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Shared low-dimensional subspaces for propagating kinetic uncertainty to multiple outputs

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ABSTRACT

Forward propagation of kinetic uncertainty in combustion simulations usually adopts response surface techniques to accelerate Monte Carlo sampling. Yet it is computationally challenging to build response surfaces for high-dimensional input parameters and expensive combustion models. This study uses the active subspace method to identify low-dimensional subspace of the input space, within which response surfaces can be built. Active subspace methods have previously been developed only for single (scalar) model outputs, however. This paper introduces a new method that can simultaneously approximate the marginal probability density functions of *multiple* outputs using a single low-dimensional *shared subspace*. We identify the shared subspace by solving a least-squares system to compute an appropriate combination of single-output active subspaces. Because the identification of the active subspace for each individual output may require a significant number of samples, this process may be computationally intractable for expensive models such as turbulent combustion simulations. Instead, we propose a heuristic approach that learns the relevant subspaces from cheaper combustion models. The performance of the active subspace for a single output, and of the shared subspace for multiple outputs, is first demonstrated with the ignition delay times and laminar flame speeds of hydrogen/air, methane/air, and dimethyl ether (DME)/air mixtures. Then we demonstrate extrapolatory performance of the shared subspace: using a shared subspace trained on the ignition delays at constant volume, we perform forward propagation of kinetic uncertainties through zero-dimensional HCCI simulations – in particular, single-stage ignition of a natural gas/air mixture and two-stage ignition of a DME/air mixture. We show that the shared subspace can accurately reproduce the probability of ignition failure and the probability density of ignition crank angle conditioned on successful ignition, given uncertainty in the kinetics.

1. Introduction

The development of detailed kinetic models involves compiling a set of elementary reactions whose rate constants can be determined from experimental measurement, reaction-rate theory, or a combination of both. For large hydrocarbon fuels, many reaction pathways and rates are determined via extrapolation from the knowledge of the reactions for smaller species, a process that inevitably contains uncertainties. Whether the collective uncertainties in kinetic models can be small enough to meet a certain level of chemical accuracy, and to satisfy the needs of combustion simulations with prescribed accuracy requirements, remains an open question.

The forward propagation of chemical kinetic uncertainties to combustion simulation results is one of the central steps towards addressing the above question. For the simulation of simple combustion problems such as homogeneous reactors or one-dimensional flames, quantifying the uncertainty in the outputs due to kinetic uncertainty, and comparing these output uncertainties with experimental data that are endowed with error bars, constitutes a comprehensive validation of a given chemical mechanism. For the simulation of practical combustion problems involving turbulence-chemistry interaction and complex boundary

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conditions, quantifying the uncertainties originating from the kinetics leads to a more rigorous assessment of the predictability of simulations.

For simple combustion problems [1–8], probabilistic methods have been developed to quantify the uncertainties in simulations arising from chemical kinetics. Most of the cited works employ non-intrusive methods, although intrusive methods have also been investigated [2]. For small mechanisms, the computational cost of each deterministic simulation is relatively low, such that classical Monte Carlo (MC) (or quasi-Monte Carlo) methods that use a large number of samples from the kinetic parameter space are affordable [5]. For large mechanisms, each deterministic simulation is computationally expensive; hence one must approximate the input parameter–to–output relationship using various response surface techniques such as the sensitivity analysis based (SAB) method [9], polynomial chaos expansions (PCE) [3,10], high dimensional model representations (HDMR) [11], artificial neural networks (ANN) [12], and combinations thereof such as ANN-HDMR [12]. These techniques have been used to facilitate forward uncertainty quantification in conjunction with MC methods. A comprehensive review of response surface methods in the context of combustion simulations can be found in [13]. In addition, PCE and HDMR provide global sensitivity indices of the kinetic parameters via a simple post-processing of the coefficients in the fitted polynomial representation. These sensitivity analyses partition the output variance among individual reactions and provide insights for model development. However, response surface methods – like all function approximation methods – face a fundamental scaling difficulty when applied to high-dimensional inputs. For example, the number of coefficients in a total-degree polynomial expansion increases exponentially with the number of input parameters; this is a symptom of the 'curse of dimensionality' [14].

