Large eddy simulation/probability density function simulations of the Cambridge turbulent stratified flame series under swirling conditions

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The large eddy simulations/probability density functions (LES/PDF) methodology is applied to the Cambridge/Sandia turbulent stratified flame series under swirling conditions. The methane/air chemistry is represented by a 16-species augmented reduced mechanism, and the in situ adaptive tabulation method is adopted to accelerate the chemistry calculation. Effects of differential diffusion and heat loss through the bluff-body surface are taken into account. The simulations are conducted for premixed (SwB3), moderately and highly stratified (SwB7 and SwB11, respectively) cases under swirling conditions. The results from LES/PDF simulations are compared with experimental measurements. The computed mean and r.m.s. profiles of velocity, temperature, equivalence ratio and mass fractions of species are in very good agreement with the measurements for all three conditions. Scatter plots and conditional means of species mole fractions and temperature are compared with the experimental data, where overall good consistency with the measurements is achieved. The recirculation zones are five times longer than those obtained under non-swirling conditions. A low-equivalence-ratio high-temperature region near the bluffbody is not captured in the computation, which is attributed to the insufficient entrainment of downstream mixtures into the recirculation zone. The parametric studies show that the differential diffusion has a negligible effect on the mean and r.m.s. results, whereas the heat loss has a considerable effect on the temperature and CO profiles close to the bluffbody.

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I. INTRODUCTION

Swirling flow is widely used to stabilize lean premixed turbulent flames in gas turbines to satisfy the low-emission constraints, and to reduce the size of the combustion devices by increasing the residence time. Despite of its effectiveness, swirling flows introduce significant challenges in terms of combustion instabilities, because they are primarily characterized by low frequency large-scale coherent flow structures that are inherently unstable. These unstable flow patterns increase the turbulent intensity and also introduce combustion oscillations, which makes it challenging to model the interaction between turbulence and chemistry. Additionally, in practical combustion devices, the limited time and length scales imposed by design constraints may prevent the fuel from mixing perfectly with the oxidizer (e.g., in gas turbines). The fuel concentration can vary spatially within the combustion chamber, which leads to partially premixed or stratified combustion, i.e., the flame front propagates through an inhomogeneous mixture composition. The inhomogeneous fuel distribution in the combustible mixture may lead to combustion instabilities due to strong fluctuation in the heat release rate. The combined effects of stratified combustion under swirling conditions introduce challenges to the numerical modeling of turbulent flames. Therefore, well-defined benchmark experimental measurement data are required for development and validation of combustion models for turbulent stratified flames under swirling conditions.

A number of numerical studies have been performed for partially premixed swirling turbulent flames using different combustion models. These studies mainly focus on gas turbine model combustors (GTMC) with different degrees of stratification in fuel concentrations. Such GTMC configurations usually include the plenum, swirler, and combustor walls, etc., which often introduces additional complexities to the model validation process. To avoid such complexities and to accelerate the model validation process, many canonical swirl burners are designed. For example, Bonaldo and Kelman have developed a weak swirl lean stratified premixed burner in an unconfined atmosphere. The stratification is provided by two concentric annular flow jets feeding the fuel with different equivalence ratios. The swirling coflow air is provided to stabilize the flame with a minimal swirl. The weak swirl is insufficient to create a recirculation zone, however, it leads the mean axial velocity to decay almost linearly. Consequently, the flame is stabilized at the position where the velocity of the fresh fuel mixture is equal to the flame speed. Nogenmyr et al. have developed a
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laboratory measurement rig where a premixed CH$_4$/air mixture is injected through a low swirl burner into a low speed co-flowing air at room temperature and pressure. The flame is stabilized in a low velocity region above the burner created by the swirling flow. The stratification in fuel concentration occurs due to the dilution of the ambient air in the shear layer, while the flame core remains premixed. The authors have also modelled the flame using the G-equation model employing two different chemistry models, i.e., flamelet and finite rate chemistry. The two chemistry models have predicted similar mean and rms flow fields, while the finite rate chemistry model resulted in closer agreement with the experiments.

Recently, the Cambridge/Sandia swirl burner has been designed by Sweeney et al.\textsuperscript{20,21} to investigate stratified turbulent flames under swirling and non-swirling conditions and provide detailed experimental measurements for validation of numerical models. The Cambridge/Sandia swirl burner has become a platform for studying highly turbulent stratified flames.\textsuperscript{22} The burner consists of a central bluffbody and two fuel streams surrounded by an air coflow. The flame is stabilized by a recirculation region behind the bluffbody. Two annular jets inject fuel/air mixtures at different equivalence ratios. The Cambridge turbulent stratified flame series under non-swirl conditions have previously been studied numerically by Nambully et al.\textsuperscript{23,24} using a filtered-laminar-flame PDF model, by Proch and Kempf\textsuperscript{25} using an artificial thickened flame model, by Brauner et al.\textsuperscript{26} using a probability density function (PDF) model based on the Eulerian stochastic field method, and by Turkeri et al.\textsuperscript{27} using a transported PDF model.

