Uncertainty Quantification of Operating Conditions on the Structure of Turbulent Premixed Flames Using Non-Intrusive Surrogate Modeling Strategy

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Premixed flames may suffer from uncertainties associated with operating conditions, chemistry, turbulence, and turbulence-chemistry interactions. These uncertainties negatively impact the confidence in the predictive capabilities of the computational tools. The use of Uncertainty Quantification (UQ) aims to quantify such uncertainties to enable improved confidence in the predicted results and reliability of computational tools. Two non-intrusive techniques exist for UQ studies: surrogate modeling and direct modeling. While the direct Monte Carlo (MC) technique offers accurate results, it tends to be computationally expensive for large-scale studies. Surrogate modeling techniques, however, are much less computationally expensive. In the present study, we use the surrogate modeling strategy to perform UQ of operating conditions on the features of laminar and turbulent premixed flames. First, we evaluate the performance of three surrogate modeling techniques, namely, stochastic collocation (SC), polynomial chaos expansion (PCE), and Gaussian process (GP) in comparison to the direct MC technique, which showed promising results with the SC and PCE approaches at a significantly much lower computational cost compared to GP and direct MC approaches. Therefore, we consider PCE as the surrogate technique to perform UQ of laminar and turbulent premixed flames by considering the equivalence ratio as the uncertain input parameter and flame speed and thickness as the output parameters. The results demonstrate the efficacy of the surrogate technique on propagating the uncertainty associated with input parameters in the output parameters.

I. Introduction

Chemically reacting turbulent flows occur in several energy conversion and propulsion devices such as internal combustion engines, swirl combustors, gas turbines, and rocket combustors. Large-eddy simulation (LES) of such flows, which exhibit the presence of unsteady flow features, is considered to be a promising approach for their investigation [1–3]. However, LES-based studies suffer from uncertainties associated with the modeling of chemistry, turbulence, turbulence-chemistry interaction, thermodynamics, physical constants, and boundary and operating conditions. Therefore, characterizing the uncertainties is necessary to improve upon the predictive capabilities of an LES, which can enhance reliability in LES-based design, control, and optimization studies. Here, a particular focus is on analyzing the effects of the uncertainties associated with the input parameters. Such input uncertainties can be embedded within the underlying mathematical model of an LES by employing probabilistic approaches to the physical system of interest [4]. In this study, the accuracy and efficiency aspects of non-intrusive approaches to account for input uncertainties are examined in the context of LES of turbulent premixed flames.

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Uncertainty quantification (UQ) is aimed to characterize the effects of input uncertainties on a system's response, i.e., the quantities of interest (QoI). In general, UQ can be classified into a forward UQ and an inverse UQ. Forward UQ [5, 6] examines the uncertainties in QoI by propagating the known statistics of the input uncertainties. On the other hand, inverse UQ [7–9], aims to quantify the input uncertainties against available observations in a manner so that the discrepancies between the computational results and the observations can be minimized. In this study, we perform forward UQ to understand the effects of uncertainties in operating conditions on the features of laminar and turbulent premixed flames. We consider the well-established Bayesian inference-based probabilistic approach in this study to obtain the statistics of QoI.

In the Bayesian inference-based approach, the input parameter space is usually explored by using the direct Monte Carlo (MC) sampling technique [10]. Although such a method is popular, a major challenge associated the MC sampling is the requirement of a large number of simulations to obtain statistical convergence. This limitation of the direct MC approach renders it computationally prohibitive for the study of chemically reacting flows. To alleviate this challenge, metamodels also referred to as surrogate models, emulators, or response surfaces have been developed, which use a limited number of expensive forward evaluations and employ a learning algorithm. Such surrogate models usually take much less computational time and maintain the input/output relation to a desirable accuracy [11, 12]. Some of the commonly used surrogate models include radial basis functions [13], moving least-squares [14], artificial neural networks [15], and stochastic spectral approaches [16–19]. The surrogate models relying on stochastic spectral techniques such as Gaussian process [20] (GP), generalized polynomial chaos expansion [21] (PCE), and stochastic collocation [22] (SC) have received greater attention in past studies when expensive forward evaluations are involved. Therefore, these three surrogate models are considered in the present study.

