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Large eddy simulations of a bluff-body burner using the thickened flame model

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ABSTRACT

The Large eddy simulation (LES) has been widely used in describing turbulent flow. Also, the dynamic thickened flame (DTF) model is an effect method in combustion simulation. In the paper, the velocity and mixture fraction of cold flow in the bluff-body burner were simulated by RANS and LES method, which were compared with the measurements to access the prediction capability. And the DTF model was used to investigate the process of flame propagation. The results show that the velocity and mixture fraction simulated by both models are in agreement with the measurements. The LES method can capture smaller vortex structures in the flow process compared with the RANS method. In the ignition process, the flame kernel moves to the bluff and anchors in the recirculation zone, then burns along the isosurface of the stoichiometric mixture fraction. The path is in agreement with the experimental results. Also, the flame structure in propagation process simulated by the DTF model can match well with the experimental results.

Keywords: Large Eddy Simulation, Ignition, Dynamic thickened flame model, Flame structure

INTRODUCTION

The ignition performance of combustor is related to the reliability of the air-engine, and the ignition process involves the atomization, turbulent flow and chemical reaction of fuel. The test method costs a lot and can only understand the ignition situation in a macroscopic way, while the numerical simulation can study the ignition characteristics in detail. The

widely used simulation method is the Reynolds-averaged Navier–Stokes (RANS) method, which has some difficulties in predicting the turbulent flow accurately. More recently, the development of Large eddy simulation (LES) has allowed detailed studies of turbulent flow. Even though the cost of such LES remains very high, the predictive capacities of the tool for turbulent flow has been clearly demonstrated.

Usually, the flame thickness is generally smaller than the computational grid size, so some geometry approaches have been proposed to deal with the issue, including flame front tracking techniques (Menon et al. 2012) and the use of filtered progress variables (Boger et al. 1998). Also, the thickened flame (TF) model is proposed to simulate the combustion process, which is most used in an LES combustion model for premixed flames (Selle et al. 2004), lifted flames (Legier et al. 2000) as well as ignition sequences (Vreman et al. 2009; Fiorina et al. 2010). Amer (Amer et al. 2016) used the TF model combined with the flamelet generated manifolds to predict the flame structure. Volpiani (Volpiani et al. 2017) adopted the TF combustion model coupled with global and local dynamic procedures to assess the influence of the dynamic model in the prediction of combustion instabilities. Later, Legier (Legier et al. 2002) proposed the dynamic thickened flame (DTF) model, which could simulate mixing, diffusion and premixed flames simultaneously and compute the thickening factor dynamically in space and time. In order to ensure a smoother distinction between the flame front and the zone close to it, some sensors were proposed to calculate the thickening factor dynamically such as the hyperbolic

tangent function of Arrhenius expression. Durand (Durand et al. 2007) used the progress variable as a sensor of DTF model, which performed well for predicting laminar flame structure when coupling with multi-step reaction mechanism. But it underestimated the effective thickening factor. Guo (Guo et al. 2018) used the hyperbolic tangent function of progress variable to calculate thickening factor dynamically, and the preheated and reaction zones were thickened effectively. Shang (Shang et al. 2010) used the DTF model to study the combustion process of non-premixed flame, whose flame front sensor was based on the heat release rate. The predicted mixture fraction, reaction products concentration by DTF model could agree with the experimental data. For the most, the efficiency functions were introduced, which played an important role in compensating the reduced surface area of the thickened flame. The value of the efficiency function affected the fuel combustion speed and heat release rate (Charlette et al. 2002; Bougrine et al. 2014). Xiao (Xiao et al. 2018) used the DTF model coupled with a single-step chemistry to investigate the premixed combustion. The prediction of unsteady premixed propane-air flame propagation was quite reliable compared with the experimental results.