The burner under swirling conditions has been modelled using different combustion models. Brauner et al.\textsuperscript{26} have reported numerical results for the stratified turbulent flames under swirling conditions. In their study, the flow fields have been predicted quite accurately, however, the numerical predictions of species show apparent discrepancies within the recirculation zone. Additionally, temperature is over-predicted within the recirculation zone and close to the bluffbody. Zhang et al.\textsuperscript{28} have studied the burner in the premixed mode under both swirling and non-swirling conditions using two different combustion models, including the dynamic thickened flame model with tabulated detailed chemistry and the presumed-PDF model with tabulated detailed chemistry. In this study, although the mean temperature and species profiles are in reasonable agreement with the experimental data, the r.m.s. profiles are lower than the measurements. Xiao et al.\textsuperscript{29} performed a numerical study using the partially stirred reactor (PaSR) model. Although the trend in the experimental
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data have been captured by the numerical results, the magnitudes of the mean temperature and main products are predicted to be lower than the measurements. Gruhlke et al.\(^{30}\) conducted a numerical study for the burner in the premixed mode using a dynamic thickened flame approach with a new post-processing method for finite-rate chemistry. The new post-processing method improves the prediction of minor species such as CO. Subsequently, Mercier et al.\(^{31}\) modeled the burner in the premixed mode under swirling condition using the filtered wrinkled flamelets model. The mean temperature profiles have been over-predicted within the recirculation zone. Additionally, the mean CO profiles have shown discrepancies compared to the measurements.

The performance of the LES/PDF methodology employing the Lagrangian Monte Carlo method in numerical solutions for predicting the effects of stratification under the non-swirling conditions has been presented in our previous study\(^{27}\). The main objective of the present computational study is to show the performance of the method under swirling conditions using the Cambridge turbulent stratified flame series. The PDF method has proven to be robust in non-premixed\(^{32–35}\), premixed\(^{36–38}\), and partially premixed\(^{39}\) combustion modes, because it involves only a few intrinsic assumptions regarding the mixture composition, flame structures, and the flame topology. In particular, the highly non-linear chemical reaction source terms are treated exactly without requiring any modeling. However, the conditional molecular diffusion terms remain in the unclosed forms, which represents the major modeling challenge of the transported PDF approach. In the context of LES, the results are less sensitive to the modeling of the conditional molecular diffusion, compared to those obtained by the Reynolds-averaged Navier Stokes (RANS) methodology. The interaction by exchange with the mean (IEM) model with mean drift term\(^{40}\) has proven to be very efficient in modeling the conditional diffusion term in several previous studies\(^{38,41–43}\).

In the present study, a hierarchy of cases, including the premixed case, the moderately and highly stratified cases, are investigated using the LES/PDF method, for the swirling conditions. The rest of the paper is organized as follows. In Section II, the governing equations and the numerical solution methodology for the LES/PDF method are presented. In Section III, the details of the experimental setup and the numerical simulations are described, followed by the presentation of the results and discussions in Section IV. Finally, conclusions from the study are summarized in Section V.
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II. METHODOLOGY

In the LES/PDF methodology, LES is employed to solve for the turbulent flow field, while the PDF method is employed to treat the turbulence-chemistry interaction. The details of the LES/PDF method have been presented in a previous paper. The main features of the method are summarized here for the sake of completeness.

A. Governing equations

In the LES method, the turbulent fields are separated into large and small scales by applying a low band-pass filtering operation. For example, the filtered density field $\bar{\rho}$ is defined as

$$\bar{\rho}(\mathbf{x},t) \equiv \int_{-\infty}^{\infty} \rho(\mathbf{y},t) G(\mathbf{y} - \mathbf{x}) d\mathbf{y},$$

where $\rho(\mathbf{x},t)$ is the density field and $G$ is the LES filter. The filtered transport equations for mass and momentum can be obtained by applying the LES filter to the instantaneous mass and momentum conservation equations. The one equation eddy-viscosity model is used to model the effects of the sub-grid scale stresses.

For variable density flows, the filtered mass density function (FMDF) of compositions is defined as

$$\mathcal{F}(\psi; \mathbf{x},t) \equiv \int_{-\infty}^{\infty} \rho(\mathbf{y},t) \delta(\psi - \phi(\mathbf{y},t)) G(\mathbf{y} - \mathbf{x}) d\mathbf{y},$$

where $\phi$ represents the $N = N_s + 1$ composition variables consisting of the mass fractions of $N_s$ species and the sensible enthalpy, $\psi$ is the sample space variable for the compositions and $\delta$ is the $N-$dimensional delta function. The Favre-filtered PDF $\tilde{f}$ is related to the FMDF as $\tilde{f} = \mathcal{F}/\bar{\rho}$. The Favre-filtered mean of a flow variable $Q$ as a function of $\phi$ can be defined as

$$\tilde{Q}(\mathbf{x},t) = \int Q(\psi; \mathbf{x},t) \tilde{f}(\psi; \mathbf{x},t) d\psi.$$