The objective of the present study is to assess the performance of well-established surrogate models, namely PCE, SC, and GP for forward UQ of premixed flames and then use the optimally performing surrogate model to perform UQ of laminar and turbulent premixed flames. The assessment study is carried out by considering freely propagating laminar premixed flame where the uncertain input parameter is considered to be a parameter in the globally reduced chemical kinetics and the QoI is considered as the laminar flame speed. Afterward, the forward UQ study of laminar and turbulent premixed flames is carried out by considering the equivalence ratio as the uncertain parameter and flame speed and flame thickness as the QoI. This article is arranged as follows. A description of forward UQ formulation and the numerical approach is discussed in Sec. II. Section III describes the computational setups considered in this study. The discussion of results pertaining to the assessment of surrogate approaches against the direct MC technique and the application of optimally performing surrogate approach for forward UQ of laminar and turbulent premixed flames are presented in Sec. V. Finally, the outcomes of this study and outlook are summarized in Sec. VI.

II. Computational Approach

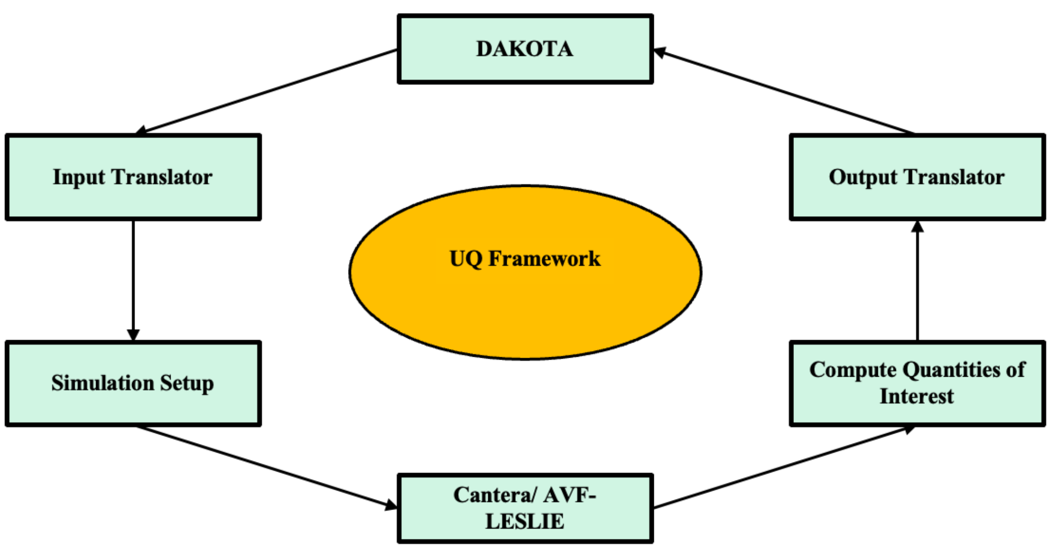

Figure 1 Computational strategy for performing forward UQ study.

A schematic of the computational approach to perform the forward UQ study is shown in Fig. 1. Overall, the approach utilizes the DAKOTA software [22] for driving the UQ study by using the solvers for laminar and turbulent premixed flames. The simulation of one-dimensional laminar flames is performed using Cantera software [23] and the simulation of turbulent premixed flames is carried out using AVF-LESLIE solver [24-27].

A. DAKOTA

The non-intrusive forward UQ is performed using a well-established open-source software referred to as Dakota [22]. Some of the well-established algorithms available in Dakota include ‘Quantification of Uncertainty for Estimation, Simu- lation, and Optimization’ (QUESO), ‘DiffeRential Evolution Adaptive Metropolis’ (DREAM), and ‘Gaussian Process Models for Simulation Analysis’ (GPMSA). Apart from the ability to conduct direct MC sampling, these approaches allow using surrogate models such as PCE, SC, and GP.