The objective of this study is to investigate the cold flow and ignition progress of bluff-body burner. The models of cold flow and combustion are presented in section 2. The cold-flow results simulated by LES and RANS methods are discussed and compared with experimental results in section 3. In section 4, the flame structures and the path of flame propagation obtained by the DTF model are analysed. Finally, section 5 concludes the paper.

BURNER DESCRIPTION AND NUMERICAL MODEL

Burner description

The burner used in present work is designed by Balachandran (Balachandran. 2005), which has two concentric circular ducts. The inner diameter of the outer duct is 35 mm, which is used to transport the air. The methane enters into the combustor through a 6-mm-internal diameter tube of wall thickness 0.5 mm. And there is a conical bluff body at the burner exist, giving a blockage ratio of 0.5. In order to make turbulence development more sufficient and eliminate the distortion of concentration calculation, the length of the combustion chamber is lengthened on the basis of the original model, $L=150\text{mm}$. The field is meshed in structured grid by ICEM. The total number of grid is up to 1.8 million. The independence of grid has been finished in reference (Yang, 2017). The structure and the grid of the bluff-body burner are shown in Fig.1.

Numerical model

Flow model

In this work, the RANS and LES methods were performed to simulate the cold flow, respectively. In the RANS method, the standard k-epsilon model is selected, and the subgrid-scale model used in LES method is the smagorinsky-lilly model. The coupled algorithm is used to

(a) Schematic view of the bluff-body burner

(b) Schematic view of the grid used for the simulations

Fig.1 Schematic view of the structure and grid of the bluff-body burner.

solve the coupling of pressure-velocity and the Second order implicit is used in LES model.

Combustion model

The dynamic thickened flame model is used in this paper, which is initiated by Butler and O'Rourke (Vreman et al. 2009; Butler et al. 1977). The basic idea of the model is increasing the thickness of the flame front by a factor to make it resolvable on coarse grids, while maintaining its flame propagation velocity. The scalar transport function is expressed as Eq. (1):

$$\frac{\partial \bar{\rho} \tilde{Y}_k}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{u} \tilde{Y}_k) = \nabla \cdot (\bar{\rho} \Xi_{\Delta} F D_k \nabla \tilde{Y}_k) + \frac{\Xi_{\Delta} \omega_k \tilde{Q}}{F} \quad (1)$$

where F and Ξ_{Δ} are the thickening factor and the wrinkling factor, respectively. The thickening factor F is expressed as a function of flame sensor Ω . The flame sensor Ω used to determine the flame position here is a "Arrhenius-like" expression, which is proposed by Legier (Legier et al. 2002). And the hyperbolic tangent function is introduced to calculate thickening factor dynamically.

$$F = 1 + (F_{max} - 1) \tanh \gamma \frac{\Omega}{\Omega_m} \quad (2)$$

$$\Omega = (Y_F)^a (Y_O)^b \exp \left(-\Gamma \frac{E}{RT} \right) \quad (3)$$

$$F_{max} = \max \left(\frac{n \Delta_{mesh}}{\delta_l}, 1 \right) \quad (4)$$

In Eq.(4), n is the number of grid point to resolve the flame structure, which is set to be 10 according to Charlette (Charlette et al. 2002). Δ_{mes} is the mesh spacing. The maximum value of F_{max} is limited to 10. In the thickening

process, the flame surface is decreased compared with the real flame. Therefore, the wrinkling factor Ξ_Δ modeled by algebraic expressions is introduced to compensate it (Eq.(5)) (Colin et al. 2000). However, the factor has some defects in limiting cases, and Charlette (Charlette et al. 2002) proposed an exponent formulation (Eq.(6)).

$$\Xi_\Delta = 1 + \alpha \Gamma_1 \left(\frac{n\Delta_{mesh}}{\delta_l}, \frac{u'_\Delta}{S_l} \right) \frac{u'_\Delta}{S_l} \quad (5)$$

$$\Xi_\Delta = \left(1 + \min \left[\max \left(\frac{n\Delta_{mesh}}{\delta_l} - 1, 0 \right), \Gamma_2 \left(\frac{n\Delta_{mesh}}{\delta_l}, \frac{u'_\Delta}{S_l}, Re_\Delta \right) \frac{u'_\Delta}{S_l} \right] \right)^\beta \quad (6)$$