The modeled transport equation for $\tilde{f}$ can be written as

$$\frac{\partial \bar{\rho} \tilde{f}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{f}}{\partial x_i} - \frac{\partial}{\partial x_i} \left( \bar{\rho} D_T \frac{\partial \tilde{f}}{\partial x_i} \right) =$$

$$\frac{\partial}{\partial \psi_\alpha} \left[ \dot{\rho} \tilde{f} \Omega(\psi_\alpha - \bar{\phi}_\alpha) \right] - \frac{\partial}{\partial \psi_\alpha} \left[ \tilde{f} \frac{\partial}{\partial x_i} (\dot{\rho} V_{\alpha,i}) \right] - \frac{\partial}{\partial \psi_\alpha} \left[ \tilde{f} S_{\alpha}(\psi) \right].$$
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where $\bar{u}_i$ and $\bar{D}_T$ are the Favre-filtered velocity and the turbulent diffusivity, respectively. The first two terms on the right-hand side are the mixing term modeled by the IEM mixing model and the transport term represented by a mean drift term, respectively. The last term in Eq. (4) represents the evolution of $\tilde{f}$ in the composition space due to chemical reactions, and it appears in the closed form. In Eq. (4), $V_{\alpha,i}$ is a corrected diffusion velocity defined as

$$V_{\alpha,i} = \begin{cases} \tilde{D}_{(\alpha)} \frac{\partial \tilde{\phi}_\alpha}{\partial x_i} - \tilde{\phi}_\alpha \bar{D}_T \frac{\partial \tilde{\phi}_\alpha}{\partial x_i} & \text{for species } \alpha, \\ \tilde{D}_{(\alpha)} \frac{\partial \tilde{\phi}_\alpha}{\partial x_i} & \text{for enthalpy}, \end{cases}$$

where $\tilde{D}_{(\alpha)}$ is the mixture-averaged molecular diffusivity of species $\alpha$ or the thermal diffusivity for the sensible enthalpy. In Eq. (5), the suffices in parentheses are excluded from the summation convention, which otherwise applies to composition indices (here $\alpha$ and $\beta$). For the molecular mixing, the scalar mixing rate $\Omega$ is modeled as

$$\Omega = C_m \bar{D} + \bar{D}_T,$$

where $\bar{D}$ is thermal diffusivity, $C_m$ is a model constant and $\Delta$ is the LES filter size. In this study, the molecular viscosity $\tilde{\mu}$, and the thermal and species diffusivities $\tilde{D}_\alpha$ are evaluated using CHEMKIN’s transport library as functions of the resolved composition and temperature.

**B. The solution methodology for LES/PDF model equations**

The finite-volume method is employed in the numerical solution of the filtered conservation equations of mass and momentum, while a Monte Carlo approach in the Lagrangian framework is adopted to obtain the numerical solution of the modeled transport equation for $\tilde{f}$ (Eq. (4)). In the Monte Carlo approach, the flow is represented by a large number of notional Lagrangian particles whose position and composition evolve by the following stochastic differential equations.

$$dX^*_j = \left( \bar{u}_j + \frac{1}{\bar{\rho}} \frac{\partial (\bar{\rho} \bar{D}_T)}{\partial x_j} \right)^* dt + \left( 2 \bar{D}_T^* \right)^{1/2} dW^*_j,$$

$$d\phi^*_\alpha = - \Omega^* \left( \phi^*_\alpha - \tilde{\phi}_\alpha^* \right) + \left[ \frac{1}{\bar{\rho}} \frac{\partial \bar{V}_{\alpha,i}}{\partial x_i} \right]^* + S_\alpha(\phi^*),$$

where $dW^*_j$ denotes the Wiener increment in the $j$ direction. The superscript $^*$ denotes the particle properties, or the LES fields evaluated at the particle locations.
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The resulting solution methodology is a hybrid method composed of (i) an Eulerian finite-volume method for solving the filtered conservation equations for mass and momentum (referred to as the LES solver), and (ii) a Lagrangian Monte Carlo method for solving the modeled transport equation for the joint PDF of compositions (denoted as the PDF solver). For the hybrid LES/PDF approach, the resolved velocity $\tilde{u}$, the turbulent viscosity $\tilde{\mu}_T$, the turbulent diffusivity $\tilde{D}_T$ and the mixing frequency $\Omega$ are calculated by the LES solver. The PDF solver advances the notional particles in the physical space and the composition space, and provides the filtered density $\tilde{\rho}$, the Favre-filtered temperature $\tilde{T}$ and mass fractions $\tilde{Y}_\alpha$ to the LES solver.

The transported specific volume (TSV) method is employed for density feedback from the PDF solver to the LES solver. For the TSV method, the filtered density $\tilde{\rho}$ used in the LES equations is obtained from a transport equation for the Favre-filtered specific volume $\tilde{\upsilon}$ as

$$\frac{\partial \tilde{\rho} \tilde{\upsilon}}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u}_j \tilde{\upsilon})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \tilde{\rho} \tilde{D}_T \frac{\partial \tilde{\upsilon}}{\partial x_j} \right) + S_{\upsilon} + \dot{\omega}_{\upsilon}, \tag{9}$$

where $S_{\upsilon}$ is obtained from the PDF solver and represents the change of Favre-filtered specific volume $\tilde{\upsilon}$ due to the molecular mixing, the molecular diffusion, and chemical reactions. The last term in Eq. (9) is a relaxation term of the form

$$\dot{\omega}_{\upsilon} = \frac{\tilde{\upsilon}_{PDF} - \tilde{\upsilon}}{\tau_{\upsilon}}, \tag{10}$$

where $\tilde{\upsilon}_{PDF}$ is the specific volume obtained from the particles in the PDF solver. $\tau_{\upsilon}$ is the relaxation time scale taken here as $\tau_{\upsilon} = 4\Delta t$, where $\Delta t$ is the time step. Once the specific volume is computed from Eq. (9), the filtered density $\tilde{\rho}$ is obtained as

$$\tilde{\rho} = \frac{1}{\tilde{\upsilon}}. \tag{11}$$

To satisfy the boundedness condition imposed by the scalar transport in Eqs. (7) and (8), the minimum-decay-factor adjustment is employed. The simulations in this study are performed using the pdfFoam solver developed entirely within OpenFOAM.

