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Sajjad Yousefian[1]
School of Engineering,
National University of Ireland, Galway,
Galway, Ireland;
Ryan Institute for Marine, Environmental and
Energy Research,
National University of Ireland, Galway,
Galway, Ireland;
MaREI, The SFI Centre for Energy,
Climate and Marine Research,
Galway, Ireland
e-mail: sajjad.yousefian@nuigalway.ie

Sandeep Jella
Siemens Energy Canada Ltd,
9505 Côte-de-Liesse Road,
Montréal, QC H9P 1A5, Canada

Philippe Versailles
Siemens Energy Canada Ltd,
9505 Côte-de-Liesse Road,
Montréal, QC H9P 1A5, Canada

Gilles Bourque
Siemens Energy Canada Ltd,
9505 Côte-de-Liesse Road,
Montréal, QC H9P 1A5, Canada;
Department of Mechanical Engineering,
McGill University,
Montréal, QC H3A 0G4, Canada

Rory F. D. Monaghan
School of Engineering,
National University of Ireland, Galway,
Galway, Ireland;
Ryan Institute for Marine, Environmental and
Energy Research,
National University of Ireland, Galway,
Galway, Ireland;
MaREI, The SFI Centre for Energy,
Climate and Marine Research,
Galway, Ireland

A Stochastic and Bayesian Inference Toolchain for Uncertainty and Risk Quantification of Rare Autoignition Events in Dry Low-Emission Premixers

Quantification of aleatoric uncertainties due to the inherent variabilities in operating conditions and fuel composition is essential for designing and improving premixers in dry low-emissions (DLE) combustion systems. Advanced stochastic simulation tools require a large number of evaluations in order to perform this type of uncertainty quantification (UQ) analysis. This task is computationally prohibitive using high-fidelity computational fluid dynamic (CFD) approaches such as large eddy simulation (LES). In this paper, we describe a novel and computationally efficient toolchain for stochastic modeling using minimal input from LES, to perform uncertainty and risk quantification of a DLE system. More specially, high-fidelity LES, chemical reactor network (CRN) model, beta mixture model, Bayesian inference and sequential Monte Carlo (SMC) are integrated into the toolchain. The methodology is applied to a practical premixer of low-emission combustion system with dimethyl ether (DME)/methane–air mixtures to simulate auto-ignition events at different engine conditions. First, the benchmark premixer is simulated using a set of LESs for a methane/air mixture at elevated pressure and temperature conditions. A partitioning approach is employed to generate a set of deterministic chemical reactor network (CRN) models from LES results. These CRN models are then solved at the volume-average conditions and validated by LES results. A mixture modeling approach using the expectation-method of moment (E-MM) is carried out to generate a set of beta mixture models and characterize uncertainties for LES-predicted temperature distributions. These beta mixture models and a normal distribution for DME volume fraction are used to simulate a set of stochastic CRN models. The Bayesian inference approach through SMC method is then implemented on the results of temperature distributions from stochastic CRN models to simulate the probability of auto-ignition in the benchmark premixer. The results present a very satisfactory performance for the stochastic toolchain to compute the auto-ignition propensity for a few events with a particular combination of inlet temperature and DME volume fraction. Characterization of these rare events is computationally prohibitive in the conventional deterministic methods such as high-fidelity LES. [DOI: 10.1115/1.4055361]

1 Introduction

Understanding the impact of the inherent variability of the operating conditions and fuel composition, as different sources of aleatoric uncertainties, is critical for the design and improvement of dry low emission (DLE) combustion systems. Quantification of aleatoric uncertainties through a stochastic framework is computationally expensive in general and prohibitive for combustion systems in particular. Using high-fidelity approaches such as large eddy simulation (LES) has been the focus of numerical simulations over the last two decades [1]. However, implementing stochastic approaches and integrating machine learning (ML) methods with LES is very challenging [2]. ML methods facilitate the understanding of underlying physics, inferring the physical parameters from experimental data, and constructing reduced-order models [3]. Therefore, a hybrid method that is computationally efficient and integrates physics-based models is needed to perform uncertainty quantification (UQ) and ML to expedite combustion systems development and improvement.

Chemical reactor network (CRN) modeling has been employed for practical combustion systems to facilitate the process of optimization and parametric studies. In this approach, a network of ideal reactors such as perfectly stirred reactors (PSRs) and plug flow reactors, or nonideal reactors such as incompletely stirred reactor (ISR) [4] and partially stirred reactor (PaSRs) [5] is used to model a combustion system. Flow-field data such as velocity, temperature, species, progress variable, or mixture fraction distributions from computational fluid dynamic (CFD) simulations or experimental measurements are employed to create a thermo-chemically representative CRN. The CRN can accommodate and solve a very detailed chemical kinetic model, compared to high-fidelity simulations, which enables the prediction of pollutant emissions. In our previous publications [6,7], we compiled a comprehensive literature review for CRN studies in the literature. An updated literature review study is presented in Fig. 1 for 65 CRN studies in the literature. The axes show the numbers of reactions and species in the kinetic mechanisms, the size of each bubble represents the size of CRN and the color illustrates the year of

[1]Corresponding author.

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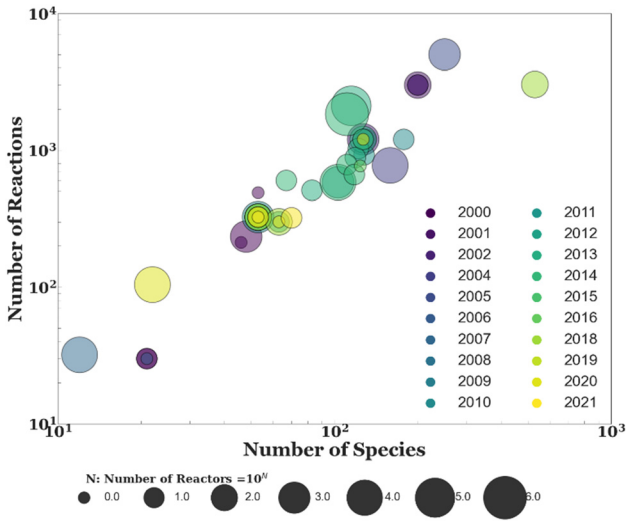

Fig. 1 Distribution of 65 CRN modeling studies in the literature. The axes show the numbers of reactions and species in the kinetic mechanisms, the size of each bubble represents the size of CRN, and the color illustrates the year of study.

study. The results highlight that CRN modeling approach is still a relevant approach in the literature.

Smith [4] and then Mobini [8] developed the concept of the ISR, where the inlet flow is not entirely premixed, unlike the PSR model. Turbulent fluctuation with time and spatial inhomogeneity in mixing is taken into account in the ISR [9]. The ISR's concept is based on a zero-dimensional approximation of the conditional moment closure (CMC) method for turbulent reacting flows [10]. This approach applies to the flows with recirculation and nonpremixed combustion in the primary zone of combustion systems. Gkantonas et al. [11] recently developed a modeling approach using a network of ISRs to simulate soot emissions in aero-engine combustion systems. The authors employed CFD results using an LES-CMC method to generate and solve the ISR network (ISRN). The results presented a computationally efficient framework with reasonable accuracy.