Both models assume that the flame wrinkling and turbulence motions can get an equilibrium at sub-grid scale, but it is not always reached (Veynante et al. 2015). Therefore, the model parameter α in Colin and β in Charlette should be specified from the resolved fields (Wang et al. 2011; Wang et al. 2012). The wrinkling factor proposed by Charlette is used in this paper. In order to reduce the computation cost, the model parameter $\beta = 0.5$ is used, which provides similar results to that of dynamic flame wrinkling model. Also, the parameter β as a dynamic parameter will be considered in the future study. δ_l is the laminar flame thickness, which is given as Eq.(7) :

$$\delta_l = 2k_1(T_2/T_1)^{0.7} / (\rho_1 C_p S_l) \quad (7)$$

where T_1 and T_2 are the temperatures in the unburned and burnt regions, respectively. ρ_1 , C_p , k_1 and S_l are the density, specific heat, thermal conductivity and laminar flame velocity of the mixture. The laminar flame velocity S_l is fitted according to the experimental data under different equivalent ratios (Poinot Thierry and Denis Veynante, 2001).

$$S_l = A + B\phi + C\phi^2 + D\phi^3 \quad (8)$$

where $A=-0.14358$, $B=-0.58978$, $C=2.56457$, $D=-1.42488$

Spark model and boundary conditions

In this paper, a source term is introduced to the energy equation to simulate spark energy deposited. The source term takes a Gaussian distribution in space and time, which can better match with the results obtained in the experiment. The spark energy source term is expressed as Eq.(9) (Metghalchi et al, 1982):

$$\dot{\omega}_s = \frac{E_{spark}}{(2\pi)^2 \sigma_t \sigma_r^3} e^{-\frac{1}{2} \left[\left(\frac{t-t_0}{\sigma_t} \right)^2 + \left(\frac{x-x_0}{\sigma_r} \right)^2 + \left(\frac{y-y_0}{\sigma_r} \right)^2 + \left(\frac{z-z_0}{\sigma_r} \right)^2 \right]} \quad (9)$$

where E_{spark} is the ignition energy of the spark model. The ignition delay time σ_t and the initial spark radius σ_r used here are 0.16 ms and 2 mm, respectively. t_0 is the sparking instant in time and (x_0, y_0, z_0) is the position of the spark.

The main case in Ahmed (Ahmed et al. 2007) is chosen to investigate the cold flow and combustion process. The bulk velocity of the air is 10 m/s, which corresponds to a Reynolds number of around 6000 based on the annular width of 5 mm. The global equivalent ratio (ϕ) is about 0.55. The time step used here is 2×10^{-5} s, which is obtained according to CFL criterion (Boileau et al. 2008; Neophytou et al. 2010).

RESULTS OF COLD FLOW

Velocity field

The inert flow of the annular bluff-body burner is simulated using the RANS and LES method before ignition simulation.

The velocity contours accepted from RANS and LES methods are listed in Fig.2. The structure of flow field simulated by RANS is highly symmetrical, shown in Fig.2(a). There is also a symmetry in the time-averaged (about 20ms) flow field simulated by LES, shown in Fig.2(b). The length of the recirculation zone is about 28.5mm, which matches well

(a) RANS-velocity contour (b) LES-averaged velocity contour (c) LES-transient velocity contour

Fig.2 Velocity contour simulated by RANS and LES. White line: isoline of zero axial velocity.

with the experimental results (about 25mm). The instantaneous result of flow field simulated by LES at 52ms in Fig.2(c) shows that many small vortex structures can be captured. The existence and the interaction between the small vertexes play an important role in the flame propagation and stability.