C. Thermal boundary condition

The bluffbody wall is modeled as a fixed-temperature boundary in this study. A temperature profile that is measured experimentally by Euler et al. is prescribed over the bluffbody.
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surface. In the PDF solver, the heat loss is taken into account by adjusting the mean sensible enthalpy in the cells adjacent to the bluffbody surface. The mean sensible enthalpy at the wall surface is calculated using the mean species mass fractions obtained from the particles and the measured wall temperature. After computing the mean sensible enthalpy at the wall, the sensible enthalpy of particles is updated according to mixing and transport that are calculated using the IEM mixing model and the mean drift term, as described in the particle composition equation (Eq. (8)). Figure 1 shows the stencil used to interpolate mean properties onto the particle locations and to compute the mean drift terms in the boundary cells.

III. EXPERIMENTAL CONFIGURATION AND SIMULATION DETAILS

The Cambridge/Sandia swirl burner was designed to investigate the effect of stratification under swirling and non-swirling operating conditions. In this study, we focus on the swirling conditions as the non-swirling cases have been studied previously. A schematic of the burner is shown in Fig. 2. The burner consists of a central bluffbody surrounded by two annular fuel jets, i.e., the inner and outer jets, outside of which an air coflow is supplied to reduce the entrainment of the ambient air. For the inner and outer jets, the inlet bulk velocities are 8.31 m/s and 18.7 m/s, corresponding to Reynolds numbers of 5,960 and 11,500, respectively. The swirling flow is applied through the outer jet. The swirl number, defined as the ratio of mean tangential velocity to the mean axial velocity ($S = U_{tg}/U_z$), has the value of 0.79. The air coflow is laminar with an inlet velocity of 0.4 m/s. Three different stratification configurations, including premixed (SwB3), moderately stratified (SwB7), and highly stratified (SwB11) cases, are summarized in Table I. The stratification ratios, defined as the ratio of the equivalence ratios at the inner and outer jets ($\phi_{inner}/\phi_{outer}$) for the cases of SwB7 and SwB11, are set as two and three, respectively, to investigate the effect of stratification systematically. Velocity measurements are provided by Zhou et al., and the temperature and mass fraction measurements are provided by Sweeney et al.

The cylindrical computational domain spans 300 mm in the axial $z$—direction and 200 mm in the radial $r$—direction. The domain is discretized using a non-uniform $256 \times 128 \times 96$ cylindrical grid. The grid is concentrated near the nozzle in the axial direction and in the shear layer between the fuel jets in the radial direction.
FIG. 1. The stencil of the computational cells adjacent to the bluffbody surface. The circles denote the cell vertices used to compute mean properties at particle locations, while the squares represent the face centers used to calculate the mean drift terms. The empty symbols denotes the properties calculated using the experimental temperature profiles while the filled symbols denotes the properties obtained from the particles.

FIG. 2. A schematic of the stratified bluffbody burner.

TABLE I. Equivalence ratios of the two annular jets.

| Case | $\phi_{\text{inner}}$ | $\phi_{\text{outer}}$ | $\phi_{\text{inner}}/\phi_{\text{outer}}$ |
|------|-----------------------|------------------------|------------------------------------------|
| SwB3 | 0.75                  | 0.75                   | 1                                        |
| SwB7 | 1                     | 0.5                    | 2                                        |
| SwB11| 1.125                 | 0.375                  | 3                                        |

For the fuel jets, the instantaneous inlet velocities are obtained from two auxiliary turbulent non-swirling and swirling annular periodic pipe simulations for the inner and outer jets,
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respectively. In the pipe flow simulations, the axial and tangential velocities are corrected at each time step against the effect of numerical diffusion. A top-hat profile of 0.4 m/s is specified for the air coflow. At the bluffbody and wall-lips, the no-slip boundary conditions are applied. The non-adiabatic boundary condition is applied to the surface of the bluffbody using the experimentally measured temperature profiles as described in Section II C. Zero-gradient boundary conditions are imposed for all the fields at the outlet and at the far field.

Approximately 20 particles per cell are employed in the PDF solver. The mixing model parameter, $C_m$, is selected as $C_m = 25$. The methane/air combustion is represented by an augmented reduced mechanism (ARM1). In situ adaptive tabulation (ISAT) is adopted to accelerate chemistry integration. An error tolerance $\epsilon_{tol}$ of $5 \times 10^{-5}$ is employed in ISAT and this error tolerance has been found to be sufficiently low to ensure accurate solutions in similar simulations. The simulations are parallelized using a domain decomposition method and performed using 192 cores. A constant time step of $\Delta t = 4 \times 10^{-6}$ s corresponding to a Courant number of approximately 0.2 is employed. The simulations are first run for fifteen flow-through times based on the inner fuel stream velocity to reach a statistically-stationary state, and another ten flow-through times are performed to collect the statistics. The normalized computational cost is approximately 380 $\mu$s per grid cell per time step.

