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Development of three-feed stream steady laminar flamelet model in OpenFOAM: Assessment for a reacting jet issuing into a hot and diluted coflow

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Abstract

A three-feed stream steady laminar flamelet model has been implemented in OpenFOAM as a part of the development of a numerical framework for simulations of non-premixed flames under transcritical and supercritical conditions (i.e., in rocket engines or in direct fired supercritical carbon dioxide gas turbine combustors). The developed code is adopted to simulate a reacting jet issuing into a hot and diluted coflow (i.e., HM3 flame) with RANS approach. A good agreement observed in the comparison of available experimental data and previous studies with data obtained from the present study proves that the implementation of the model is proper, and the developed framework can be used for turbulent non-premixed flames with a reasonable computational cost. This is an important step toward the development of the three-feed stream steady laminar flamelet model for reacting flow simulations under high pressure conditions.

1 Introduction

Recently, significant interest and research efforts have been dedicated to direct-fired supercritical carbon dioxide (sCO_2) power cycle (i.e., Allam-Fetvedt power cycle) [1] due to its friendliness and high thermal efficiency. The sCO_2 power cycle includes a gas turbine combustor having two distinct characteristics compared to conventional ones. It has an extremely high pressure operating condition (i.e., 200 to 300 atm) and a third pure sCO_2 stream injecting directly into the combustor to cool down the combustion chamber. This requires a three-feed stream model for numerical simulations of the sCO_2 gas turbine combustor if a flamelet-based combustion model is used.

The steady laminar flamelet model (SLFM) which was mainly advanced by Peters [2] is one of the most fundamental and simple models in the family of flamelet-based combustion models [3,4]. It has been widely used and well established for numerical investigations of turbulent non-premixed combustion [5-7] due to its computational efficiency. However, the SLFM has been shown to be inadequate to characterize the flame in some practical cases including three injected streams such as a burner configuration in the work of Dally et al. [8] on MILD combustion. To solve the problem, Ihme and See [9] extended Flamelet/Progress Variable (FPV) [10] accounting for three-feed stream (3s) model in large eddy simulation (LES) of a reacting jet issuing into a hot and diluted coflow (i.e., HM3 flame). Based on the idea, Indelicato et al. [11] applied successfully 3s-SLFM to simulate sCO_2 KAUST burner in OpenFOAM (OF) [12] using Reynolds-averaged Navier-Stokes (RANS) approach. However, their developed OF code including 3s-SLFM is not available for public use.

flameletFoam which is already available on github now [13] is OF-based (OF-2.x) solver consisting of SLFM for turbulent non-premixed combustion in both RANS and LES context developed by Muller and coworkers [14]. However, it does not include 3s-SLFM and is only applicable for ideal gas cases. Until now, there is no 3s-SLFM available for public use especially for sCO_2 combustion. In that context, our long-term objectives are to develop real-fluid based 3s-SLFM in OF-6 based on the work of Muller et al. [14]. We have finished the development of real-fluid models [15]. Thus, the main objective of this work is to validate the implemented 3s-SLFM in the context of RANS through assessment of a reacting jet issuing into a hot and diluted coflow which was performed experimentally by Dally et al. [8].

2 Theoretical modeling

2.1 Steady laminar flamelet model

The SLFM is based on the view of the turbulent flame as an ensemble of thin laminar diffusion flames, generally referred to as flamelets. This model is greatly supported by concepts of a scalar dissipation rate χ and a mixture fraction Z. The scalar dissipation rate is a function of the mixture fraction and can be parameterized by its value at stoichiometric mixture χ_{st} [2, 14]. The mixture fraction characterizes the stoichiometry of a mixture of fuel and oxidizer such that $Z = 1$ in the fuel side and $Z = 0$ in the oxidizer side. In the SLFM, flamelets are calculated in a pre-processing step. Then flamelet solutions are tabulated to form a library (i.e., flamelet library) using Favre presumed probability density function (PDF) since the species mass fraction and temperature can be characterized as a function of mixture fraction and stoichiometric scalar dissipation rate (i.e., $T(Z, \chi_{st})$, $Y_i(Z, \chi_{st})$) [2, 14]. As the results, the mean value of a scalar is calculated as:

