Nonlinear large-eddy simulation of a Cambridge stratified swirlingflame

XiangQian[a], HaoLu[a,b], Chun Zou[a,b], Hong Yao[a,b]

[a]State Key Laboratory of Coal Combustion,

[b]School of Energy and Power Engineering,

Huazhong University of Science and Technology, Wuhan 430074, China

1 Introduction

Swirling combustion technology has been widely used in industrial combustion devices, such as gas turbines, internal combustion engines, and furnaces, owing to the fact that swirling flow can enhance fuel and air mixing and reduce flame length [1]. However, the appearance of oscillations and instabilities in swirling burner makes it particularly challenging to accurately simulate the interactions between turbulence and combustion. The Cambridge stratified swirl burner series [2, 3] provideabundant experimental data under a series of operating conditions, including different swirl numbers and stratification levels, and thus can be used to validate turbulence and combustion approaches. Recently, numerical studies have been carried out for the flames under non-swirl conditions [4-6] and swirling conditions [7]. A recent large-eddy simulation (LES) study by Brauner et al. [7] hasshown the overestimationof the temperature in the central regions of swirling flames is very serious(~400K), and they and their co-workers have also shown that, at the 14th international workshop of measurement and computation of turbulent nonpremixed flames (2018), changes of the combustion model are not critical to solving this issue.

In LES, subgrid-scale (SGS) model is one of the keys to accurately simulate turbulent flames. Modeling studies have shown that nonlinear SGS models can capture strong anisotropies in turbulent flows, thus yielding a more accurate set of results in flows with strong shears [8-11]. Recent LESs of turbulent flames [12, 13] have shown that the usage of the gradient-type structural SGS models is able to provide better predictions of turbulent mixing.Owing to the strong shear generated in high-velocity nozzles under high swirling configuration, nonlinear SGS models would be a better option to study the high-swirling case.

The aim of this study is to investigate the influence of high swirl in the SwB3 case by using a gradient-type structural SGS stress model [9, 11-13], which is one of the recently developed nonlinear SGS models. The following section describes our study’s numerical framework, including a description of the case and the simulation details. Then the LES results are presented and discussed.

2 Model Description

2.1 LES Governing Equations

Correspondence to: haolu@hust.edu.cn; zouchun@hust.edu.cn

In this study, we get the resolved governing equations by applying the filtering operation to the continuity equation, the momentum equations, and the transport equations of enthalpy and chemical species:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j}{\partial x_j} = 0 \tag{1}$$

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial \bar{\sigma}_{ij}}{x_j} + \bar{f}_i \tag{2}$$

$$\frac{\partial \bar{\rho}\tilde{h}}{\partial t} + \frac{\partial \bar{\rho}\tilde{h}\tilde{u}_j}{\partial x_j} = \frac{D\bar{p}}{Dt} - \frac{\partial q_j^h}{\partial x_j} - \frac{\partial \bar{q}_j}{\partial x_j} + \overline{\sigma_{ij}\frac{\partial u_i}{\partial x_j}} + \bar{s}_h + \bar{\dot{\omega}}_h \tag{3}$$

$$\frac{\partial \bar{\rho}\tilde{Y}_i}{\partial t} + \frac{\partial \bar{\rho}\tilde{Y}_i\tilde{u}_j}{\partial x_j} = -\frac{\partial q_j^i}{\partial x_j} - \frac{\partial \bar{q}_j^i}{\partial x_j} + \bar{\dot{\omega}}_i \tag{4}$$