Three parametric models are considered in this study, as shown in Table II. The non-adiabatic boundary condition described in Sec. II C is applied in Model DD-HL (baseline), while the adiabatic boundary condition is used in Models DD-AD and ED-AD. The differential diffusion effect described in Sec. II B is included in Models DD-HL and DD-AD, while the unity Lewis number assumption is applied to all species in Model ED-AD. Here, the ED model employs the unity Lewis number assumption in both the molecular mixing and the molecular transport. In contrast, the DD model takes into account the differential diffusion in the molecular transport term while using the unity Lewis number assumption in the molecular mixing term. The effect of heat loss through the bluffbody is investigated by comparing Models DD-HL and DD-AD. The effects of the differential diffusion are studied by comparing Models DD-AD and ED-AD.
TABLE II. Model variations for parametric studies.

| Model | Differential diffusion | Heat loss |
|-------|------------------------|-----------|
| DD-AD | ✓                      | ×         |
| DD-HL | ✓                      | ✓         |
| ED-AD | ×                      | ×         |

IV. RESULTS

In this section, the baseline numerical results are first validated through a hierarchical comparison with the experimental measurements, including the global characteristics in Sec. IV.A, radial profiles of mean and r.m.s. velocities in Sec. IV.B, radial profiles of mean and r.m.s. scalars in Sec. IV.C, and scatter plots of species in Sec. IV.D. Following the validation, the effect of stratification on the flame structure is discussed. The effect of differential diffusion and the effect of heat loss through the bluffbody are addressed last, through parametric studies in Secs. IV.E and IV.F, respectively.

A. The general behavior of the flames

The iso-contours of the mean axial velocity superimposed by the mean streamlines, the mean temperature and the mean equivalence ratio from Model DD-HL are presented in Fig. 3. The recirculation zones are approximately 100 mm long for all the cases, which are five times longer than those under the non-swirling conditions (not shown here; see Ref.[27]). This difference demonstrates the strong effects of swirling flow on the recirculating flow structure. The long recirculation zone brings the cold and low equivalence ratio fluid from downstream to upstream positions, which reduces the temperature and equivalence ratio within the recirculation zone closed to the centerline due to mixing. The level of reduction in temperature and equivalence ratios is higher in stratified cases, SwB7 and SwB11, than those in the premixed case, SwB3. In the stratified cases, SwB7 and SwB9, at the axial location of 10 mm, the temperature and equivalence ratio at the centerline are approximately 7% and 35%, respectively, lower than those in the vicinity of the flame front within the recirculation zone. In contrast at the same axial location in SwB3, the differences of
FIG. 3. The mean axial velocity superimposed by the time-averaged streamlines (left), the mean temperature (middle), and the mean equivalence ratio (right), from the simulations with Model DD-HL. Row 1 to Row 3: SwB3, SwB7 and SwB11.

temperature and equivalence ratio at the centerline and in the vicinity of the flame front within the recirculation zone are approximately 1% and 17%, respectively.
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The flame fronts, defined as the loci of the peak r.m.s. temperature in the radial direction, are marked by the white points in Fig. 3. The flame front in SwB3 is mainly located within the regions with uniform equivalence ratios. Far downstream at approximately 50 mm, the flame front begins to encounter slight gradients of equivalence ratio, due to mixing between the fuel streams and the air coflow. For SwB7 and SwB11, the flame fronts start to propagate into regions with the stratification much earlier, i.e., after approximately \( z = 20 \) mm, due to the differences in the equivalence ratios between the inner and outer jets.

The effect of the heat loss through the bluffbody can be observed in the vicinity of the bluffbody surface. The temperature within this region is significantly reduced due to the heat loss effect, which will be further discussed in Sec. IV F.

B. Velocities

The mean and r.m.s. of the resolved axial, radial and tangential velocities are examined in this section to further validate the model predictions. The radial profiles obtained from SwB3, SwB7 and SwB11 at three different axial locations are compared with the experimental measurements, as shown in Figs. 4 to 8. The mean resolved axial velocity profiles agree well with the experimental data. Slight discrepancies are observed close to the centerline at downstream locations in SwB7 and SwB11. The mean tangential velocity profiles match very well with the experimental measurements as shown in Fig. 5. However, the peak values are over-predicted by approximately 10% at \( z = 10 \) mm. The mean resolved radial velocities show good consistency with the experimental data for all three cases, as shown in Fig. 6. Deviations are more obvious at the downstream locations. The peak values are over-predicted by less than 10% and the profiles are slightly shifted outward from the centerline, indicating that stronger expansion towards the radial direction due to the swirling flow is predicted by all three model combinations.

The profiles of the r.m.s. of the resolved axial, tangential and radial velocities agree well with the experimental profiles for all the three cases, as shown in Figs. 7 to 8, respectively. As shown in Fig. 7, the peaks of the r.m.s. axial velocity are over-predicted at \( z = 50 \) mm within the recirculation zone, and the over-prediction is more prominent in the stratified cases. The over-prediction of fluctuating velocity might be caused by the under-prediction of temperature within the recirculation zone, which will be further discussed in Sec. IV C.
FIG. 4. Radial profiles of the mean resolved axial velocity at different axial locations. Symbols: experimental data; red solid line: Model ED-AD; blue dot dashed line: Model DD-AD; black solid line: Model DD-HL.

The r.m.s. radial velocity profiles in Fig. 9 are slightly shifted outward, which is consistent with the observed shift in the mean radial velocity profiles in Fig. 6.