B. Cantera

Cantera is an open-source software [23], which can be used for solving problems involving chemical kinetics, thermodynamics, and transport processes. We use this solver to simulate freely propagating one-dimensional (1D) laminar premixed flame. The software can be interfaced with different programming languages. We have employed a Python-based interface of this software to perform the simulations.

C. AVF-LESLIE

AVF-LESLIE is a well-established three-dimensional (3D) parallel, multi-species compressible reacting flow solver [24-27]. It is a multi-physics simulation tool capable of performing simulation of reacting/non-reacting flows. It has been extensively used in the past to study a wide variety of flow conditions, including acoustic flame-vortex interaction, premixed flame turbulence interaction, non-premixed combustion, and compressible turbulence. It utilizes a finite volume-based spatial discretization on a structured grid using the generalized curvilinear coordinates and is second-order accurate in space and time. The solver can handle arbitrarily complex finite-rate chemical kinetics. The mixture-averaged transport properties, the finite-rate kinetics source terms, and the thermally perfect gas-based thermodynamic properties are obtained using the Cantera software [23]. The parallelization of the solver is based on the standard domain decomposition technique based on the message-passing interface library.

III. Computational Setup

We consider three test cases in the present study. These cases are labeled as cases A, B, and C. While cases A and B correspond to freely propagating 1D laminar premixed flames, Case C is a turbulent premixed flame where an initially planar and laminar premixed flame interacts with a decaying isotropic turbulent flow.

Case A: This case is considered to establish the reliability of surrogate modelling techniques, where we assess the performance of PCE, SC, and GP approaches in comparison to the direct MC method. We consider a 1D laminar methane/air premixed flame with a reference temperature of 570 K and pressure of 1 atm (see Fig. 2). We employ a finite-rate chemical kinetics approach by using a globally reduced chemical kinetics comprising 1-step and 5-species [28], where the reaction-rate model is specified as:

$$\dot{w} = Ae^{-E_a/R_u T}[F]^a[O]^b$$

In this study, the uncertain input parameter was determined to be the pre-exponential factor $A \in [A_{min},\ A_{max}]$, where $A_0 = 2.4 \times 10^{16}$ is the nominal value reported in the literature. We consider the laminar flame speed (S_L) to be the QoI.

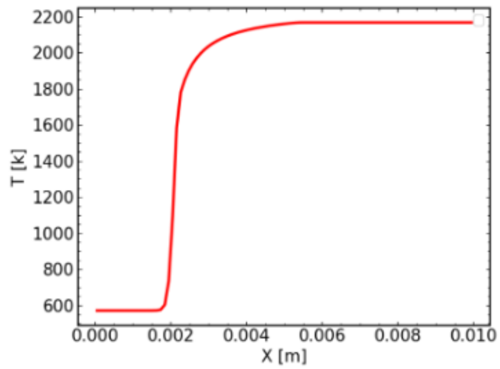

Figure 2 1D laminar premixed flame with reactants on the left and products on the right.

Case B: This test case is like Case A, where the primary difference in the uncertain input parameter and the QoI. Specifically, the equivalence ratio ϕ is considered as the uncertain input parameter and laminar flame speed and thickness are considered as the QoI. Here, the finite-rate kinetics is accounted by employing a 4-step and 8-species chemical mechanism [29].

Case C: This case corresponds to the interaction of an initially premixed laminar flame with a decaying isotropic turbulence. Figure 2 shows a schematic of this configuration, where the initial flame front is specified near the center of the computational domain with reactants and products on its left and right sides, respectively. The extent of the computational domain is a cube of size $L = 0.0055$ m. The flow field is initialized using an isotropic turbulent flow field and is superimposed with a one-dimensional planar flame solution obtained at equivalence number ϕ, reference temperature of 570 K, and pressure of 1atm. These conditions are chosen based on past studies of such flames [30,31]. A characteristic-based inflow-outflow boundary condition is used in the streamwise direction, and a periodic boundary condition is used along the spanwise and transverse directions. For the forward UQ study, ϕ is considered as the uncertain input parameter and turbulent consumption speed is considered as the QoI.