Construction of reduced-order models such as CRN and ISRN provides a computationally inexpensive representation of the original high-fidelity models. However, their computational cost is still high for UQ studies. Surrogate models or metamodels based on ML methods deliver a more efficient framework for these studies [12]. The use of ML methods has recently increased in the field of combustion. Gaussian process [13,14], polynomial chaos expansion [7,15–17], Markov chain Monte Carlo (MCMC) [7,18], neural network approaches such as artificial neural network [18–20], convolutional neural network [21], and deep neural network [22,23] are the most commonly used methods for the ML of physics-based combustion models in the literature. ML-based surrogate models then can be employed to conduct forward and inverse UQ studies.

Raman and Hassanaly [1] conducted a comprehensive literature review on the methods for reduced-order modeling, surrogate modeling, uncertainty sources and UQ methods for numerical simulation of combustion systems. Zhaou et al. [2] also performed another literature review study and broadly investigated ML methods for combustion modeling.

In a recent study for lean-premixed and hydrogen-enriched combustion systems, a probabilistic framework was developed by authors [7] to perform Bayesian inference and UQ study for epistemic uncertainties. The experimental results for the most probable flame location in a benchmark DLE system were employed to develop a physics-based CRN. Two surrogate models were developed for exit temperature and NO_x using this CRN model. Then a Bayesian calibration approach was implemented on these surrogate models and experimental data using the MCMC approach to predict unknown heat transfer rate as well as volumes of main flame and postflame zones. The method provided a fast, robust, and consistent approach to reduce epistemic uncertainties for the design and optimization of practical and industrial low-emission combustion systems.

In this study, a novel stochastic and Bayesian inference toolchain is developed that provides a computationally efficient and integrated framework to convert a high-fidelity CFD model into a stochastic framework for uncertainty and risk quantification in practical and low-emission combustion systems. A limited number of high-fidelity CFD simulations are employed to quantify uncertainty due to inherent variability in the inlet temperature and di-methyl ether (DME)-enriched fuel composition in a combustion system. DME is used a surrogate representing the change of reactivity due to the higher order alkanes, limiting the number of components to take into account. The ultimate goal is to capture the propensity of auto-ignition due to the stochastic nature of these input parameters. A computationally efficient toolchain is developed and implemented using the results of LES simulation of a benchmark configuration at relevant gas turbine conditions. A set of methods such as deterministic CRN modeling, beta mixture modeling for uncertainty characterization through expectation-method of moment (E-MM), stochastic CRN modeling, and sequential Monte Carlo (SMC) through a Bayesian framework for surrogate modeling are utilized in the toolchain. A method is also proposed for risk quantification based on the results of stochastic modeling.

2 Description of Methods

2.1 Overview. Figure 2 presents the flowchart of the stochastic and Bayesian inference toolchain developed in this study. It includes CRN construction, deterministic and stochastic CRN modeling, uncertainty characterization, uncertainty analysis and rare event or auto-ignition characterization. A framework is also proposed for risk quantification.

In the first step, a benchmark DLE combustion system is selected. In the second step, nonreacting LES simulation of the baseline configuration is obtained at a carefully selected condition representative of the problem of interest. In the third step, a partitioning approach is developed and implemented on the LES results in the ParaView [24] to extract the required information required to construct a CRN. The CRN is implemented in CANTERA [25] using a series of PSRs and flow controllers. In the fourth step, the CRN model is solved as a deterministic model to calculate the temperature and species time evolution within the PSRs [25]. Using volume-averaged LES data, this deterministic CRN model is then calibrated and validated for temperature and equivalence ratio values. The validated CRN model is then used as a starting baseline for stochastic modeling.

In the fifth step, the uncertainty in temperature distribution resulting from the averaging of the LES-predicted temperature

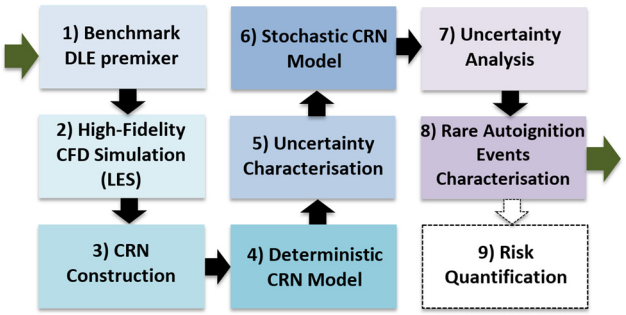

Fig. 2 Flowchart of stochastic and Bayesian inference toolchain

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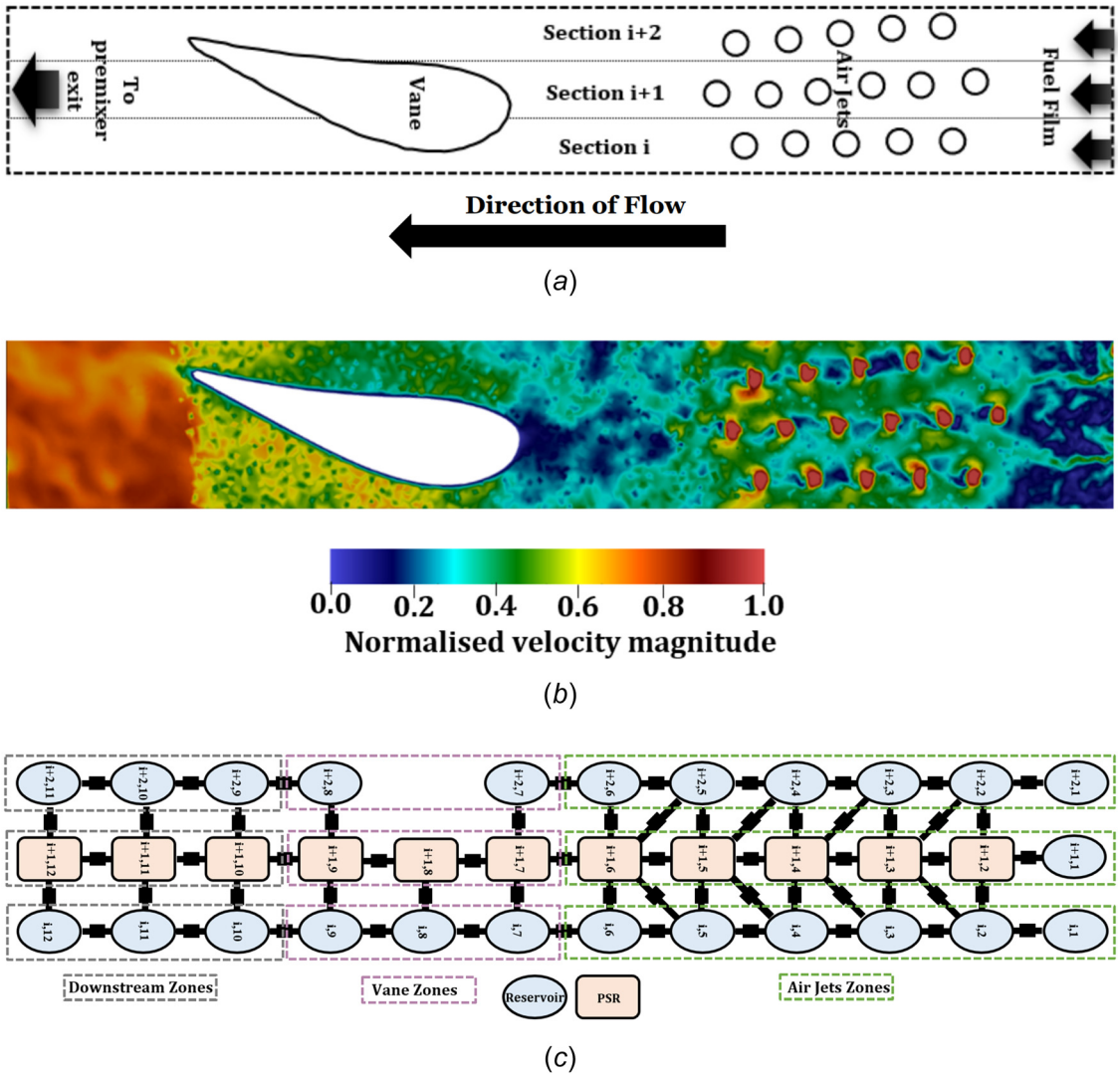