C. Scalars

The mean temperature $T$, equivalence ratio $\phi$ and mass fractions $Y$ of CH$_4$, CO$_2$, O$_2$ and CO are compared with the experimental measurements at four axial locations in Figs. 10-12. The mean temperature profiles are overall in very good agreement with the measurements for all the cases. The mean temperature at $z = 10$ mm is over-predicted by approximately 100 K by Model DD-HL for all the cases. Further downstream at $z = 50$ and 60 mm, the temperature profiles for SwB3 are well-predicted, whereas the peak values of the temperature profiles are under-predicted by approximately 200 K for SwB7 and SwB11 at the same locations. As observed in Fig. 3, the center of the recirculation zones are located approximately at $z = 60$ mm for all the cases. The strength of the recirculating flow field can have
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![Radial profiles of the mean resolved tangential velocity at different axial locations.](image)

FIG. 5. Radial profiles of the mean resolved tangential velocity at different axial locations. Symbols: experimental data; red solid line: Model ED-AD; blue dot dashed line: Model DD-AD; black dashed line: Model DD-HL.

strong effects on the temperature profiles at those locations. Therefore, the discrepancies of temperature at \( z = 50 \) and \( z = 60 \) mm can be attributed to the discrepancies in the prediction of the recirculating zone.

The equivalence ratio profiles exhibit overall good agreement with the measurements for all the three cases. At downstream locations of \( z = 30, 50 \) and \( 70 \) mm, the equivalence ratio profiles are under-estimated in SwB7 and SwB11. The under-predicted equivalence ratios within the recirculation zones are consistent with the observed under-prediction of temperature at the same locations, and may result from the strong effect of mixing with downstream airs within the recirculation zone.

The mean \( \text{CH}_4 \) profiles are in good agreement with the measurements for all the three cases at all the axial locations. The \( \text{CO}_2 \) and \( \text{O}_2 \) profiles are well predicted in the premixed case of SwB3. In SwB7 and SwB11, the \( \text{CO}_2 \) and \( \text{O}_2 \) profiles are in good agreement with the experiment at \( z = 10 \) mm, however, \( \text{CO}_2 \) is slightly under-predicted and \( \text{O}_2 \) is slightly over-predicted within the recirculation zone close to the flame front (approximately \( r = 25 \)).
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FIG. 6. Radial profiles of the mean resolved radial velocity at different axial locations. Symbols: experimental data; red solid line: Model ED-AD; blue dot dashed line: Model DD-AD; black solid line: Model DD-HL.

mm in Fig. 3 at \(z = 50\) and \(60\) mm. For SwB3, the profiles of CO are well predicted at all axial locations. The peak values of the CO profiles are in very good agreement with the experiment at \(z = 10\) mm, while they are slightly under estimated at downstream locations. For the cases of SwB7 and SwB11, the profiles of CO are well predicted at \(z = 10\) mm, while the CO profile is under predicted at the downstream locations.

Lastly, the total r.m.s. of temperature, equivalence ratio and mass fractions of CH\(_4\), CO\(_2\), O\(_2\) and CO are presented in Figs. 13-15 and compared with the measurements. The total r.m.s. of the scalars is defined as \(Y_{\alpha,rms} = \left(\langle \tilde{Y}_{\alpha}^2 \rangle - \langle \tilde{Y}_{\alpha} \rangle^2 \right)^{1/2}\), where \(\langle \cdot \rangle\) denotes the time averaging. All the profiles are overall in good agreement with the measurements. At downstream locations, the fluctuations are slightly lower than those obtained from the measurements, however, the trends in the experimental data are well captured at these locations. The r.m.s. of the equivalence ratio, O\(_2\), CO\(_2\), and CO are under-predicted at \(z = 50\) and \(60\) mm for all the three cases. This may be explained by the slightly coarsened grid resolution in this region. Although the species concentration is evolved by the Lagrangian
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FIG. 7. Radial profiles of the r.m.s. of the resolved axial velocity at different axial locations. Symbols: experimental data; red solid line: Model ED-AD; blue dot dashed line: Model DD-AD; black dashed line: Model DD-HL.

particles in the numerical solution procure, the mean properties used in the mixing model are computed at the grid nodes. Therefore, grid resolution has an impact on the distribution of the equivalence ratio.

D. Scatter plots

To further validate the numerical results, mole fractions of all experimentally-measured species, CO$_2$, H$_2$, CO, CH$_4$, H$_2$O, O$_2$, and the equivalence ratio, $\phi$, are presented in the temperature space at $z = 10$ mm, shown as scatter plots in Figs. 16-18. The mean values conditional on temperature, $\langle X_\alpha | T \rangle$, obtained from the simulations are also compared with the experimental data. The plots are color-coded by the equivalence ratio. The scatter plots are generated using the notional Lagrangian particles from five different time snapshots. The scatter plots from the LES/PDF simulations are in good agreement with the experimental data. The plots from the simulations are slightly narrower in the temperature space than
FIG. 8. Radial profiles of the r.m.s. of the resolved tangential velocity at different axial locations. Symbols: experimental data; red solid line: Model ED-AD; blue dot dashed line: Model DD-AD; black dashed line: Model DD-HL.

those in the experimental measurements, indicating faster mixing rates predicted by the numerical simulations. However, the trends of all species are well captured.