where $\tau_{ij} = \bar{\rho}(\widetilde{u_i u_j} - \tilde{u}_i\tilde{u}_j)$ is the SGS stress tensor, $q_j^h = \bar{\rho}(\widetilde{h u_j} - \tilde{h}\tilde{u}_j)$ is the SGS heat flux, $q_j^i = \bar{\rho}(\widetilde{Y u_j} - \tilde{Y}\tilde{u}_j)$ is the SGS flux of the species i, $\bar{\sigma}_{ij}$ is the filtered molecular shear-stress tensor, $\bar{f}_i$ is the external force such as the gravitational force, $\bar{q}_j$ is the filtered molecular heat flux, $\bar{q}_j^i$ is the filtered molecular diffusion of the species, $\bar{s}_h$ is the external heat source (such as radiation), and $\bar{\dot{\omega}}_h = -\sum_{i=1}^{N_i} \bar{h}_i\bar{\dot{\omega}}_i$ is the heat released from reactions, where $\bar{\dot{\omega}}_i = M_{\omega,i}\sum_{r=1}^{N_r} \bar{\dot{\omega}}_{i,r}$ is the filtered mass reaction rate of the species per unit volume and must be modeled with a combustion model. The filtered molecular shear-stress tensor for a Newtonian fluid $\bar{\sigma}_{ij}$ is usually modeled as $\bar{\sigma}_{ij} = \hat{\sigma}_{ij} = \mu(\tilde{T})(2\tilde{S}_{ij} - \frac{2}{3}\delta_{ij}\tilde{S}_{kk})$, and the deviation is negligible. Similarly the filtered molecular heat flux $\bar{q}_j$ can be modeled as $\bar{q}_j = \hat{q}_j = -\frac{C_p\mu(\tilde{T})}{P_r}\frac{\partial \tilde{T}}{\partial x_j}$and the filtered molecular diffusion $\bar{q}_j^i$can be modeled as $\bar{q}_j^i = \hat{q}_j^i = -\frac{\mu(\tilde{T})}{S_c}\frac{\partial \tilde{Y}^i}{\partial x_j}$. For simplicity, we adopt Pr = 0.7 and Sc = 0.7 in this study.

2.2 SGS Modeling

The turbulence parameterization constitutes the most critical part of the turbulent flow simulations. It is well known that LES solutions can be sensitive to the given type of SGS model. The recently introduced nonlinear models do not rely on the Boussinesq hypothesis, and have shown an evident improvement over results obtained from traditional eddy-viscosity models in a variety of flows [8], particularly for flows with large shears, including boundary layer, mixing layer, and spray combustion. We adopt the recently developed nonlinear gradient-type structural SGS stress model and SGS flux modelwritten as

$$\tau_{ij} = 2\bar{\rho}k_{sgs}\left(\frac{\tilde{G}_{ij}}{G_{mm}}\right) + \bar{\rho}\nu_{sgs}^u\nabla^2\tilde{S}_{ij} \text{and} q_i = |q|\left(\frac{\tilde{G}_{ij}}{\tilde{G}_{\theta,i}}\right) \tag{5}$$

where $k_{sgs}$is the SGS kinetic energy, $|q|$is the magnitude of the SGS flux vector, $\tilde{G}_{ij} = \frac{\partial \tilde{u}_i}{\partial x_k}\frac{\partial \tilde{u}_j}{\partial x_k}$ and$\tilde{G}_{\theta,i} = \frac{\partial \tilde{u}_i}{\partial x_k}\frac{\partial \tilde{\theta}}{\partial x_k}$are the gradient terms, θ is any given scalar, and $|G_\theta| = \sqrt{G_{\theta,1}^2 + G_{\theta,2}^2 + G_{\theta,3}^2}$. Moreover,we adopt hyper viscosity, $\nu_{sgs}^u = C_k'\Delta^3\sqrt{k_{sgs}}$,instead of regular SGS viscosity to overcome the traditional eddy viscosity's excessive dissipativeness at large scales. We use an empirical constant $C_k' = 0.008$ [9]. The local equilibrium hypothesis relies on a sufficiently large statistical sample that usually does not exist at the SGS level in a complex flow. Thus, we solve the transport equation of the SGS kinetic energy

$$\frac{\partial k_{sgs}}{\partial t} + \tilde{u}_j \frac{\partial k_{sgs}}{\partial x_j} = -\frac{\tau_{ij}}{\bar{\rho}} \frac{\partial \tilde{u}_i}{\partial x_j} - C_c \frac{k_{sgs}^{3/2}}{\Delta} + \frac{\partial}{\partial x_j}\left[\left(\frac{\nu_{sgs}}{\sigma_k} + \nu\right)\frac{\partial k_{sgs}}{\partial x_j}\right] \tag{6}$$

where, $\nu_{sgs} = C_k' \sqrt{k_{sgs}} \Delta$, and the three terms on the right-hand side represent, respectively, the production,dissipation, and diffusion of the SGS kinetic energy. The typical values for the constants are $C_k = 0.05$,$C_c = 1.0$,$\sigma_k = 1.0$ [9]. Following Lu and Porte-Agel [11], the magnitude of the SGS flux vector can be evaluated as,

$$|q| = H(P_\theta)H(P)\frac{\bar{\rho}}{Sc}\frac{2\Delta^2}{C_{\varepsilon\theta}^2}\left(-\frac{G_{\theta,k}}{|G_\theta|}\frac{\partial \tilde{\theta}}{\partial x_k}\right)\left(-\frac{G_{ij}}{G_{mm}}S_{ij}\right) \tag{7}$$

where H(x) is the Heaviside step function defined as H(x) = 0 if x < 0 and H(x) = 1 if x ≥ 0,

$P = -\tau_{ij}\tilde{S}_{ij}$,$P_\theta = -q_i \frac{\partial \tilde{\theta}}{\partial x_i}$, $C_{\varepsilon\theta} = 1$.