Fig. 3 (*a*) A schematic section of premixer [29], (*b*) LES results for normalized velocity distribution, and (*c*) corresponding CRN model in Cantera

distribution within the inlet reactor volume is characterized using a beta mixture model. In this study, DME is added to methane to modify the auto-ignition characteristic, and to represent higher hydrocarbon in natural gas. The volume fraction of DME is modeled using a normal distribution in the inlet reactor. A joint distribution is generated using the beta mixture model for temperature and the normal distribution for DME volume fraction. A set of samples is then extracted from this joint distribution through a low-discrepancy sequence approach. In the sixth step, a stochastic analysis is performed using the set of samples and repeatedly solving the deterministic CRN to obtain a distribution of output temperature. The quantified temperature distributions from stochastic CRN modeling in each PSR are used in step seven for uncertainty analysis. In the eighth step, the Bayesian inference is implemented on the calculated temperature distributions for surrogate modeling using SMC to calculate the probability of rare events or auto-ignition events in the premixer. The computed failure probability is then used in the optional ninth and final step to perform a risk quantification study.

2.2 Description of Benchmark Case. The benchmark combustion system in this study is a premixer developed for an aero-derivative gas turbine DLE combustion system. This premixer replicates aspects of practical DLE gas turbine combustors' operating conditions. Experimental and numerical studies have been carried out in this premixer to study combustion instability [26–28] and auto-ignition propensity [29]. This premixer is self-stabilized and has a set of guide vanes to generate a swirling flow at its outlet [28]. Multiple air jets and vanes are employed in the premixer to inject air into a cross-stream of gaseous fuel and generate swirl, respectively. A schematic section of the premixer geometry, direction of flow, and arrangement of air jets and vane are illustrated in Fig. 3(*a*).

2.3 High-Fidelity Non-Reacting Computational Fluid Dynamic Simulation (Large Eddy Simulation) of Premixer. Previously, a reactive LES by Jella et al. [29] was used to study auto-ignition chemistry at low temperature and high pressure, characteristic of the mixing section of DLE premixers. The authors used chemical explosive mode analysis to identify zones of the premixer that could be susceptible to auto-ignition events for different CH_4 and DME fuel mixtures. A new LES was carried out in this study to simulate the (nonreactive) flow field in the premixer for a mixture of air and 100% CH_4 as fuel. Figure 3(*b*) shows the results for normalized velocity distribution. The results of these simulations were then used to develop a stochastic CRN model. The nominal computational grid cell size in the premixer is of the order of 0.2 mm. The convective Courant–Friedrichs–

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Lewy number was restricted to values lower than 0.5 by selecting an appropriate time-step. More details about the LES simulation setup and results can be found in Ref. [29]. It should be noted that the strength of the proposed CRN method is that it does not require a reactive LES as an input. Hence, typical computational resources can be dedicated to obtaining high fidelity nonreactive flows, which provide well-converged higher order statistical distributions of the mixing field. The computational cost for a nonreacting and reacting LES using 30×10^6 mesh cells is 14,400 and 38,400 CPU hours, respectively. The computational cost especially for the reacting case is a prohibitive task to perform stochastic modeling that requires a large number of simulations.

2.4 Methodology for Constructing Chemical Reactor Network and Deterministic Modeling. Steps number three and four in Fig. 2 are employed for deterministic CRN modeling of the premixer based on LES results. As described in the third step of the toolchain in Fig. 2, a partitioning approach is employed in ParaView to divide the computational domain into 16 sections. Each section consists of three zones to cover air jet holes, vane and downstream regions in the premixer, as shown in Fig. 3(*c*). Then each section is further subdivided into a set of volumes, and volume-averaged LES properties are calculated. Each volume includes a group of computational cells from LES simulation. Available features in ParaView such as Slice are employed for portioning and dividing each partition into a set of volumes. A set of PSRs and reservoirs is mapped onto the volumes and connected through some mass flow controllers. Figure 3(*c*) also shows a schematic of the CRN model for a section. Each reactor is characterized by an index i,j represents the section's number and $j = 1, \ldots, n$ shows the reactor's number. The blue and red reactors represent reservoirs and PSRs, respectively.

This CRN model is constructed for each section and then Eqs. (A1) and (A2) (Appendix) as conservation equations are solved for each PSR using CANTERA based on the volume-averaged properties. Mass flow controllers are also employed to connect PSRs using Eq. (A3) (Appendix). Each PSR is connected to the adjacent sections using a set of mass flow controllers as shown in Fig. 3(*c*). The exchange of mass flow rates between reactors is calculated using the Surface Flow feature in the ParaView. More details about the process of partitioning, CRN construction, calibration, and validation are provided using a flowchart in Fig. 8 (Appendix). The air jet zones are critical parts for CRN construction due to the air jet holes. Therefore, each volume in the air jet zone includes a single air jet hole.