$$\tilde{\phi} = \int_0^\infty \int_0^1 \phi(Z, \chi_{st}) P(Z, \chi_{st})\, dZ\, d\chi_{st} \qquad (1)$$

where ϕ can be temperature or mass fraction of species. The joint PDF $P(Z, \chi_{st})$ is decomposed assuming statistical independence:

$$P(Z, \chi_{st}) = P(Z) P(\chi_{st}) \qquad (2)$$

The shape of the PDF for the scalar dissipation rate is modeled with simple Dirac function (δ-function) while presumed β-PDF is adopted for mixture fraction:

$$P(\chi_{st}) = \delta(\chi - \chi_{st}) \qquad (3)$$

$$P(Z) = Z^{\alpha-1}(1-Z)^{\beta-1} \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \qquad (4)$$

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where Γ is the gamma-function, α and β the parameters of β-PDF depending on the mean mixture fraction $\tilde{Z}$ and its variance $\widetilde{Z''^2}$ as $\alpha = \tilde{Z}(\tilde{Z}(1-\tilde{Z})/Z''^2 - 1)$, and $\beta = (1-\tilde{Z})(\tilde{Z}(1-\tilde{Z})/Z''^2 - 1)$.

The main advantage of the SLFM approach is that flamelets are coupled to the turbulent flow by only a few controlling parameters such as the mixture fraction, its variance and the scalar dissipation rate. Thus, the chemical kinetics can be solved separately from the turbulent flow. In the turbulent CFD code, only three controlling parameters need to be solved instead of solving the full energy and species equations in multi-dimensional domain. Then the local species composition and temperature can be retrieved from the flamelet library. This feature massively reduces the computational cost for the practical turbulent simulations. The detailed governing equations can be found in [14].

2.3 Three-feed stream SLFM

The single mixture fraction formular was shown to be inadequate to characterize a burner that has three-feed streams such as the HM3 [8] or the sCO_2 gas turbine combustor [11]. In that context, Ihme and See proposed a three-feed stream model to identify the different compositions of oxidizer streams by introducing an additional scalar, W, representing the oxidizer split such that $W = 0$ and $W = 1$ in the coflow and the shroud air stream, respectively. W is independent of mixture fraction and is constant in each flamelet, and is calculated as [9]:

$$W = \frac{Y_O - Y_O^{(0)}}{Y_O^{(1)} - Y_O^{(0)}} \quad (5)$$

where Y_O is elemental mass fraction of oxygen, superscripts (0) and (1) denote the coflow and shroud air stream, respectively.

In the present work, we implement the same three-feed stream model but for SLFM instead of FPV combustion model as in [9] Consequently, the temperature as well as species mass fraction can be expressed as a function of mixture fraction, stoichiometric scalar dissipation rate, and W ($\phi = \phi(Z, \chi_{st}, W)$. Then the mean value of a scalar (in the same manner as SLFM approach) is calculated as:

$$\tilde{\phi} = \int_0^1 \int_0^\infty \int_0^1 \phi(Z, \chi_{st}, W) P(Z, \chi_{st}, W)\, dZ\, d\chi_{st} dW \quad (6)$$

The joint PDF $P(Z, \chi_{st}, W)$ is decomposed assuming statistical independence:

$$P(Z, \chi_{st}, W) = P(Z)P(\chi_{st})P(W) \quad (7)$$

The shape of the PDF for W and the scalar dissipation rate are modeled with δ-function while the shape of the PDF is approximated using presumed β-PDF for mixture fraction as presented in Section 2.1. It is of importance to note that the library is four-dimensional (4-D) after integration. To use its integrated data, it also requires a 4-D linear interpolation.

In the turbulent code, an additional transport equation for W is solved along with the set of governing equations for mass, momentum conservation, and controlling parameters.

$$\frac{\partial \bar{\rho}\tilde{W}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j \tilde{W}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\left(\mu + \frac{\mu_t}{Sc_t}\right)\frac{\partial \tilde{W}}{\partial x_j}\right) \quad (8)$$

where μ and μ_t are laminar and turbulent viscosity, respectively.

