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A Pareto-efficient combustion framework with submodel assignment for predicting complex flame configurations

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ABSTRACT

The selection of an appropriate combustion model for the numerical prediction of reacting flows remains an outstanding issue. Often, expert knowledge or experimental data is required to make an informed decision in selecting a suitable model. Furthermore, the computational cost that is associated with the application of a certain combustion model introduces another constraint in the selection process. By addressing these issues, the objective of this work is to develop a Pareto-efficient combustion (PEC) framework for application to complex chemically reacting flows under consideration of user-specific input about quantities of interest, desired simulation accuracy and computational cost, and a set of combustion models. PEC utilizes a Pareto efficiency, and introduces a manifold drift term as a measure for determining the adequacy of using a certain combustion-manifold model to predict selected quantities of interest. Since underlying model assumptions are encoded in the manifold, PEC restricts the application of submodels within its intended use. Further, the proposed approach for evaluating the manifold drift provides a rigorous method for combining different combustion models – as long as they can be described by a manifold. As such, this formulation represents a general description for the selection of combustion models, thereby overcoming potential limitations of flame-topology indicators and regime-specific combustion models. The capability of the PEC-framework is demonstrated in application to a tribrachial flame. By considering combustion models from the class of reaction-transport manifolds (inert mixing, equilibrium, flamelet/progress variable, and flame-prolongation in ILDM) and chemistry manifolds (using detailed and skeletal mechanisms), it is shown that PEC locally adapts the submodel fidelity within the user-defined threshold for selected quantities of interest. A parametric analysis is conducted to illustrate the dynamic range of the PEC-framework in accommodating Pareto-efficient submodel arrangements.

1. Introduction

Despite significant progress in combustion modeling, considerable challenges remain in the mathematical description and the simulation of chemically reacting flows. Reasons for this are the physico-chemical complexity, which is associated with the consideration of fluid dynamics and turbulence, the conversion of a large number of chemical species that evolve at vastly different spatio-temporal scales and concentration magnitudes, heat-release and dilatational effects due to exothermic reactions, the description of multiphase processes associated with liquid spray-phase and supercritical combustion processes, and long-range effects such as radiation and thermoacoustic interactions. While often only a subset of these processes is examined in laboratory experiments, they require consideration in practical combustion systems such as gas turbines, internal combustion engines, rocket motors, and furnaces.

Because of the computational complexity that is required to represent the oxidation of realistic fuels using detailed chemical kinetic models, lower-dimensional manifold representations are frequently used to reduce the dimensional complexity [1]. Common to these techniques is the representation of the thermochemical state space in terms of a reduced set of scalars whose evolution is described by the solution of transport equations. Different manifold techniques for combustion applications have been developed [1], and they can be distinguished in chemistry manifolds [2–5], reaction-transport manifolds [6–9], thermodynamic manifolds [10–12], and empirical manifolds [13–16].

Over recent years, several combustion models have been proposed, and many of those models rely on fundamentally different modeling approaches and approximation levels. Different categorizations have been introduced to distinguish among those models. The most common categorization is based on the

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combustion-regime representation [17–21], distinguishing between the asymptotic limits of premixed and non-premixed combustion. More recently, concept-based categorizations have been introduced by differentiating between so-called flamelet-like and PDF-like methods [1]. A more general classification is to distinguish between topology-free and topology-based combustion models.

Topology-free combustion models make limited assumptions about the flame structure, and are therefore agnostic to the underlying combustion regime. These models require the solution of transport equations for all species, and employ different representations to describe scalar mixing and reaction chemistry. Examples for topology-free combustion models are finite-rate chemistry models, the eddy-dissipation concept [22], and probability-density function (PDF) methods [23,24]. Since these models are not constrained to a particular combustion regime, they are considered to be applicable to a wider range of combustion problems. Topology-free models enable the consideration of different combustion-physical processes, such as the higher-dimensional manifold representation of the reaction chemistry, multi-stream systems, or non-adiabatic effects. However, these models are computationally expensive, require special treatment of non-local diffusion processes, and employ special discretization methods to overcome the higher-dimensional formulation in space-time-composition space. Often, topology-free models make use of chemistry manifolds to reduce the computational complexity.

Topology-based combustion models exploit the topological structure of the flame. The flame structure is then represented in terms of reaction-transport or mixing manifolds, which are obtained from the solution of representative flame configurations, such as laminar counterflow diffusion flames, freely propagating premixed flames, or one-dimensional embedded flame elements. The solution of these representative flame configurations is either evaluated prior to the simulation and stored in chemistry libraries or during the simulation to incorporate specific flow-field effects. Examples of topology-based combustion models are the class of flamelet models, including the Burke–Schumann solution [25], the steady laminar flamelet (SLF) formulation [26], the flame-prolongation in intrinsic lower-dimensional manifold (FPI) [7], the flamelet-generated manifold (FGM) method [27], and the flamelet/progress variable (FPV) formulation [9,28].