The fourth step in Fig. 2 is then implemented to complete the deterministic modeling. In this step, the developed CRN is solved using detailed chemistry for the conditions corresponding to the LES simulations. The results are then validated using the extracted volume-averaged LES data from Ref. [29]. An iterative approach is then conducted as described in Fig. 8 (Appendix) to calibrate CRN and characterize the optimum number of volumes, as shown in Fig. 3(*c*). The minimum number of volumes is employed to save computational costs for reactive simulations using detailed chemistry while achieving the required accuracy. The difference between the number of PSRs is due to the position of vanes in the computational domain. Each PSR is also connected to the adjacent sections using a set of reservoirs and mass flow controllers.

2.5 Uncertainty Characterization Using Beta Mixture Modeling. Uncertainty characterization of LES-calculated temperature distributions is an essential requirement for stochastic modeling due to the impact of temperature on auto-ignition propensity. This section describes a methodology for the uncertainty characterization of LES-calculated temperature distributions as the fifth step of the toolchain in Fig. 2. A beta mixture modeling using expectation method of moment (E-MM) approach is implemented in this study for the uncertainty characterization of high-fidelity CFD data in general and temperature in particular. The method provides a flexible formulation that mathematically describes the fluctuations of LES-calculated temperature distributions. The E-MM approach is used to calculate α, β, and π parameters for a beta mixture model. This approach for uncertainty characterization in the fifth step of toolchain is based on a hybrid parameter estimation developed by Schröder and Rahmann [30].

Reactors i,1, $i+1$,1 and $i+2$,1 in Fig. 3(*c*) represent inlet reservoirs for CRN modeling. Each inlet reservoir is constructed using the method described in Fig. 8 (Appendix) and includes a set of computational cells. Each computational cell consists of LES-calculated data. As a result, a distribution can be extracted from for each parameter such as temperature and species mass fractions in an inlet reservoir. The E-MM approach for beta mixture modeling is implemented for the normalized LES-calculated temperature distributions in the inlet reservoirs as follows:

$$\frac{T_\omega(\boldsymbol{x})}{T_{\max}} = \sum_{j=1}^{c} \pi_j . b_{\alpha_j,\beta_j}(\boldsymbol{x}) \tag{1}$$

where π_j is mixture of coefficients, $\sum_j \pi_j = 1$ and $\pi_j \geq 0$, c is the number of components, and α_j, β_j are component parameters and $\alpha_j, \beta_j > 0$. ω represents all of these parameters and referred to as model parameters. ω is estimated from input LES-calculated temperature data of $\boldsymbol{x} = [x_1, x_2, \ldots, x_n]$ in the inlet reactors, and this process is characterized as the parameter estimation problem [30].

A Gaussian distribution is also assumed for the DME volume fraction with a mean value, μ, of 40%

$$v_{\mathrm{DME}}(\boldsymbol{x}) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} \tag{2}$$

The standard deviation, σ, is selected in a way that the minimum and maximum values for the DME distribution are 30% and 50% of volume fraction, respectively.

2.6 Stochastic Modeling and Uncertainty Analysis. A joint distribution is then defined to combine the beta mixture model for temperature distribution and the Gaussian distribution for the DME volume fraction. An advanced sampling approach based on a low-discrepancy sequence is then implemented on the joint distribution to define an input sampling space for the stochastic CRN modeling. The baseline and deterministic CRN model is then simulated for each sampling point. This task is computationally prohibitive to implement using a high-fidelity CFD approach such as LES since hundreds of simulations are required. The developed CRN model facilitates this process as a computationally efficient baseline to simulate the sampling space.

The results of stochastic modeling are the temperature distributions in each reactor. In contrast to the deterministic modeling where a single volume-averaged value was calculated, in each reactor, the result of stochastic modeling is the probability distribution of temperature in each reactor. These probability distributions characterize the uncertainty in terms of low and high-temperature values in each reactor. At low-temperature conditions, there is no auto-ignition event and the final temperature is close to inlet air temperature. However, at high-temperature conditions, there is an auto-ignition event.

2.7 Characterization of Rare Events Using Bayesian Inference Approach. Rare events or failure events are usually defined as having small probabilities on order or lower than 10^{-3} [31]. Hassanaly and Raman [32] performed a comprehensive review study for rare and extreme events as well as tools for characterizing these events for turbulent combustion applications. The traditional methods such as standard Monte Carlo Simulation (MCS) are computationally very inefficient to calculate the probability of failure, p_F, even if each simulation is moderate to low

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computational cost. The total required number of samples to achieve an accuracy of $\delta < 1$ is $N = \left(p_F \delta^2\right)^{-1}$ [31]. It means that to calculate a probability of the order of 10^{-3} with an accuracy of 10%, there is a need to evaluate 10^5 samples in the standard MCS.

Variance reduction techniques such as importance sampling (IS) are developed to overcome this problem in the standard MCS [33]. The subset simulation method is an advanced and adaptive stochastic method for rare event simulation. In this method, the rare event is decomposed into a sequence of events [34]. The rare event probability, p_F, is calculated as a product of probabilities for the more frequent events or subsets. The concept of conditional probability is implemented to calculate the rare event probability [35]

$$p_F = \prod_{j=1}^{L} P(F_j F_{j-1}) = \prod_{j=1}^{L} p_j \tag{3}$$

where $F_1, \ldots, F_{L-1}$ are intermediate failure domains and $(F_j F_{j-1})$ is the conditional probability. If $j = 1$ then $p_1 = P(F_1 F_0) = P(F_1)$ that can be straightforwardly calculated by the MCS. Otherwise, if $j \geq 2$, the MCS is not efficient to calculate p_j since independent samples are required to generate from the conditional distribution of $\pi(.F_{j-1})$ [35]. Alternatively, Markov chain Monte Carlo (MCMC) can be used to generate samples from the conditional distributions of $\pi(.F_{j-1})$. These conditional samples gradually capture the intermediate rare events up to the ultimate and target rare events [36].

MCMC and IS are also implemented in Bayesian inference problems based on Bayes' theorem [37]. The approach introduces sequential importance sampling or the SMC method [38]. In the SMC method, a set of weighted particles are sequentially implemented. This method was initially designed for time-dependent problems and inference in dynamical systems [39]. The estimation of rare events can be performed within the framework of the SMC method [37]. This method combines different statistical methods such as importance sampling, tempering and an MCMC. In tempering, an auxiliary parameter of β is defined in the Bayes' theorem to control the sampling process. The original Bayes' theorem and the tempering approach is described in the following equation:

$$p(\theta|y) = \frac{p(T|\theta) \cdot p(\theta)}{p(y)} \rightarrow p(\theta|y)_\beta \propto p(y|\theta)^\beta \cdot p(\theta) \tag{4}$$

where $p(\theta|y)$ is the posterior distribution, $p(T|\theta)$ is a likelihood, $p(\theta)$ is prior, and $p(y)$ is an observation from experiments or stochastic modeling. When $\beta = 0$, the posterior $p(\theta|y)_{\beta=0}$ is the same as prior distribution of $p(\theta)$ and when $\beta = 1$ the true posterior is recovered. Therefore, β can be used to control the transition from an easy to a more complex sample distribution. In this study, the SMC sequences are generated from a prior distribution and then gradually are approached to the posterior approximation. The SMC is flexible, scalable, and straightforward to implement for sample distributions with a sequential nature, multiple peaks, and a highly variable density [37,39].