Finally, the turbulent flame structures will be evaluated by 4-D linear interpolation through the 4-D tabulated flamelet library.

3 Results and discussions

3.1 A new developed framework in OpenFOAM

Our new developed solver in OF-6 is based on the *flameletFoam* code [13] which has been validated for the Sandia flame D [16] using LES and RANS approach by Muller et al. [14]. It is of importance to note that the *flameletFoam* source code cannot be used in OF-6 since it was originally developed for OF-2.x while the structure of OF-6 and OF-2.x is different. In the present study, the source code is first modified to be compatible with OF-6. Then it is extended to account for 3s-SLFM.

In the processing step of the present study, flamelets are calculated by using either OPPDIF [17] or FlameMaster code [18]. The turbulent simulations are performed using developed solver in OF-6. All simulations are under unity Lewis and Schmidt number assumptions.

3.2 Validation of two-feed stream SLFM

To validate our implementation of SLFM in OF-6, we perform two dimensional (2-D) numerical simulation of a piloted diffusion flame (Sandia flame D) [16] using RANS method. The computational domain is axisymmetric consisting of 47,870 structured control volumes as shown in Fig. 1. It is of importance to note that this number of control volumes has been found sufficient to achieve grid-independent solutions. The numerical outflow conditions are imposed at $x = 100D_{ref}$ where $D_{ref} = 7.2$ mm is the main jet diameter. GRI-3.0 chemical mechanism [18] is used for evaluating chemical reactions. The detailed boundary and setting conditions can be found in [14, 16]. A flamelet library is prepared by using OPPDIF [17].

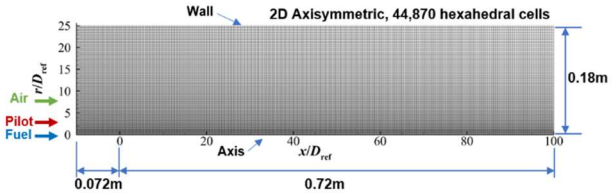

Figure 1: The computational domain of the Sandia flame D

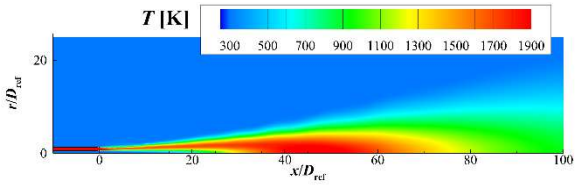

Figure 2: The distribution of temperature of the Sandia flame D obtained by the developed framework.

Figure 2 shows the temperature distribution of Sandia Flame D generated by the developed platform in OF-6 using SLFM. One dimensional (1-D) profiles of the temperature and mixture fraction along the centerline obtained from the present work are then compared with experimental data by Barlow et al. [16] as shown in Fig. 3 and Fig. 4. As a result, a very good agreement between the solutions from our developed platform and the benchmark data [16] can be observed. This result implies that our SLFM implementation in OF-6 is proper and applicable for

simulations of turbulent non-premixed flames.

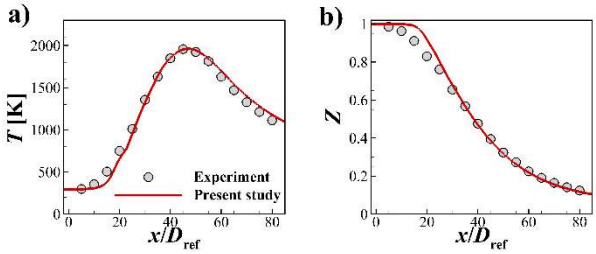

Figure 3: Axial profiles of temperature (a) and mixture fraction (b) obtained from the present study (lines) compared with experimental data (symbols) from Barlow et al. [16].

