities of interest. Due to various assumptions invoked by different combustion models, methods of verifying these assumptions are likely to have the same degree of variety. Such variety limits the capability of cross-model comparisons as well as distinguishing, within each model, relative contributions of different assumptions. In regard to quantities of interest, considerable differences can often be observed in terms of the resilience of different species to complex combustion modes [16]. For instance, due to the reduced computational complexity, flamelet-type models are often employed in simulations of practical combustion systems such as gas turbines, internal combustion engines, rocket motors, and furnaces. Despite the presence of mixed and multiple combustion regimes in these systems, reasonable accuracy of important flow-field quantities, such as major species and heat release, have been obtained. This seemingly contradictory result can be demonstrated by a test case, shown in Fig. 1. Two flames of the same equivalence ratio ($\phi = 1.4$) are considered here: a 1D freely propagating premixed flame (dashed lines) and a moderately stratified flame (solid lines). The detailed configuration of the stratified flame is discussed in [17]. Given the very good agreement in the mass fraction profiles of H_2O and CH_4, the stratified flame can be considered as being "adequately" described by the freely propagating flame in the premixed regime as far as these major species are concerned. However, large deviations of minor species mass fractions, such as CO and NO, indicate that the deviation from the premixed asymptote is highly significant, so that the stratified flame cannot be modeled by a purely premixed flame. Therefore, coarse-grained regime indicators that are solely based on major species mass fractions or progress variable are insufficient to guide model selection for high-fidelity simulations. Furthermore, this result also suggests that the generic notion of a premixed or non-premixed combustion region in a mixed-regime combustion environment can misrepresent the underlying combustion physics.

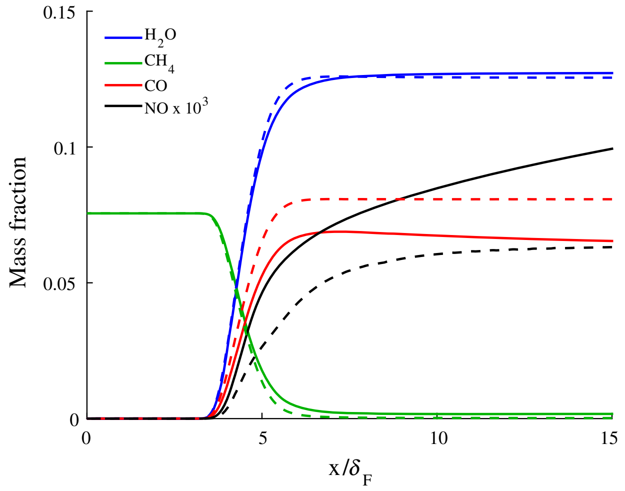

Fig. 1. Comparisons of H_2O, CH_4, CO, and NO mass fractions between a freely propagating premixed flame (solid) and a moderately stratified flames (dashed). The initial conditions are methane/air mixture at ambient condition and the equivalence ratio of $\phi = 1.4$ for both cases.

These issues lead us to a different approach that seeks to asses the "model adequacy", which is to test the compatibility between the combustion model and the local flow-field representation. This compatibility metric can be quantified by a so-called drift term, $\mathscr{D}_\phi$, which is based on the analysis of the manifold geometry and the state-space dynamics on it [1,18]. Quantifying the incompatibility provides a direct assessment of the model's applicability and the species-specific error that is introduced by the manifold without prior knowledge of the true solution. This is essentially a bootstrapping technique. In addition, it is important to emphasize that this technique evaluates the compatibility of a given manifold representation and does not seek to assess the assumptions by which this manifold is constructed. As a result, the method is universal and applicable to all models under the lower-dimensional manifold abstraction, including reaction–diffusion methods, chemical manifolds, among others.

This drift term was derived as a key component of the Pareto-efficient combustion (PEC) framework [17]. Utilizing the drift term, the PEC-framework can dynamically determine the local utilization of different manifold-based combustion models in simulations of chemically reacting flows. In addition, the aforementioned analysis was extended to detect incompatibilities between locally adjacent combustion models. Three user-specified inputs are required for the PEC-framework: a set of candidate combustion models, a set of quantities of interest, and a penalty term for specifying the accuracy-efficiency requirement. The decision on the submodel utilization then takes into consideration both the local error introduced by the manifold models and the associated computational cost in applying the submodels. The resulting procedure has the following features:

- Various manifold-based combustion models can be employed in different regions of a reacting flow simulation to describe local combustion processes of different complexity.
- The choice of combustion models is Pareto-efficient, accommodating the accuracy-efficiency preference that is specified by the user.
- The local accuracy of a particular model is assessed with respect to the quantities of interest.
- Conservation properties and smoothness of the quantities of interest across model interfaces are preserved.

The objective of the present study is to extend the drift term to LES equations. The main focus of this work is to introduce the drift term as a stand-alone indicator of the model compatibility. This extension is essential towards the application of the PEC-framework to LES of turbulent reactive flows. A detailed analysis is conducted on a piloted turbulent flame with inhomogeneous inlets. The configuration is adopted from the experiments performed in [19–21], where both premixed and non-premixed combustion processes take place. Large eddy simulations using both