2.3 Combustion Modeling

The main difficulty in LES of turbulent combustion is calculating the filtered chemicalsource term.In this study, we adopt a constant volume partially stirred reactor (PaSR) [14, 15] approach of a computational cell, where reactions occur in a fraction of its volume. In the PaSR approach, each computational cell is split into two zones: all reactions occur in one zone, the other zone has noreactions. The reaction rate of the computational cell is determined by,

$$\overline{\dot{\omega}}\left(\bar{\rho}, \tilde{T}, \tilde{Y}_1\right) = \kappa\, \dot{\omega}\left(\bar{\rho}, \tilde{T}, \tilde{Y}_1\right) \tag{8}$$

where $\dot{\omega}\left(\bar{\rho}, \tilde{T}, \tilde{Y}_1\right)$is the reaction rate computed on the basis of PSR assumption and the fraction of the reactor in the cell, κ, is assumed to be proportional to the ratio of the chemical reaction time, τ_c, to the total conversion time in the reactor (i.e. the sum of the turbulent micro-mixing time, τ_{mix}, and the reaction time),

$$\kappa = \frac{\tau_c}{\tau_{mix} + \tau_c} \tag{9}$$

This nonlinear LES framework integrates these gradient-type structural SGS models for turbulent flows with strong anisotropies and a PaSR approach [14, 15] coupled with a reduced (from GRI-Mech) methane oxidation mechanism, DRM19 mechanism [16], involving 21 species and 84 reaction steps.

2.4 Simulation Description

The Cambridge stratified swirl burner was designed to investigate flames in premixed and stratified regimes, with or without swirl. The burner is stabilized at a central bluff body surrounded by two annular fuel jets. The burner dimensions are illustrated in figure1 (left). The inlets from the innermost to the outermost are the inner fuel inlet, the outer fuel inlet, and the air coflow, respectively. The bulk velocity of the inner and outer inlets are 8.31 m/s and 18.7 m/s, respectively, and the velocity of the air coflow is 0.4 m/s. Here we only consider high swirling case with purely premixed inlet conditions.

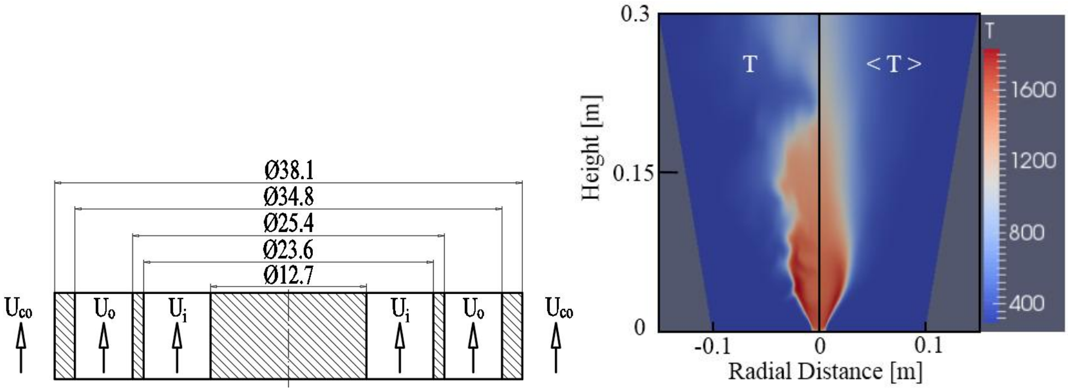

Fig. 1: (Left): schemetic of the burner (dimensions in mm); (Right): instantaneous (left half) and time-averaged (right half) temperature contours in the SwB3 case.

The computational domain spans 300 mm in the axial z-direction and 150 mm in the radial r-direction. The mesh size used in the study is 80×90×72 in axial, radial and circumferential directions, respectively. The grid is concentrated near the nozzle along the axial direction and in the shear layer between the fuel jets in the radial directions.