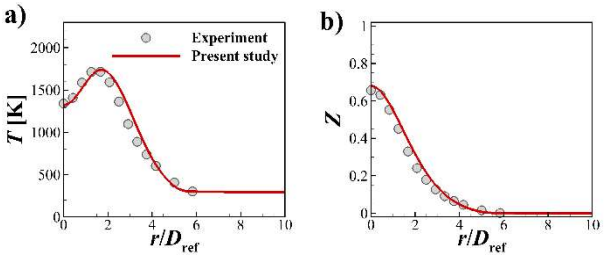

Figure 4: Radial profiles of temperature (a) and mixture fraction (b) obtained from the present study (lines) compared with experimental data (symbols) from Barlow et al. [16] at location of $x/D_{ref} = 30$.

3.3 Simulations of HM3 flame

To verify our extension of the developed code for 3s-SLFM, RANS simulations of 2D axisymmetric hot and diluted coflow flame (HM3) [8], a well-known flame configuration for which extensive validation data is available, are performed using both SLFM and 3s-SLFM. In this configuration, fuel consisting of 50%/50% hydrogen-methane mixture is supplied in the central pipe with a diameter of $D_{ref} = 4.25$ mm. The bulk exit velocity of the fuel is $U_{ref} = 73.5$ m/s (i.e., the Reynolds number of 9500). The hot diluted coflow of which mass flow rate was reported with 4.8 g/s (i.e., velocity of 3.2 m/s) is provided through the pilot nozzle with an outer diameter of $D_P = 82$ mm. The shroud air enters though the outer stream by wind tunnel with an exit velocity of 3.2 m/s. The computational domain includes 29,496 structured control volumes in which grid-independence of numerical simulations are already achieved as shown in Fig. 5. The detailed boundary conditions for numerical simulations are summarized in Table 1. Chemical reactions are evaluated by GRI-3.0 [19]. The FlameMaster code [18] is used to generate the flamelet library for both two-feed stream case (referred to as Case 1) and three-feed stream case (referred to as Case 2). It is worth noting that the mixture fraction calculated using Bilger's formular [20], Z_b, is used in Case 1 while Z is used in Case 2.

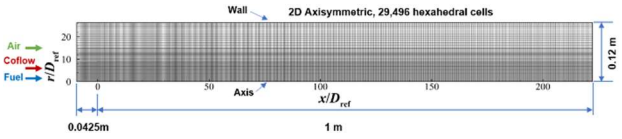

Figure 5: The computational domain of the HM3.

Figures 6 and 7 illustrate comparisons in the temperature and mixture fraction contour of the HM3 flame, respectively, obtained in the present study using both two-feed stream SLFM and three-feed stream SLFM. It is qualitatively observed that temperature solutions predicted by SLFM are much higher than those predicted by 3s-SLFM in the coflow stream, leading to the large difference in the flame temperature and flame length in the overall domain. The computational cost of Case 2 is slightly higher than that of Case 1 (i.e., 1.08 times higher).

Table 1: The reference parameters for numerical simulations taken from Dally et al [8], and from Ihme and See [9], where Z_b used for two-feed stream simulations is mixture fraction calculated by Bilger's formula [20].

Parameter	Fuel	Coflow	Air
T [K]	305	1300	300
Z	1	0	0
W	0	0	1
Z_b	1	0.03	0
U[m/s]	73.5	3.2	3.2
Compos.[a]	H_2/CH_4 = 50/50 (% by volume)	$H_2O/CO_2/N_2/O_2$ = 6.5/5.5/79/9 (% by mass)	O_2/N_2 = 21/79 (% by volume)

a. Compositions.

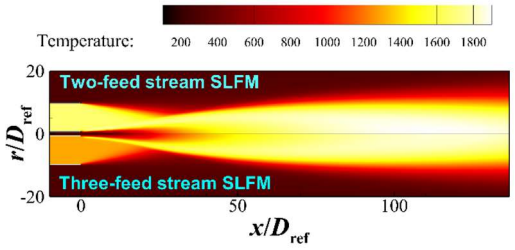

Figure 6: The temperature distribution of HM3 flame using SLFM (upper portion) and 3s-SLFM (lower portion) in RANS context.