A multivariate Gaussian function with two modes is defined for the results of temperature distribution. Two modes are selected since there are two peaks for temperature distribution and each peak represents a Gaussian distribution. The first peak falls in the low-temperature region, and the second peak falls in the high-temperature region that representing the auto-ignition events. This multivariate Gaussian function defines a surrogate model for the temperature distribution. In the next step, the SMC method is utilized to calculate the weights and mean values of the Gaussian function and the probability of the auto-ignition propensity.

The main steps of the SMC method to characterize the multivariate Gaussian function consist of (1) initializing β at zero, (2) sampling from the prior, (3) increasing β to achieve an effective sample size, (4) computing the importance weights, (5) obtaining a new set of samples based on the importance weights, (6) computing the covariance for the multivariate Gaussian function, (7) running a set of Metropolis chains, (8) repeating from step 3 to achieve $\beta \geq 1$, and (9) characterizing a set of samples from the posterior.

3 Results and Discussion

3.1 Deterministic Chemical Reactor Network Modeling. The deterministic CRN model is solved in the CANTERA for CH_4/air mixture. A skeletal mechanism is employed for stochastic CRN modeling to simulate auto-ignition events for CH_4/DME/Air mixtures. This skeletal mechanism consisting of 38 species and 238 reactions was generated using the directed relation graph method [40] from a detailed mechanism developed by Burke et al. [41] for CH_4/DME blend as fuel. The skeletal mechanism was compared to the parent, detailed mechanism in the previous study by Jella et al. [29] and was found to accurately model ignition delay time for $p = 1 - 40$ atm, $T = 600 - 1600$ K, and $\Phi = 0.5 - 1.5$.

The results of volume-averaged temperature in each PSR are validated using the CFD-extracted data. As discussed, an iterative approach is conducted for this process to achieve an optimum number of PSRs for CRN modeling that is presented in Fig. 3(*c*). Figures 4(*a*) and 4(*b*) shows the comparison of CRN and CFD results for normalized volume-averaged values of temperature and equivalence ratio for sections 1 and 2, respectively. Similar results are obtained from other sections.

There is a very satisfactory agreement between CRN and CFD results with a mean absolute percentage error of below 1% in each section. The results show that a minimum number of 12 PSRs in sections 1 and 2 is required to achieve a very satisfactory accuracy as well as saving computational costs for reactive simulations. This is the minimum number of PSRs which can be employed to save computational cost as well as achieving the required accuracy. The difference between the number of PSRs is due to the position of vanes in the computational domain. Each PSR is also connected to the adjacent sections using a set of reservoirs and mass flow controllers.

The results have been normalized based on the maximum temperature and equivalence ratio. There is no ignition event in the CFD results and consequently in the CRN modeling results. Therefore, the maximum temperature is close to the inlet condition. The developed CRN provides an accurate reduced-order model compared to the detailed LES model to predict flow field and mixing features in the premixer. The reactors number 2 to 6, 7 to 9, and 10 to 12 represent the air jets, vane and downstream zones, respectively, as shown in Fig. 3(*c*). Fuel is introduced from inlet reactors (e.g., 2,1; 3,1; 4,1) and then constantly mixed with pure air injected from holes through reactors number 2 to 6 in the air jets zones. More agreement between the CRN and LES results in the vane and downstream zones indicates that the mixing of air and fuel is practically complete in these zones. This validated CRN modeling approach is a deterministic reference model for stochastic CRN modeling.

3.2 Beta Mixture Modeling. The E-MM method is applied to the CFD-extracted data from the inlet volume in each section to develop a set of beta mixture models for temperature distribution. These beta mixture models are employed to characterize the variability or aleatoric uncertainty for temperature distribution in stochastic CRN modeling. The CFD-calculated temperature distribution is standardized for beta mixture modeling. Min–max scaler is used to constraint CFD data into a range between 0 and 1.

$$T_{\text{std}} = \frac{T - T_{\min}}{T_{\max} - T_{\min}} \tag{5}$$

Figure 5 shows the results of beta mixture modeling in two inlet reservoirs. A histogram distribution for standardized temperature distribution based on LES-extracted data is presented in this

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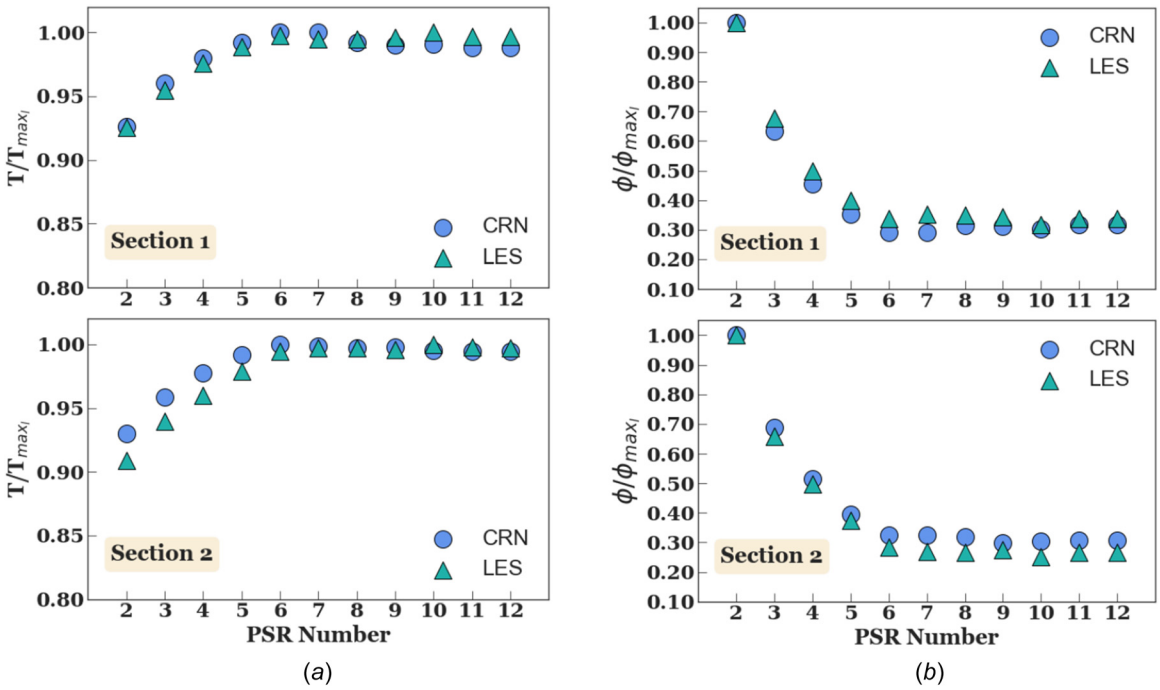

Fig. 4 Comparison of CRN and CFD results for (*a*) normalized volume-averaged values of temperature and (*b*) normalized volume-averaged values of equivalence ratio

figure. A set of beta distributions and a mixture of distributions are mapped on the histogram distribution.