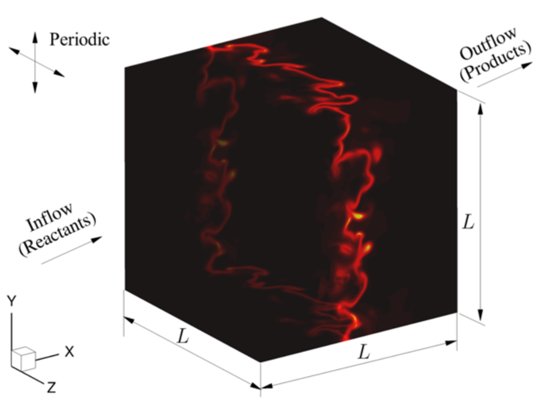

Figure 3 Schematic of the turbulent premixed flame configuration.

IV. Results and Discussion

A. Assessment of Surrogate Models

To evaluate the uncertainty of reaction parameter A on laminar flame speed, a range was specified for the variation of A with a uniform distribution. The mean was set at a value of 2.4e16 with a standard deviation of 1.33e16. The lower and upper bounds were given to be 9.06e14 and 4.71e16, respectively. For the MC approach, 5000 evaluations were run, while the surrogate modelling techniques emulated 5000 evaluations.

The results of the initial study showed promising results for both PCE and SC approaches. PCE and SC yielded the same values of mean, standard deviation, skewness, and kurtosis. GP did not offer as much accuracy as the other two surrogate modelling techniques. Tabulated results of the assessment at a sparse grid level of 4 can be found in Figure 2. With PCE yielding accurate results the fastest, it was chosen to be the surrogate modelling approach moving forward.

Sparse Grid Level 4						
Method	**Time (s)**	**Mean**	**Standard Deviation**	**Skewness**	**Kurtosis**	**Evaluations**
Monte Carlo	9005.87	0.492	0.127	-0.624	-0.0312	5000
Polynomial Chaos Expansion	17.51	0.49	0.127	-0.614	-0.0519	9
Stochastic Collocation	17.7	0.49	0.127	-0.614	-0.0519	9
Gaussian Processing	121.8	0.424	0.167	-0.287	-1.079	60

Table 1: Comparison of statistics of QoI obtained using surrogate modeling techniques with the statistics obtained using the direct MC technique.

B. Forward UQ of Laminar Premixed Flame

For this study, we consider two quantities of interest, namely, the laminar flame speed and the laminar flame thickness (thermal thickness). A range for the equivalence ratio ϕ was considered to be within 0.6 to 1.2 with a mean of 0.9. The standard deviation of ϕ is calculated based on a uniform distribution, which is specified as 0.173. We examine the sensitivity of the results by considering a sampling of ϕ based on normal and uniform distribution with the same range and standard deviation of ϕ. Overall, in each case, with the input parameters specified for Dakota software, the laminar premixed flame solution is obtained at 9 values of ϕ from which 5000 samples are calculated using surrogate technique to obtain the statistics of QoI.

Figures 4 and 5 show the normalized histogram of the flame speed and flame thickness when using a normal and a uniform distribution of the uncertain input parameter. Qualitatively, we observe a similar behavior of the histogram in the two cases. In particular, the flame speed is negatively skewed, whereas the flame thickness is positively skewed. Quantitatively, the statistics of the QoI summarized in Table 2 and 3 demonstrate some sensitivity to the types of distribution (uniform or normal) of the uncertain input parameters. However, this sensitivity is greater particularly for the higher-order statistics such as skewness and kurtosis. The computational cost of the case with normal distribution is lower compared to the case with uniform distribution, which is associated with the convergence of the simulation of 1D laminar premixed flames using Cantera.