The experimental data points extend to smaller values in the equivalence ratio space than those obtained from the LES/PDF simulation, particularly at \( T > 1500 \) K. For the premixed case SwB3, the lowest equivalence ratio is smaller than the value from the premixed jets, suggesting entrainment of downstream air and/or diluted mixture deep into the recirculation zone. The lowest equivalence ratios observed in the cases of SwB7 and SwB11 above \( T = 1500 \) K also result from the same entrainment mechanism.

The conditional means from the simulations are overall in good agreement with those obtained from the experimental data. The conditional means of \( \text{H}_2 \), \( \text{CO} \) and equivalence ratio are slightly underestimated for temperature lower than approximately 1500 K, while the conditional means of \( \text{CO}_2 \), \( \text{CH}_4 \), \( \text{H}_2\text{O} \), and \( \text{O}_2 \) are well predicted within this region in the temperature space. Considerable discrepancies are observed between the conditional means from the experimental and the numerical results for temperatures higher than 1500 K,
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FIG. 9. Radial profiles of the r.m.s. of the resolved radial velocity at different axial locations. Symbols: experimental data; red solid line: Model ED-AD; blue dot dashed line: Model DD-AD; black dashed line: Model DD-HL.

mainly because the simulations over-predict the equivalence ratio at these temperatures.

To further understand the physical locations of discrepancy in conditional means, the scatter plots of CO mass fraction as a function of temperature are color-coded by the radial positions at $z = 10$ mm for SwB3, SwB7 and SwB11, as presented in Fig. 19. The points with radial locations smaller than 5 mm are colored by black to highlight the points close to the centerline. As observed in Fig. 19, the points with low equivalence ratios are located closed to the centerline. Considering the recirculating flow fields given in Fig. 3, the points closed to the centerline mainly are entrained from the locations with lower equivalence ratio downstream. Therefore, accurate prediction of the recirculation region is important for correct prediction of the scalars. Compared to the shorter recirculation region observed in Turkeri et al.\textsuperscript{27}, the cases with swirling flow in this study are more challenging computationally. The extent of the computational domain and the outlet boundary conditions can potentially impact the states within the recirculation zone, which subsequently impact the flame stabilization. Although not shown in the paper due to space consideration, the scatter
FIG. 10. SwB3: The radial profiles of the time-averaged resolved temperature and the resolved mass fractions of CH$_4$, CO$_2$, O$_2$ and CO at five axial locations of z = 10, 30, 50, 60 mm. Symbols: experimental data; red solid line: Model ED-AD; blue dot dashed line: Model DD-AD; black solid line: Model DD-HL.

plots at further downstream locations have similar agreement with the experimental data.
FIG. 11. SwB7: The radial profiles of the time-averaged resolved temperature and the resolved mass fractions of CH$_4$, CO$_2$, O$_2$ and CO at four axial locations of $z = 10, 30, 50, 60$ mm. Symbols: experimental data; red solid line: Model ED-AD; blue dot dashed line: Model DD-AD; black solid line: Model DD-HL.
FIG. 12. SwB11: The radial profiles of the time-averaged resolved temperature and the resolved mass fractions of CH$_4$, CO$_2$, O$_2$ and CO at four axial locations of $z = 10$, 30, 50, 60 mm. Symbols: experimental data; red solid line: Model ED-AD; blue dot dashed line: Model DD-AD; black solid line: Model DD-HL.
FIG. 13. SwB3: The radial profiles of the r.m.s. temperature and the r.m.s. mass fractions of CH$_4$, CO$_2$, O$_2$ and CO at $z = 10, 30, 50, 60$ mm. Symbols: experimental data; red solid line: Model ED-AD; blue dot dashed line: Model DD-AD; black solid line: Model DD-HL.
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FIG. 14. SwB7: The radial profiles of the r.m.s. temperature and the r.m.s. mass fractions of CH₄, CO₂, O₂ and CO at z = 10, 30, 50, 60 mm. Symbols: experimental data; red solid line: Model ED-AD; blue dot dashed line: Model DD-AD; black solid line: Model DD-HL.
FIG. 15. SwB11: The radial profiles of the r.m.s. temperature and the r.m.s. mass fractions of CH$_4$, CO$_2$, O$_2$ and CO at $z = 10$, 30, 50, 60 mm. Symbols: experimental data; red solid line: Model ED-AD; blue dot dashed line: Model DD-AD; black solid line: Model DD-HL.
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E. Effect of differential diffusion

The effect of differential diffusion is examined by comparing the results obtained from Models DD-AD and ED-AD. It should be emphasized that only the resolved molecular differential diffusion is considered by the models employed here. The mean and the r.m.s. velocity as well as the scalar profiles from Models DD-AD and ED-AD are very close to one another for SwB3, SwB7 and SwB11 at all the axial locations, as shown in Figs. 4-15. Therefore, resolved molecular differential diffusion is found to have insignificant impact on the mean velocity and scalar profiles under the swirling conditions. This is in contrast with the non-swirling conditions, where differential diffusion has been found to slightly modify the velocity profiles by shortening the recirculation zone behind the bluffbody. When the recirculation zone is created by both the bluffbody and the swirling flow, differential diffusion seems to play a secondary role in affecting the size of the recirculation zone compared to the non-swirling conditions.