The results show that a combination of four beta distributions is required to predict CFD-calculated temperature distribution. Components of each beta distribution, α_j, β_j, as well as mixture coefficients, π_j, for the beta mixture model is presented in this figure. The results show a very satisfactory performance of the beta mixture model to characterize the CFD-calculated temperature distribution. Similar results are obtained for other inlet reactors (e.g., 2,1; 3,1; 4,1). The developed method in this section is a generic approach and can be implemented for uncertainty characterization of CFD results in other applications and case studies.

3.3 Stochastic Chemical Reactor Network Modeling. Results of uncertainty characterization for temperature distribution in the inlet volumes (e.g., 2,1; 3,1; 4,1) using beta mixture models are employed to develop a stochastic CRN model. A blend of pure methane and DME was used for experimental auto-ignition studies. Therefore, beta mixture models are combined with a uniform distribution for DME concentration by volume to generate a set of composed distributions. A composed distribution is a distribution that can be written in terms of one-dimensional marginal distribution functions. The minimum and the maximum values for DME concentration in the uniform distribution are 30% and 50% by volume, respectively.

Figure 6 shows the results of stochastic CRN modeling for the reactors in sections 1 and 2 as defined in Fig. 3(*c*). All calculated data for normalized temperature distribution in each reactor is illustrated by circular points using a strip plot in this figure. Each strip plot, which consists of 480 datapoints is complemented by a box-and-whisker plot as well. Each box represents the quartiles for normalized temperature distribution, while the whiskers show the rest of the distribution. Quartiles divide data into quarters or four segments according to where the numbers fall on the number line. Outliers or values notably different from other data points are not included in the whiskers. Similar results can be obtained from other sections. PSR 1,2 to PSR 1,6 and PSR 2,2 to PSR 2,6 represent air jets zones, PSR 1,7 to PSR 1,9 and PSR 2,7 to PSR 2,9 correspond to the vane zones and PSR 1,10 to PSR 1,12 and PSR 2,10 to PSR 2,12 cover downstream zones after vanes.

The results in Fig. 6 present the trend of mixing, diffusion processes, chemical reactivity, and temperature distribution in the premixer. There is a high level of nonuniformity in the mixture and temperature distribution in PSR 1,2 and PSR 2,2. This is due to the very rich fuel content and the beginning of the process of mixing hot air from holes in the air jets zone with cold fuel from inlet reactors. The level of mixing, temperature homogeneity and average temperature increase from PSR 1,3 to PSR 1,6 and PSR 2,3 to PSR 2,6 that cover the whole air jets zones. The maximum amount of mixing between air and fuel and temperature homogeneity is achieved at the end of air jets zones in PSR 1,6 and PSR 2,6.

The results in Fig. 6 show a few outliners in PSR 1,7 to PSR 1,9 and PSR 2,7 to PSR 2,9 at very high temperatures. These reactors are located in the vane zone as shown in Fig. 3(*b*). As a result, this zone is a critical location for auto-ignition due to variable input conditions. In the previous study by Jella et al. [29], similar results were obtained in terms of the location of auto-ignition at 40% DME using reactive LES for the same premixer. Therefore, the stochastic CRN model provides an accurate prediction for the location of auto-ignition.

PSR 1,10 to PSR 1,12 and PSR 2,10 to PSR 2,12 in downstream zones after vanes show a very well-mixed condition and uniform temperature distribution. There are some outliners in PSR 1,10, PSR 1,11 and PSR 2,10, PSR 2,11 due to the auto-ignition events in PSR 1,9 and PSR 2,9, respectively. The high-temperature gas after the auto-ignition events in PSR 1,9 and PSR 2,9 reactors is mixed with the cold flow downstream in PSR 1,10, PSR 1,11 and PSR 2,10, PSR 2,11. The cold flow is coming from the adjacent section into these reactors. PSR 1,10, PSR 1,11 and PSR 2,10, PSR 2,11 are located right after the vane section in the downstream zone as shown in Fig. 3(*b*). Similar results are obtained from other sections.

The results show that the implemented framework is well suited to evaluate the stochastic nature of the mixing-diffusion process taking into account the chemical reactivity. The stochastic approach efficiently characterizes the small number of extreme events for auto-ignition that cannot be captured through a deterministic and high fidelity model. The computational cost for a reacting CRN evaluation is 28.8 CPU hours which is considerably lower than 38,400 CPU hours for a reacting LES.

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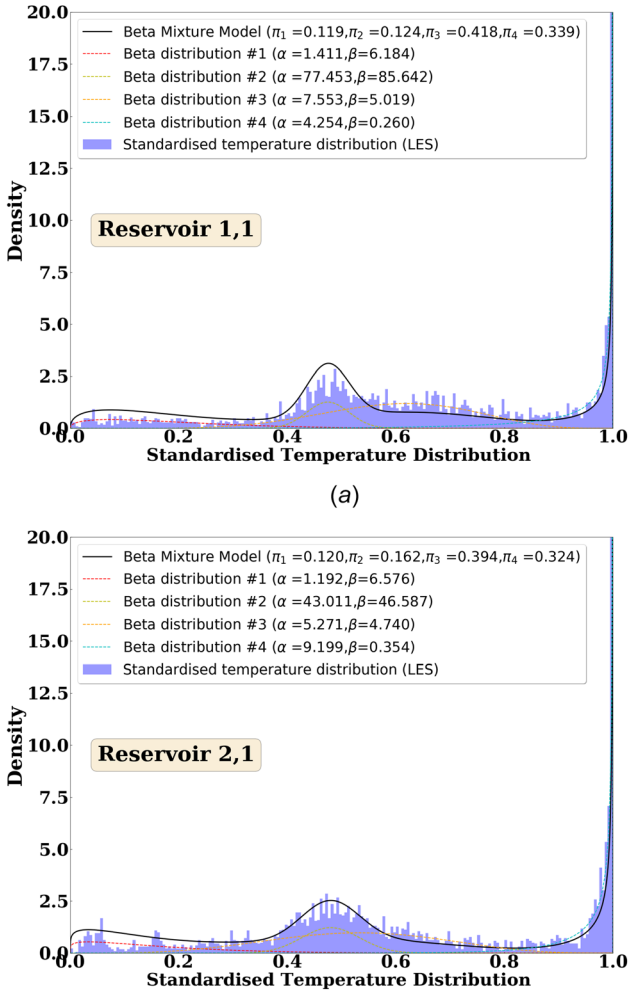

Fig. 5 Results of the E-MM approach for beta mixture modeling for LES-calculated temperature distribution in (*a*) reservoir 1,1 and (*b*) reservoir 2,1