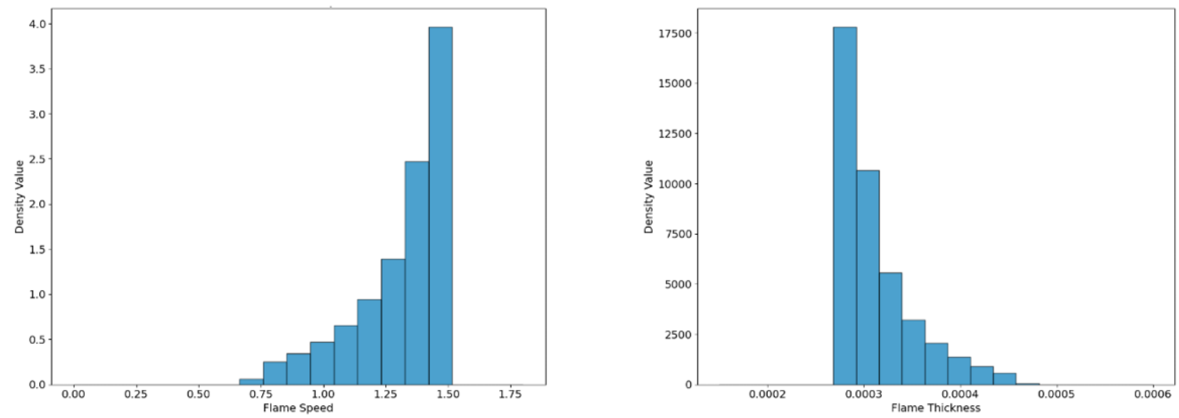

Figure 4: Normalized histogram of the flame speed and flame thickness obtained using the forward UQ study of the laminar premixed flame by using a normal distribution of the uncertain equivalence ratio.

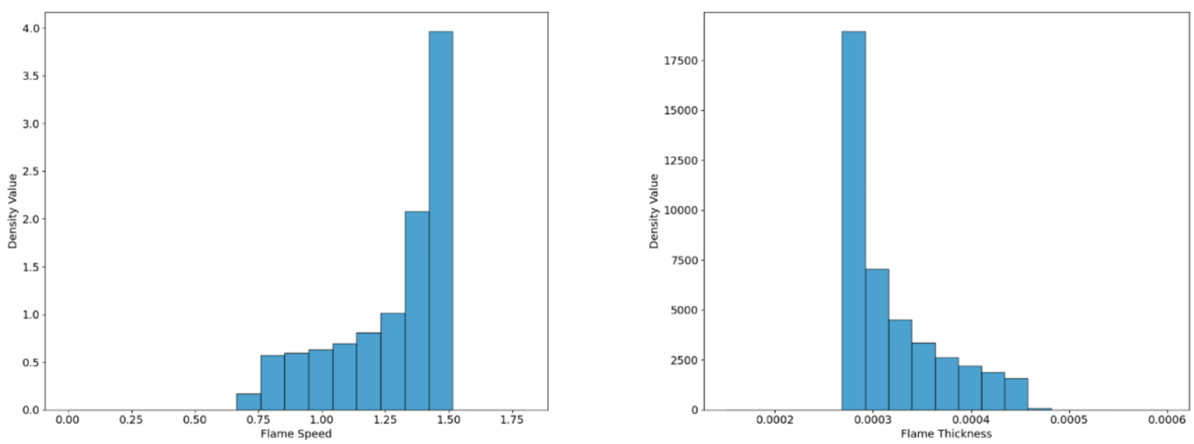

Figure 5: Normalized histogram of the flame speed and flame thickness obtained using the forward UQ study of the laminar premixed flame by using a uniform distribution of the uncertain equivalence ratio.

Table 2: Statistics of the flame thickness obtained from the forward UQ study of laminar premixed flame.