For the fuel jets, the mean inlet velocities ofjets are obtained through pipe simulations of periodic boundary. Then turbulence was added to the mean velocity profiles. The inlet velocity of the air coflow is set to be the uniform velocity profile of 0.4 m/s. At the bluff body and the wall-lips, no-slip boundary conditions are applied. The temperature of the bluff body is from the experiment data that was measured by Euler et al. [17]. All statistical quantities were collected, typically, for a period of 5–10 flow through times, based on the jet bulk velocity, after the initial flow was allowed to reach a statistically steady state.For a general view of this case, figure 1 (right) shows instantenous and time-averaged resolved temperature of the flow.

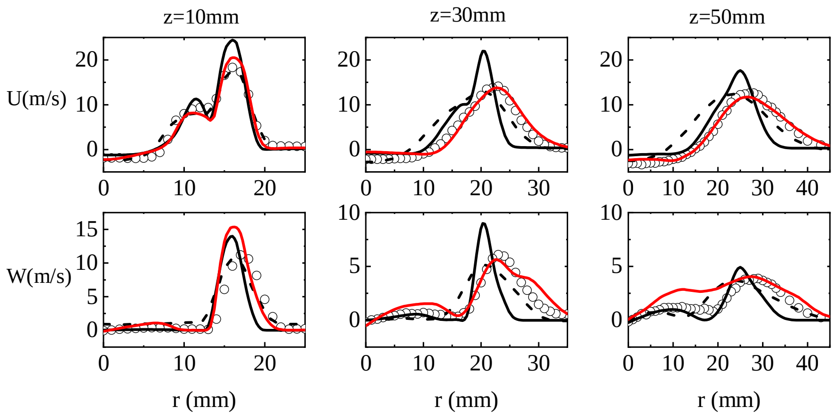

Fig. 2 Radial profiles of mean axial and tangential velocity at three downstream locations. Red solid line: the GM/PaSR results; black solid line: the SM/PaSR results;black dashedline: the LES/PDF results in Brauner et al. [7]; black circle: experiment data.

3 Result and Discussion

In this section, we present a comparison of the mean velocities,temperature and the mass fraction of $CH_4$and O_2 between the experimental measurements [2, 3] and the LES results. The LES results are obtained using the current gradient-type model (GM)/PaSR approach,the Smagorinsky model (SM)/PaSR approachand the LES/PDF approach using the dynamic Smagorinsky SGS model as reported by Brauner et al [7].

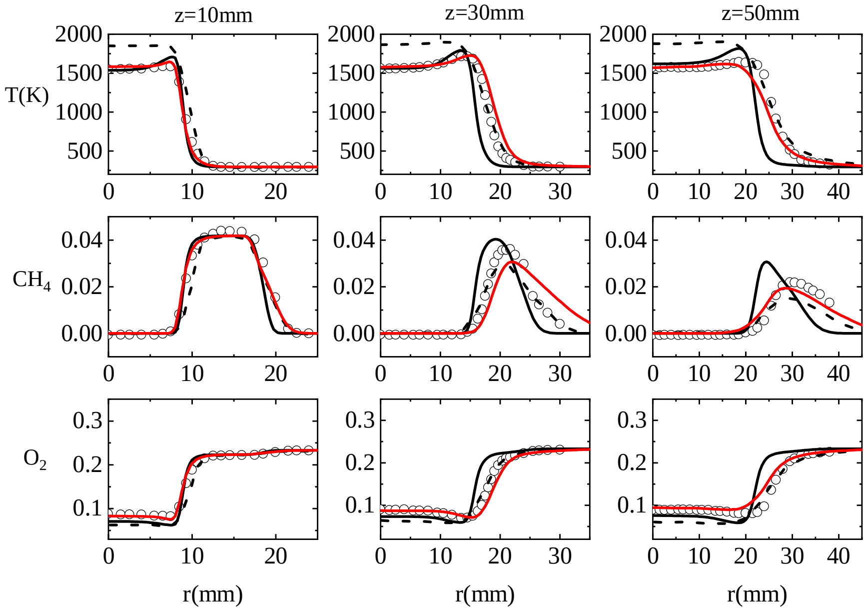

Fig. 3 Radial profiles of mean temperature, CH_4, and O_2 at three downstream locations. Symbol description follows the presious figure.

The mean velocities, temperatureand the mass fraction of CH_4 and O_2 at axial locations z=10mm, 30mm and 50mm are compared with the experimental data as shown in figures 2 and 3. The mean temperatureand CH_4, O_2 mass fractions profiles are in satisfactory agreement with the measurements.The mean axial and tangential velocity profiles are in good agreement with the experiment data, including in the recirculation zone of the bluff-body wake. It is clearly evident, that comparing with the previous LES/PDF results, the current nonlinear LES delivers significantly improved predictions.