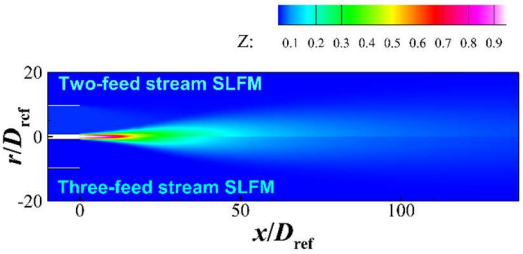

Figure 7: The mixture fraction distribution of HM3 flame using SLFM (upper portion) and 3s-SLFM (lower portion) in RANS context.

Figure 8 shows the quantitative comparisons of temperature and mass fraction of CO_2 profiles at a location of $x/D_{ref} = 7.1$ between the present results and experimental data [8] as well as those of a previous study by Ihme and See [9] using FPV-LES. It can be seen that the present results using SLFM (RANS) are very close to the reference solutions (mean values) obtained by [9] using FPV (LES) in both two-feed stream and three-feed stream cases although adopted turbulent and combustion models are different. This evidently implies that our implementation of SLFM as well as 3s-SLFM are proper. Moreover, using 3s-SLFM gives more accurate predictions than utilizing SLFM in the HM3 burner. Particularly, the calculated results obtained from the two-feed stream model are overpredicted in the coflow-region. This is also consistent with the work of Ihme and See [9]. The overprediction is originated from the fact that the composition of both the coflow and the air stream cannot be adequately represented by a single mixture fraction. This is a

limitation of two-feed stream flamelet-based models [9].

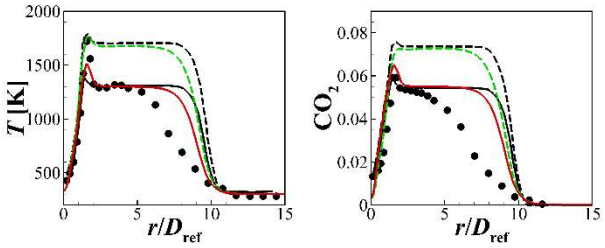

Figure 8: Comparison of radial profiles of temperature and mass fraction of CO_2 at an axial location of $x/D_{ref} = 7.1$ in the HM3 flame. Symbols: experimental data by Dally et al. [8], black dashed lines: simulated data using two-feed stream FPV (LES) by Ihme and See [9], green dashed lines: the present work using two-feed stream SLFM (RANS), black solid lines: simulated data using three-feed stream FPV (LES) by Ihme and See [9], red solid lines: the present work using three-feed stream SLFM (RANS).

4 Conclusions

A three-feed stream steady laminar flamelet model has been implemented in OpenFOAM-6 based on the work of Muller et al. [14] and Ihme and See [9]. The developed code was then adopted to run RANS simulations of three-feed stream burner configuration (i.e., HM3 flame) under MILD combustion conditions. A good agreement observed in the comparison of the present work and available experimental data [8] and previous studies [9] proves that the developed framework can be used for turbulent non-premixed flame simulation with low computational cost and reasonably good accuracy. The comparison between simulated results obtained using SLFM and 3s-SLFM illustrated that the three-feed stream model provides significantly improved predictions for the flame structure and temperature in the HM3 flame configuration.

Acknowledgment

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Nomenclature

D_{ref}	main jet diameter [m]
r	radial axis [m]
Sc_t	turbulent Schmidt number [-]
T	Temperature [K]
U	velocity [m/s]
W	oxidizer split factor [-]
U_{ref}	main jet velocity [m/s]
x	axial axis [m]
Y_i	mass fraction of i-th species [-]
Z	mixture fraction [-]
Z_B	Bilger's mixture fraction [-]
Z''^2	mixture fraction variance [-]
χ_{st}	stoichiometric scalar dissipation rate [s^{-1}]
ρ	density [kg/m^3]
μ	molecular dynamic viscosity [kg/m-s]
μ_t	turbulent viscosity [kg/m-s]