The construction of reaction-transport manifold models introduces assumptions that are specific to the representation of the flame topology. It is therefore important to appreciate that these assumptions are directly encoded in the topology of the manifold. As such, the trust region of a particular combustion model is defined by its manifold.

Reaction-transport manifolds are parameterized in terms of a reduced set of scalars, typically consisting of mixture fraction, progress variable, enthalpy, strain or scalar dissipation rate. Because of the reduced dimensionality, these models are limited in describing certain combustion processes. To accommodate additional phenomena, these reaction-transport manifolds have been extended to consider effects of wall-heat losses [29–31], radiation [32], autoignition [33–35], multi-stream systems [36–38], and the representation of mixed- and multi-mode combustion regimes [39,40]. While promising, these approaches face potential shortcomings: First, the validation of these extensions relies on data that might not be representative for the practical problem under consideration. Second, these model extensions may substantially increase the complexity, thereby deteriorating the accuracy in capturing the combustion behavior for which the original model was intended. Third, without prior knowledge it is not known which combustion-physical processes require consideration. Fourth, the manifold extension introduces additional unclosed contributions such as cross-dissipation terms or correlations that require modeling. Finally, extended manifold models are applied globally although the combustion-physical processes for which they are developed are confined to a localizes region, such as the autoignition region at the flame base or the near-wall region that is affected by heat transfer and flame/surface coupling.

Common to all applications is the issue of selecting a particular combustion model for simulating a certain flame configuration. This selection is typically guided by factors such as knowledge about the underlying combustion physics, operating conditions, quantities of interest (QoI), computational expenses, necessary model implementation efforts, and – to some extend – also by the bias of the user. Often different models provide comparable predictions for flame configurations that are represented by canonical flames, single combustion regimes, high Damköhler or low Karlovitz numbers, and simple gaseous fuels. Since, however, these combustion models invoke specific assumptions and approximations, their predictive capability reduces with increasing combustion-physical complexity.

Tasked with examining a new combustion configuration, evaluating the impact a burner-design modification has on the pollutant emissions, or assessing the potential of a new combustor concept, a practitioner faces the questions:

- Which combustion model is most adequate to accurately predict a certain quantity of interest?
- How to assess and control the accuracy of a combustion simulation in situ?
- How to balance computational cost and model accuracy during the simulation?
- How to accurately represent combustion-physical processes that are specific to a particular burner?

By addressing these questions, the objective of this work is to develop a novel Pareto-efficient combustion (PEC) framework for the dynamic utilization of different manifold representations to describe chemically reacting flows. Specifically, by combining different manifold representations, PEC enables the general adaptation of combustion submodels to the underlying flow-field representation, thereby providing an accurate description of the combustion-physical complexity. The key attributes of PEC consist in (i) the user-specific selection of a set of combustion models that can be represented by a manifold (such as chemistry, mixing, or reaction-transport manifolds), (ii) a quantity of interest such as temperature, carbon monoxide, nitric oxide, and other pollutants or intermediate species, and (iii) a cost function to describe the desirable cost and accuracy in representing the QoI. Subject to this information, a particular manifold candidate is locally selected that minimizes the cost function. PEC provides direct error control and dynamically adapts the model fidelity so that regions of different combustion-physical complexity are represented by the most appropriate model formulation; regions that are adequately represented by inert mixtures, equilibrium compositions, or quasi one-dimensional premixed or diffusion flame structures are modeled using computationally efficient reaction-transport manifold models, and topologically complex and multi-dimensional combustion processes that control flame dynamics, ignition, flame stabilization, extinction, and blow-out are described using models at higher fidelity. The flexibility in the selection of the penalty term on the cost function enables the consideration of the computational cost, since the demand for the simulation accuracy and computational expenses can vary at different stages during the model application. Beyond the specification of the set of manifolds candidates, QoI, and cost function with penalty term, PEC requires no additional user input. The local selection of the submodel is determined using the manifold drift function as metric for the model accuracy. Therefore, PEC can accommodate different combustion submodels without the requirement for expert knowledge on the model selection. Quantities of interest and desirable model accuracies are usually known requirements on the combustion simulation.

The proposed Pareto-efficient combustion modeling framework has the following main ingredients: (i) a metric for examining the