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# Model form uncertainty quantification in turbulent combustion simulations: Peer models

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ABSTRACT

Turbulent combustion simulations invoke a number of component models for chemical kinetics, turbulence, flame structure, etc., each of which has an error associated with its structural form and contributes to overall uncertainties in simulation results. These model form errors arise from the necessity of making assumptions in deriving a model. Conventional approaches to estimating model form errors rely on an *ad hoc* additive error that is then calibrated against experimental or computational data. These approaches inherently neglect any *a priori* knowledge of physics in developing the model error estimate. Instead, in this work, an inherently physics-based approach to estimating model form error is developed based on the notion of "peer" models. In the generic approach, the error in a candidate model is determined by taking the difference between it and an equally plausible alternative "peer" model with a different set of assumptions. The generic approach is applied in this work to the modeling of the subfilter mixture fraction dissipation rate, which is typically modeled as the ratio of the subfilter mixture fraction variance and a time scale. The typical time scale approximation invokes a turbulent time scale, and a "peer" model is proposed in which a chemical time scale is invoked to estimate the model form error. Using stochastic collocation, the subfilter mixture fraction dissipation rate model form error as well as the uncertainty in a model parameter are propagated through LES calculations of the Sandia D Flame utilizing the steady flamelet model. The results indicate that the mixture fraction, temperature, and carbon monoxide uncertainties increase with downstream distance due to an increase in the relative subfilter mixture fraction variance and increased sensitivity to the time scale approximations, which diverge in magnitude with downstream distance. Uncertainties in these quantities arising from the model form error are shown to be more significant than uncertainties arising from the model constant uncertainty. For the temperature, uncertainties due to chemical kinetic rate uncertainty are shown to be slightly smaller than uncertainties due to the subfilter mixture fraction dissipation rate model error; for the carbon monoxide mass fraction, uncertainties due to chemical kinetic rate uncertainty are twice as large as uncertainties due to the subfilter mixture fraction dissipation rate error since carbon monoxide is more kinetically-controlled than the temperature.



## 1. Introduction

Uncertainties in turbulent combustion simulations arise from three distinct sources: uncertainties in boundary or operating conditions, uncertainties in component model parameters such as chemical kinetic rate coefficients, and structural uncertainties associated with the form of component models. The first source of uncertainties, that is, those associated with boundary conditions, have been widely addressed in individual works and in collective workshops such as TNF [1]. In cases where accurate experimental measurements of boundary conditions are not available, authors often explicitly quantify the sensitivity of simulation results to boundary condition variables; in cases where accurate experimental measurements of boundary conditions are available, these can be directly (statistically) imposed in simulations (see, e.g., [2–4]). The latter two sources of uncertainties could be considered either simulation uncertainties or model errors. In the model development community, the prevailing view of these uncertainties is model errors, and the ultimate goal of model validation is to determine where, when, and why model errors are large in an effort to either determine the limits of model applicability or identify model components that require additional refinement.

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However, an alternative view is to accept these errors as uncertainties and develop algorithms to estimate the model error and quantify the subsequent prediction uncertainty.

Efforts in turbulent combustion modeling have focused primarily on the second class of uncertainties, that is, parametric uncertainties in component model coefficients, and have applied formal uncertainty propagation techniques. Due to the large number of component models involved in a turbulent combustion simulation, treating the coefficients of some of the component models as uncertainties can assist in isolating the model error associated with one of the component models. Mueller et al. [5] first applied formal uncertainty propagation techniques to turbulent combustion simulations by developing a method to propagate the uncertainties in chemical kinetic rate coefficients through a Large Eddy Simulation (LES) calculation of a turbulent partially premixed piloted jet flame. Their results showed that the simulation uncertainties in temperature and species mass fractions due to uncertainties in the chemical kinetic rate coefficients were comparable to the discrepancies with the experimental measurements. The implication is that, due to the uncertainty associated with combustion chemistry, the discrepancies between the flamelet-based LES model and the experimental measurements were insufficient to invalidate the combustion model. Related approaches for uncertainties in chemical kinetic rate coefficients are being pursued by other groups [6]. In a later work, Khalil et al. [7] propagated parametric uncertainties associated with subfilter transport models, that is, the Smagorinksy constant and subfilter Prandtl and Schmidt numbers, through LES calculations of a turbulent nonpremixed bluff body flame. Their results showed that there was significant uncertainty in the velocity and scalar fields due to the uncertainty in the subfilter transport models. Interestingly, their results showed that the uncertainties in the mean axial velocity and root-mean-square scalars were attributed to uncertainty in the Smagorinsky constant while the uncertainties in the root-mean-square axial velocity and mean scalars were attributed to the uncertainties in the subfilter Prandtl and Schmidt numbers. These results highlight the fact that the relative contributions of model uncertainties are a strong function of the quantity of interest, and model uncertainties may not be apparent in all quantities of interest (i.e., in the cited work, focusing only on the mean scalar fields would have led to the conclusion that uncertainties associated with the Smagorinksy constant are unimportant).