F. Effect of heat loss through the bluffbody

The effect of heat loss through the bluffbody is examined by comparing results obtained from Models DD-HL and DD-AD. The mean and the r.m.s. velocity profiles from the two models are very similar to one another, as shown in Figs. 4-15, which indicates that heat loss has negligible effect on the velocity profiles. The temperature profiles from Model DD-HL are in better agreement with the experimental data than those from Model DD-AD at \( z = 10 \) mm for all the cases. Model DD-HL over-predicts the mean temperature by approximately 100K while Model DD-AD over-predicts by approximately 300K close to the centerline in SWB7 and SwB11 at \( z = 10 \) mm.

The mean CO profiles from Model DD-HL are in very good agreement with the experimental measurements, while Model DD-AD over-predicts CO mass fractions by approximately 25% at \( z = 10 \) mm. This is mainly due to the higher temperature predicted by Model DD-AD.

The mean equivalence ratio profiles from Models DD-HL and DD-AD are very similar in the premixed case, SwB3. For the moderately stratified case SwB7, Model DD-HL produces slightly lower profiles than those from Model DD-AD at \( z = 10 \) mm. For the highly stratified
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case, SwB11, the result from Model DD-HL is in better agreement with measurements than those from Model DD-AD at \( z = 10 \text{ mm} \), while Model DD-AD predicts 5% higher the equivalence ratio than the measurements at that axial location.

The mean mass fraction of \( \text{CH}_4 \), \( \text{CO}_2 \) and \( \text{O}_2 \) from Model DD-HL are in slightly better agreement with measurements than those from Model DD-AD within the recirculation zone \( (r < 12 \text{ mm}) \) at \( z = 10 \text{ mm} \). Comparing to \( \text{CO} \), mass fractions of \( \text{CH}_4 \), \( \text{CO}_2 \) and \( \text{O}_2 \) demonstrate lower levels of sensitivity to the heat loss effect.

For all scalar profiles, Models DD-HL and DD-AD predict very similar results at further downstream locations of \( z = 30, 50 \) and \( 70 \text{ mm} \), which indicates a negligible effect of heat loss at those locations. The r.m.s. profiles of temperature, equivalence ratio, and mass fractions of \( \text{CH}_4 \), \( \text{CO}_2 \), \( \text{O}_2 \) and \( \text{CO} \) from Models DD-HL and DD-AD are also very close to one another at all the axial locations.

V. CONCLUSION

LES/PDF simulations of the Cambridge/Sandia stratified turbulent flames under swirling conditions have been performed with finite-rate chemistry. The premixed (SwB3), the moderately stratified (SwB7), and the highly stratified (SwB11) flames are simulated using the same set of models and parameters. The mean and the r.m.s. velocity fields are well predicted, using the baseline model parameters. The radial profiles of the mean and the r.m.s. temperature, equivalence ratio, and species mass fractions are in overall good agreement with the experimental measurements.

The scatter plots of species and their conditional means exhibit very good consistency with the measurements. Entrainment of the lower equivalence ratio mixture from downstream to the recirculation zone is under-predicted near the bluffbody surface at \( z = 10 \text{ mm} \), but over-predicted further downstream for the two stratified cases. Consequently, the equivalence ratio and temperature are over-predicted near the bluffbody surface and under-predicted further downstream. The lengths of recirculation zone are approximately five times those of the non-swirling conditions. A unique challenge of the swirling bluffbody stabilized flames is the downstream boundary condition, which can have a more significant impact on the composition of the recirculation zones under swirling conditions.

The results obtained with and without differential diffusion show that the differential
diffusion considered in the mean drift term has a negligible effect on the length of the recirculation zone, as well as on the mean and the r.m.s. velocity and scalar profiles for SwB3,
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FIG. 17. SwB7: Scatter plots of mole fractions of CO$_2$, H$_2$, CO, CH$_4$, H$_2$O, O$_2$ and $\phi$ as a function of temperature from the experimental measurements and the LES/PDF simulation with DD-HL model at $z = 10$ mm, color-coded by the equivalence ratio. Black solid line: conditional mean of species mole fractions from the experiment; red dashed line: conditional mean of species mole fractions from the simulation.

SwB7 and SwB11. Compared to the non-swirling conditions, the length of the recirculation
FIG. 18. SwB11: Scatter plots of mole fractions of CO$_2$, H$_2$, CO, CH$_4$, H$_2$O, O$_2$ and $\phi$ as a function of temperature from the experimental measurements and the LES/PDF simulation with DD-HL model at $z = 10$ mm, color-coded by the equivalence ratio. Black solid line: conditional mean of species mole fractions from the experiment; red dashed line: conditional mean of species mole fractions from the simulation.

zone is more influenced by the swirling conditions than the existence of a bluffbody and
FIG. 19. Scatter plots of mass fractions of CO as a function of temperature obtained from the experimental measurements (top) and the LES/PDF simulation with DD-HL model (middle) at $z=10$ mm, color-coded by the radial positions. The conditional mean temperature at $z=10$ mm is shown in the bottom row. The particles that are close to the centerline (i.e., radial locations smaller than 5 mm) are colored by black. Black solid line: conditional mean of CO from the experiments; red dashed line: conditional means of CO from the simulations.

differential molecular diffusion.

The effect of heat loss through the bluffbody wall is examined through a parametric study. It is found that taking into account the heat loss through the bluffbody significantly improves the prediction of mean temperature and CO mass fraction close to the inlet. Additionally, the inclusion of heat loss has a negligible impact on the results at further downstream locations.

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DATA AVAILABILITY STATEMENTS

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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