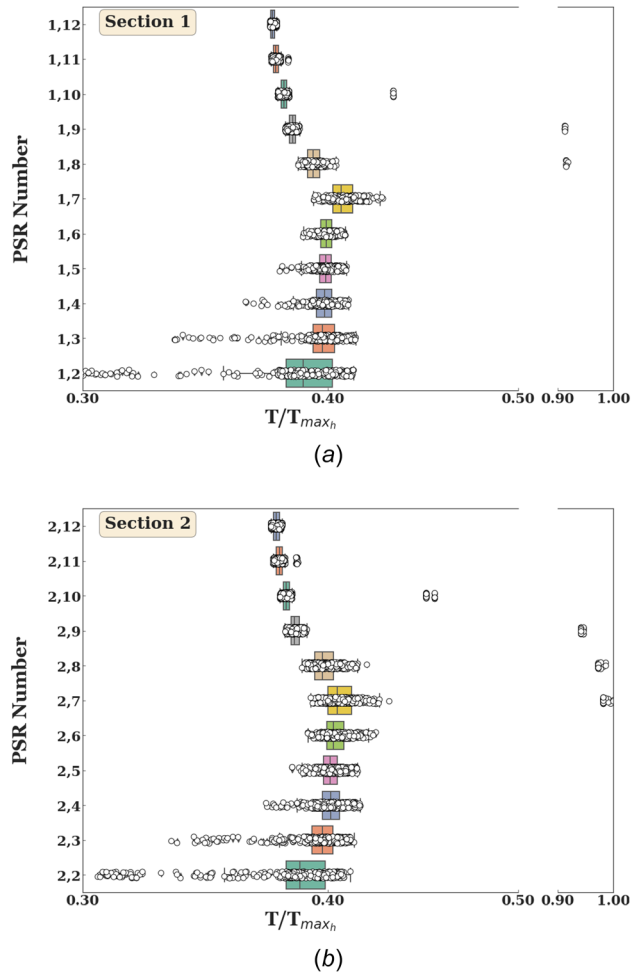

Fig. 6 Strip and box-and-whisker plots for normalized temperature distribution in each reactor of sections 1 (*a*) and 2 (*b*). Rare events are outside the whiskers.

3.4 Characterization of Auto-Ignition Event. A more detailed analysis is conducted for auto-ignition events in this section based on the eighth step in Fig. 2. The results of stochastic modeling indicated that there are a small number of failure or auto-ignition events in PSR 1,7 to PSR 1,9 and PSR 2,7 to PSR 2,9. The multivariate Gaussian approach and Bayesian inference through the SMC simulation are implemented on the results of stochastic modeling for critical reactors. A surrogate model is developed for the temperature distribution in these reactors, and then the probability of auto-ignition is calculated using SMC approach. The results of temperature distribution in PSR 2,9 are used for the analysis in this section as one of the critical reactors in terms of auto-ignition event. There are two distinct peaks for temperature distribution in this reactor. The peak on the left with a much higher probability corresponds to the safe events without auto-ignition. However, the peak on the right with a much lower probability represents a few autoignition events. A multivariate Gaussian function with two modes is assumed for the temperature distribution. The SMC approach is implemented to compute the weight of each mode and covariance matrix. Figure 7 presents the temperature distribution in PSR 2,9 and the results of SMC simulation. A set of curves as posteriors are mapped on the temperature distribution in this figure as the results of SMC simulation.

Predicted kernel density estimations posterior values are in light blue, and the mean posterior value is in dark blue. The results show a very satisfactory performance of the SMC approach to recover each mode and the relative weights. As a result of SMC simulation, the computed temperature distribution from stochastic CRN model can be converted into a bivariate Gaussian function as a surrogate model. The probability of the ignition event can be calculated using this surrogate model which is 0.004. Similar results can be obtained for other critical reactors with auto-ignition events.

Table 1 presents more details for the mean value, standard deviation and weight of each peak in Fig. 7.

As described in Sec. 3.3, the required number of reactive simulations to characterize the auto-ignition events is 480. Performing this number of simulations using LES framework is computationally prohibitive to validate the auto-ignition probability. The calculated probability for the auto-ignition event can be utilized for risk quantification. As presented in Fig. 2, the risk of auto-ignition can be quantified by multiplying the probability of auto-ignition by its severity or consequence. The severity of auto-ignition in a combustion system depends on its cost at different conditions such as minor, noticeable, critical, and disastrous consequences. The quantification of the consequences of auto-ignition and estimation of related costs are beyond the scope of this study.

4 Conclusions

In this study, a novel stochastic and Bayesian inference toolchain was developed that provides a computationally efficient and integrated framework to convert a high-fidelity CFD model into a stochastic framework for uncertainty and risk quantification in practical and low-emission combustion systems. A quantified assessment of the probability of auto-ignition inside a premixer as a benchmark low-emission combustion system was performed,

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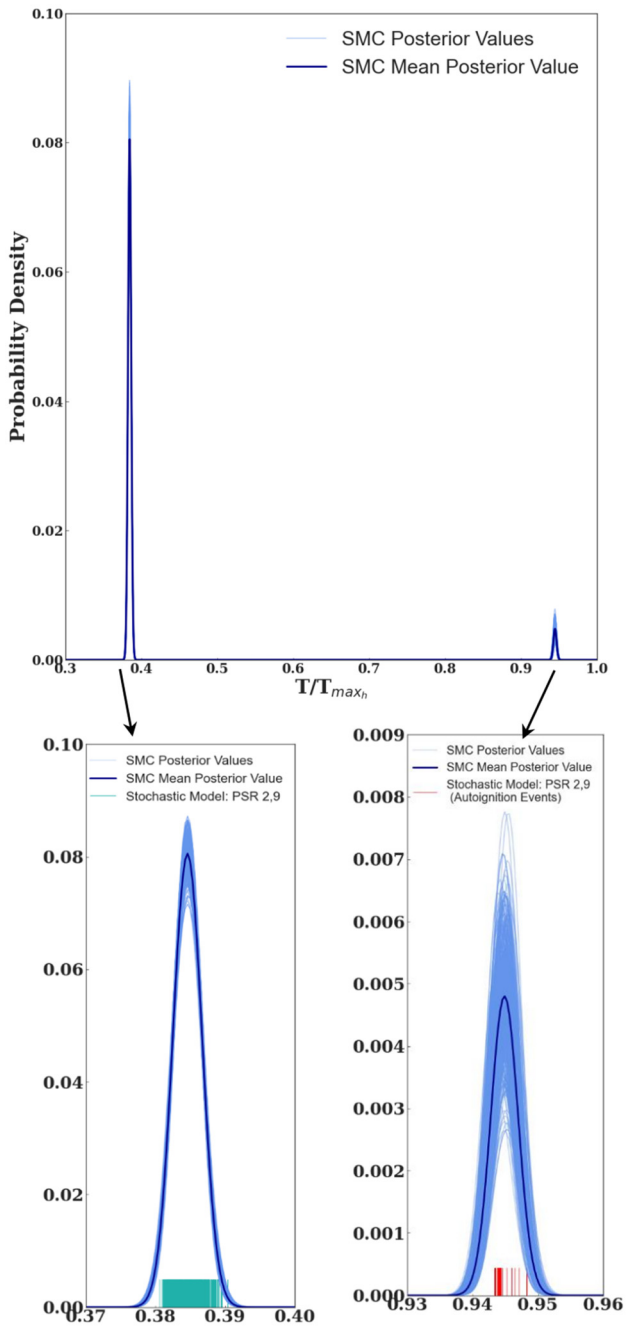

Fig. 7 Results of SMC simulation. Light blue color and dark blue color represent the posterior and the mean posterior values. The second peak on right shows auto-ignition events.