4 Conclusion

The present study integrates the recently introduced gradient-type structural SGS approach and the PaSR combustion approach to simulate a Cambridge stratified swirl flame.In LES modeling, the structural apprach is an alternative to the eddy-viscosity/diffusivity approach. Using the structural approach, one can predict the SGS terms without assuming the energy must flow from resolved scale to subgrid scale, and this feature is helpful for accurate predictions of cross-scale interactions in turbulent flames. Results show that the proposed nonlinear LES framework yields a great improvement in the predictions of the temperature and CH_4, O_2 mass fractionsprofiles, and the mean profiles of axial and tangential velocities are in satisfactory predictions.

The gradient method does not require convolution integration to achieve spatial filtering, thus, the computational cost of the framework is similar to the cost of the standard eddy-viscosity/diffusivity approach, such as the Smagorinsky model. These features make this LES framework an attractive tool for simulation of flames in complex flows. Furture work would extend it to address more turbulent flames.

Acknowledgments

This reserach was supported by the National Natural Science Foudation of China (51776082). Computing resources were provided by the National Supercomputer Center in Guangzhou.

References

[1] Johanson MR, Littlejohn d, Nazeer WA, Smith KO, Cheng RK (2005), A comparison of the flowfields and emissions of high-swirl injectors and low-swirl injectors for lean premixed gas turbines, Proc. Combust. Inst.

[2] Sweeney MS, Hochgreb S, Dunn MJ, Barlow RS. (2012). The structure of turbulent stratified and premixed methane/air flames I: Non-swirling flows. Combust. Flame 159:2896.

[3] Sweeney MS, Hochgreb S, Dunn MJ, Barlow RS. (2012). The structure of turbulent stratified and premixed methane/air flames ii: Swirling flows. Combust. Flame 159 :2912.

[4] Proch F, Kempf AM.(2014). Numerical analysis of the Cambridge stratified flame series using artificial thickened flame LES with tabulated premixed flame chemistry. Combust. Flame.161：2627.

[5]Mercier R, Schmitt T, Veynante D,Fiorina B.(2015). The influence of combustion SGS submodels on the resolved flame propagation. Application to the LES of the Cambridge stratified flames.P.Combust.Inst. 35：1259.

[6] Turkeri H,Zhao XY, Pope SB, Muradoglu M.(2019) Large eddy simulation/probability density function simulations of the Cambridge turbulent stratified flame series. Combust. Flame.199：24.

[7] Brauner T, Jones WP, Marquis AJ. (2016). LES of the Cambridge Stratified Swirl Burner using a Sub-grid pdf Approach.Flow Turbul. Combust.96:965

[8] Lu H, Rutland CJ.(2016). Structural subgrid-scale modeling for large-eddy simulation: A review. ActaMech. Sin. 32 : 567.

[9] Lu H, Rutland CJ, Smith LM. (2008). A posteriori tests of one-equation LES modeling of rotatingturbulence. Int. J. Mod. Phys. 19:1949.

[10] Lu H, Porte-Agel F. (2010). A modulated gradient model for large-eddy simulation: application to a neutral atmospheric boundary layer. Phys. Fluids. 22: 015109.

[11] Lu H, Porte-Agel F. (2013), A modulated gradient model for scalar transport in large-eddy simulation ofthe atmospheric boundary layer, Phys. Fluids 25:015110.

[12] Lu H, Zou C, Shao S, Yao H (2019), Large-eddy simulation of MILD combustion using partially stirred reactor approach, Proc. Combust. Inst.

[13] Lu H, Chen WZ, Zou C, Yao H (2019), Large-eddy simulation of Sandia Flame F using structural subgrid-scale models and partially-stirred-reactor approach, Physics of Fluids

[14] Chomiak J, Karlsson A (1996), Flame liftoff in diesel sprays, Twenty-Sixty Symposium (International) on Combustion/The Combustion Institute 26

[15] Nordin P (2001), Complex chemistry modeling of diesel spray combustion, Ph.D. Thesis, Chalmer University of Technology

[16] Kazakov A, Frenklach M, DRM19 reaction mechnism, http://www.me.berkeley.edu/drm/

[17] Euler M, Zhou R, Hochgreb S, Dreizier A (2014), Temperature measurements of the bluff body surface of a swirl burner using phosphor thermometry, Combustion and Flame, 161