Distribution	Time (s)	Mean (m)	Standard Deviation (m)	Skewness	Kurtosis
Normal	45.52	0.000311	0.0000398	1.44	1.65
Uniform	76.1	0.000318	0.0000509	1.09	0.0089

Table 3: Statistics of the flame speed obtained from the forward UQ study of laminar premixed flame.

Distribution	Time (s)	Mean (m/s)	Standard Deviation (m/s)	Skewness	Kurtosis
Normal	45.52	1.31	0.0177	-1.31	0.911
Uniform	76.1	1.27	0.0217	-1.01	-0.278

C. Forward UQ of Turbulent Premixed Flame

Now, we perform the forward UQ study of the turbulent premixed flame. Similar to Case B, we consider a range of $\phi \in [0.6, 1.2]$ with a mean of 0.9. The standard deviation of ϕ is specified to be 0.173. We consider the normalized turbulent consumption speed to be the QoI in this problem. Overall, 9 3D simulations are performed using the values of ϕ sampled from a normal distribution and 5000 samples of QoI are obtained using the surrogate PCE technique.

Figure 6 shows the normalized histogram obtained for this case. We can observe that compared to the results obtained for the laminar flame speed of the laminar premixed flame in Sec. V (B), the behavior of the histogram is different, which can be attributed to the effects of turbulence-chemistry interaction. Specifically, the histogram shape is broader with a marginally positive skewness. This results into a higher standard deviation compared to the laminar flame, which is evident from the statistics of this case summarized in Table 4.

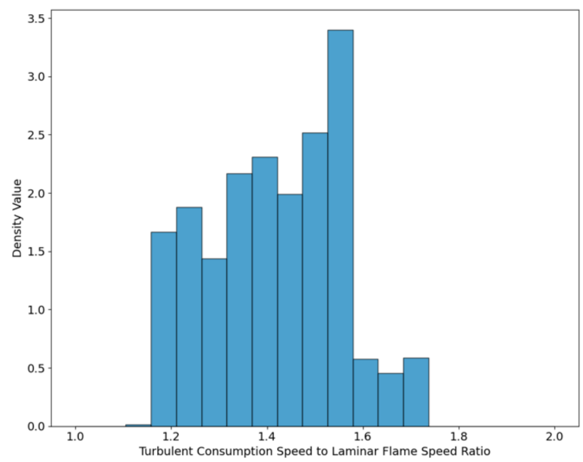

Figure 4: Normalized histogram of the ratio of turbulent consumption speed and laminar flame speed obtained using the forward UQ study of turbulent premixed flame.

Table 4: Statistics of the normalized consumption speed from the forward UQ of turbulent premixed flame.

Mean	Standard Deviation	Skewness	Kurtosis
1.42	0.136	0.00764	-0.861

V. Conclusions

Quantification of uncertainties associated with operating conditions that are prevalent in turbulent combustion can allow for a greater confidence level in the prediction of quantities of interest. However, performing UQ using a direct strategy tends to be computationally prohibitive. Therefore, alternate efficient strategies are needed to examine the effects of uncertainties. In this study, we assessed the performance of computationally efficient surrogate non-intrusive techniques for carrying out forward UQ of premixed flames.

For the forward UQ study, we consider both laminar and turbulent premixed flames. First, we compared surrogate approaches, namely, PCE, SC, and GP with the direct MC approach by considering laminar premixed flame, where we observed that the PCE approach yielded accurate and efficient results. For the UQ study of this case, the chemical kinetics parameter was considered to be the uncertain parameter and the laminar flame speed was considered to be the QoI. Afterward, we used the PCE as a surrogate technique to examine the effects of uncertainty in the equivalence ratio on the speed and thickness of laminar and turbulent premixed flames. Overall, the statistical behavior of flame speed was altered, possibly due to the presence of turbulence-chemistry interaction in turbulent premixed flame configuration.

The results in this study demonstrated the efficacy of the employed computational framework, which can be used to perform UQ of broader class of turbulent flows to examine the statistical behavior of output quantities of interest on the uncertain input parameters.

Acknowledgments

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