Various methods can be used to reduce the dimension of the input parameter space and thus accelerate the construction of response surfaces. Local sensitivity analysis and screening methods have been used in [11,15-17] to identify the reactions that contribute most to uncertainties in the outputs. Subsequent response surface construction and MC analysis will then only involve these important reactions. Recently, the active subspace (AS) dimension reduction method has attracted much attention in uncertainty quantification (UQ) applications, such as airfoil design [18], battery modeling [19], hydrologic modeling [20], and so on. The term "active subspace" first appeared in the thesis by Russi [21]. Further discussion of active subspace methods, including numerical implementation issues, can be found in Constantine [22]. While sensitivity analysis aims at identifying which of the input parameters are important for explaining the variability of the output, the AS approach identifies important directions in the input space that are linear combinations of the input parameters. Since the subspace is not constrained to be aligned with the canonical basis, as is the case for standard sensitivity analysis, the AS approach can lead to more efficient dimension reduction. Given a particular scalar output of interest, written as a function of the input parameters, the important or "active" directions are identified via the dominant eigendirections of a matrix defined as the second moment of the gradient of this function. A certain number of gradient evaluations, at distinct sample points in the input parameter space, are required to obtain good estimates of this dominant eigenspace. This number grows weakly with the input parameter dimension (e.g., with the log of the dimension [23]). Additionally, since most legacy combustion codes do not use the adjoint method to efficiently compute the gradient of a simulation output, the gradients themselves must be estimated by either finite differences or local linear fitting. Consequently, the number of simulation runs required will be at least linearly proportional to the dimension of the input parameters [22].

The number of simulations that can be undertaken, however, is severely limited for expensive models; multi-dimensional turbulent combustion simulations can take days to weeks for each sample of the kinetic parameters. In the work of Mueller et al. [24] for large eddy simulations (LES) combined with a steady flamelet model, high dimensional kinetic uncertainties are propagated into a low-dimensional flamelet table, and then injected into the LES solver. Specifically, the uncertainty in the kinetic parameters leads to uncertainties in the tabulated profiles of density, temperature, and species concentration. Only the density is needed to evolve the LES governing equations, which proceeds by random sampling of density profiles indexed by a single stochastic dimension. The uncertainties in the profiles of temperature and species concentration can be determined by combining the uncertainties of the tabulated profiles of the flamelets and the uncertainties of the mixture fraction from the flow solver. This UQ algorithm has been demonstrated with Sandia Flame D [25], showing that the uncertainty due to the rate constants is large enough to account for nearly all of the discrepancies between the LES/flamelet results and experimental measurements. The approach, although efficient, is nevertheless only applicable to simulations with flamelet-like combustion models.

In this work, using a heuristic approach analogous to that employed for the reduction of detailed chemical mechanisms, we propose to identify low-dimensional subspaces of the uncertain kinetic parameters using representative (and cheap) simulations of homogeneous reactors and one-dimensional laminar flames. These subspaces are then used to quantify the impact of kinetic uncertainty in the expensive target combustion simulation. This UQ approach is also compatible with a wide variety of turbulent combustion models.

Of course, training with many different cheap combustion problems will, in general, yield many different input subspaces. A way of combining subspaces obtained from *multiple* distinct outputs is then required for our overall UQ approach to work. One could identify the active subspace for each training model and then take a union of these subspaces in a straightforward way (e.g., via Gram-Schmidt orthogonalization), but at the price of increasing the dimensionality of the subspace. We will instead formulate a *shared subspace* method that yields a subspace whose dimension is no larger than the maximum dimension of the active subspace of each individual training model. This shared subspace has the property of being able to reproduce the *marginal* probability density function of the output of each training model. We will then use the shared subspace to propagate uncertainty through the complex/expensive combustion model.

The rest of the paper is organized as follows. In Section 2, we recall the active subspace method and introduce our shared subspace methodology; then we describe our approach for training the shared subspace from multiple model outputs. In Section 3, we demonstrate the performance of the active subspace for a single output and the shared subspace for multiple outputs of the training models, using mechanisms for hydrogen, methane, and dimethyl ether (DME) combustion. Then we evaluate performance of our approach for a zero-dimensional HCCI simulation. The conclusion is in Section 4.

2. Methodology

This work focuses on the uncertainties in the reaction rates. Following previous works [1–3,7,8], the rate constants of reactions are presumed to be independent and the rate constant of an individual reaction, e.g., reaction j, is characterized by a lognormal distribution with a nominal value k_{j0} and a temperature-independent uncertainty factor UF_j. We interpret one third of the uncertainty