The third class of uncertainties, that is, structural uncertainties associated with the form of component models has received far less attention. The only works to date have followed the same basic *data-based* approach that is commonplace in a variety of domains. First, an additive stochastic model "mismatch" or "inadequacy" term is "embedded" into a component model [8,9] as a representative model for the model form uncertainty. Second, this "mismatch" term is calibrated against experimental data. Finally, this calibrated model uncertainty is propagated through a turbulent combustion simulation to assess the effects of this uncertainty on various quantities of interest. The first such work following this basic algorithm applied to turbulent combustion modeling, from Mueller and Raman [10], sought to assess the effects of upstream combustion model errors on downstream predictions of soot volume fraction in a turbulent nonpremixed piloted jet flame. The error in the combustion model was limited strictly to the temperature, and the additive model "inadequacy" term was simply estimated from the baseline model's discrepancy with available experimental measurements. The results showed that the resulting uncertainty in the downstream soot volume fraction prediction was comparable to the experimental uncertainties in those measurements. More recent works have introduced more sophisticated calibration techniques based on Bayesian inference [6].

While useful in better understanding the relationships between input and output uncertainties in turbulent combustion simulations, *data-based* approaches suffer from two fundamental flaws as a general framework for quantifying model form uncertainty. First, the model form uncertainty estimate is only as good as available data, and data is inherently limited. There is no guarantee that a model "inadequacy" calibrated against a given data set is general, and, in many instances, an estimate of the uncertainty of a component model is required when there is no available experimental data for this "inadequacy" calibration. Second, purely *data-based* approaches essentially discard *a priori* knowledge of physics, especially fundamental constraints. As an example, in the authors' previous work cited above [10], the temperature error was presumed to be Gaussian, that is, an unbound temperature, which violates fundamental laws of thermodynamics. Admittedly, in practice, this is latter point is sometimes not a major concern. For this cited example, the probability of a temperature far below an environmental temperature or far above the equilibrium flame temperature would be vanishingly small, although not strictly zero.

Therefore, rather than relying on *data-based* model "inadequacy" calibration, a new *physics-based* approach is required for estimating model form uncertainty. Unlike *data-based* approaches, *physics-based* approaches have the potential to be widely applicable since they will be based on general physical principles rather than available data. In this paper, a *physics-based* approach is developed that presumes no knowledge about the specific assumptions that lead to a model. The approach will be demonstrated within the context of turbulent combustion modeling, but the generic approach can be extrapolated to any domain of interest. However, as with any *physics-based* approach, the specific application details of the generic approach will be different in other domains.

In this paper, the *physics-based* approach is detailed in the next section. The approach invokes a "peer" model to develop an estimate for the uncertainty in a model and is applied specifically to the modeling of the subfilter mixture fraction dissipation rate, a key parameter in turbulent combustion models. In the following two sections, the approach is used to quantify the prediction uncertainties in a Large Eddy Simulation (LES) calculation of turbulent partially premixed piloted jet flame. Uncertainties resulting from the subfilter mixture fraction dissipation rate model are compared with prediction uncertainties resulting from parametric uncertainties in chemical kinetic rate coefficients, quantified in previous work [5].

## 2. Model form uncertainty quantification: "Peer" models

Consider a candidate model $\mathcal{M}$, which relates any number of input variables $x$ to some output quantity of interest $\mathcal{M}(x)$. The model is only an approximation to first principles $\mathcal{F}$ due to a combination of a reduced set of input variables and a presumed functional dependence on the input variables. The model error $\varepsilon$ results from these two facts and, without loss of generality, can be defined as the difference between the model and first principles:

$$\mathcal{F}(x,y) = \mathcal{M}(x) + \varepsilon(x,y)\,, \tag{1}$$

where $y$ are additional input variables that the first principles relationship $\mathcal{F}$ may depend on that the model $\mathcal{M}$ does not consider. The first principles relationship $\mathcal{F}(x,y)$ is generally not explicitly known and follows implicitly from other relationships such as the governing equations. As a result, the model error $\varepsilon(x,\ y)$ is unknown and must be estimated. In *data-based* approaches, the model error is calibrated against a finite number of realizations of the first principles relationship $\mathcal{F}(x,y)$, but, as discussed above, such data are not always available. The requirement that