Table 1 Results of SMC simulation

Temperature range	Mean value	Standard deviation	Weight
Low (without auto-ignition)	0.384	0.220	0.944
High (with auto-ignition)	0.944	0.905	0.056

and unsafe sections have been identified. This hybrid and multipurpose computational tool also facilitate integrating physics-based models with ML methods for combustion applications. The selected combination of reduced-order models and ML methods enable to capture of the stochastic nature of the transient convection–diffusion-reaction mixing process due to inherent variations in inlet conditions such as temperature and fuel composition in a real gas turbine premixer. A large number of 480 simulations were carried out using the stochastic framework for detailed chemistry to characterize a small number of auto-ignition events. This task is computationally impossible using high-fidelity CFD approaches such as LES. Therefore, the developed framework provides a fast, robust, accurate, and consistent process to guide the modification, optimization, and virtual prototyping of low-emission combustion systems, especially for industrial applications. The future study will focus on (1) characterizing the severity or consequence of a failure event in terms of cost to quantify associated risk, (2) increasing stochasticity by integrating mixture models for mixture fraction or equivalence ratio with temperature distribution and fuel composition, and (3) implementing novel fuels such as hydrogen, ammonia/hydrogen and hydrogen-enriched natural gas into the toolchain.

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Nomenclature

Letters

A = pre-exponential factor
b = beta probability distribution
I = indicator function
L = number of subsets/likelihood
n = number of input variables
N = number of samples/terms
p = probability
P = pressure
Q = heat loss
r = rare event
R = reaction
T = temperature
V = variance
w = importance weight
W = responsibility weight

Greek Symbols

α = component parameter for beta distribution
β = component parameter for beta distribution
Γ = gamma function
δ = accuracy parameter
ε = threshold value
θ = input parameter
μ = expected (mean) value
π = mixture coefficient
ρ = density
τ = residence time
ϕ = equivalence ratio
ω = net production rate

Subscripts

F = failure
max = maximum
min = minimum
std = standardized
t = term
α = species

Abbreviations

CFD = computational fluid dynamics
CMC = conditional moment closure
CRN = chemical reactor network
DLE = dry low emission

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DME = di-methyl ether
IS = importance sampling
ISR = incompletely stirred reactor
LES = large eddy simulation
MCMC = Markov chain Monte Carlo
MCS = Monte Carlo simulation
ML = machine learning
MLE = maximum likelihood estimation
MM = method of moments
NO_x = nitrogen oxides
PaSR = partially stirred reactor
PSR = perfectly stirred reactor
SMC = sequential Monte Carlo
UQ = uncertainty quantification

Appendix

In the following, the method for partitioning the LES domain as well as the construction, calibration, and validation process of the CRN model is presented in Fig. 8. This figure presents more details about step 3 in Fig. 2 using Paraview and CANTERA.

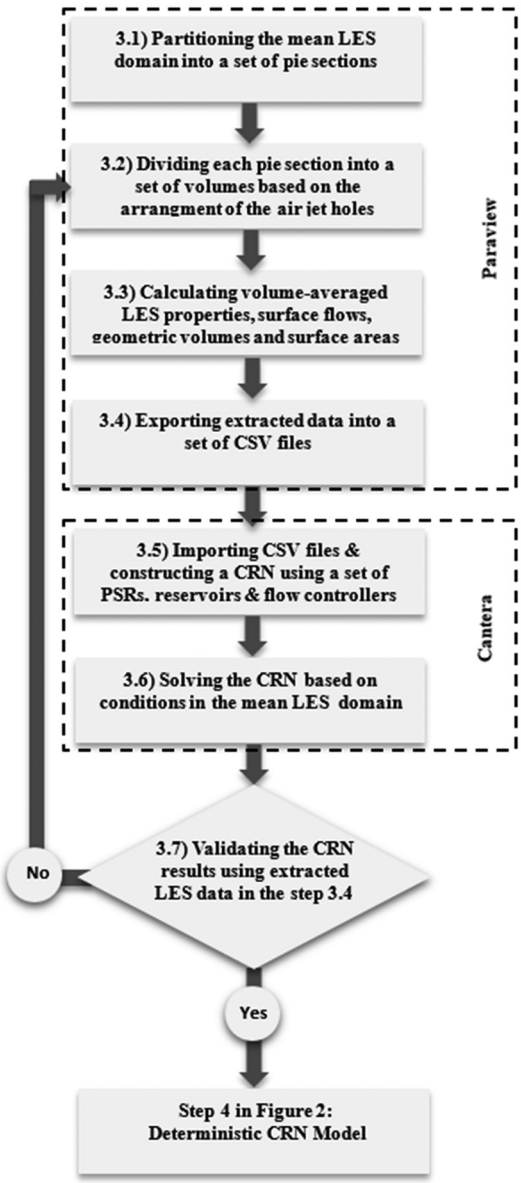

Fig. 8 Details of step 3 in Fig. 2 for partitioning LES domain and construction, calibration and validation process of CRN model using Paraview and CANTERA

The steady-state conservation equations for mass and energy in a single PSR are as follows [42]:

$$\dot{\omega} MWV + \dot{m}(Y_{i,\text{in}} - Y_{i,\text{out}}) = 0 \tag{A1}$$

$$\dot{Q} = \dot{m}\left(\sum_{i=1}^{N} Y_{i,\text{out}} h_i(T) - \sum_{i=1}^{N} Y_{i,\text{in}} h_i(T_{\text{in}})\right) \tag{A2}$$

where V is volume, $\dot{m}$ is mass flowrate, $\dot{Q}$ is heat loss, h is molar enthalpy, Y is mass fraction, MW is molecular weight, T is temperature, and $\dot{\omega}$ is the net production rate. A mass flow controller is used as a connection between two PSRs. This controller maintains a specified mass flowrate independent of upstream and downstream conditions using the below equation:

$$\dot{m} = \max(\dot{m}_0 g(t), 0) \tag{A3}$$

where $\dot{m}_0$ is a constant value and $g(t)$ is a function of time.

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