The axial and radial velocity in different axial positions (5mm, 15mm, 25mm, 35mm) are compared with measurements, shown in Fig 3. The results show that the tendency of velocity distribution simulated by RANS and LES models can be well in agreement with the experimental results. It indicates that the RANS method has a certain practical value in simulating cold flow. The results of large eddy simulation are more consistent with the experimental results, especially in the region near the wall and the shear layer. In a word, large eddy simulation is more accurate than RANS in predicting cold flow.

(a) Axial velocity

(b) Radial velocity

Fig.3 Radial profile of velocities at different axial positions. Symbols: experimental results; Red line: LES simulation; Black line: RANS simulation.

Mixture fraction field

The time-averaged contour plots of the mixture fraction from the experiment and the simulation results are shown in Fig.4. The distribution of mixture fraction is similar. The stoichiometric mixture fraction (ξ_{st}) counter surrounds the recirculation zone and crosses the symmetry axis at about 26.5mm, which is in agreement with the experimental results. The quantitative comparison is listed in Fig.5.

As shown in Fig.5, the variation tendency and the mixture fraction (ξ) simulated by RANS and LES are almost the same in the recirculation zone. The value of ξ inside the recirculation zone is about 0.08, which is in the flammable range. Moreover, the values simulated by LES model near the downstream of 15mm are closer to the measurement compared with the RANS model. That is to say that the LES model can be more reliable to predict the cold flow than the RANS model.

(a) Experimental results

(b) LES results

Fig.4 Contours of the mixture fraction. Red line: isoline of stoichiometric mixture fraction.

Fig.5 Radial profile of mixture fraction at different axial positions. Symbols: experimental results; Red line: LES simulation; Black line: RANS axial positions.

RESULTS OF IGNITION AND FLAME STRUCTURE

The thickened flame model coupled with the global reaction mechanism is used to simulate the combustion process. The aim of the section is to investigate the veracity of the thickened flame model in predicting the flame propagation. The flame structure in different times are compared between simulation and experiments. A detailed analysis is proposed in the next section.

Fig.6 The instantaneous temperature after ignition. The isosurface corresponds to 890K. Red line: isoline of stoichiometric mixture fraction.

Flame kernel development

The three-dimensional contours of temperature in different time are listed in Fig.6. After ignition for about 1ms, the kernel nearly anchors at the ignition location for the low negative axial velocity (closed to 0m/s). The flame moves to the edge of bluff quickly at about 5.8ms. And the flame-surface wrinkling caused by turbulence can be observed, which does not decrease a lot due to the function of wrinkling factor. Later, the flame develops in the recirculation zone and the fuel burns along the isosurface of the stoichiometric mixture fraction.

Flame structure

The planar temperature of the flame simulated by the thickened flame model is shown in Fig.7, and the experimental result is shown in Fig.8. The kernel barely moves during 1ms for the axial velocity at the position of the spark is closed to 0m/s. With the increasing of the axial velocity, the kernel moves to the bluff quickly in about 3ms. Due to the mixture in recirculation zone is rich (0.08), so the size of kernel changed slowly. At about 12ms, the kernel achieves near the bluff and then spreads along with the isosurface of the stoichiometric mixture fraction. The path of flame propagation and the flame structure are in line with the OH measurement. However, the flame evolution is faster than the experimental results between during the period of 1-3ms. The reason for that may be that the strain rate is not considered in flame propagation.

Fig.7 The instantaneous of temperature after ignition. The images cover a region of 70 × 50mm. (Simulation results)

Fig.8 The instantaneous of temperature after ignition. The images cover a region of 70 × 50mm. (Experimental results)

CONCLUSIONS

The cold flow and ignition progress of an annular bluff-body burner have been simulated in this paper. The main conclusions are listed as follows:

(1) The cold flow simulated by RANS and LES model are in agreement with measurements. The distribution of velocity and mixture fraction simulated by the LES model can better fit to the experimental results compared with the RANS model, especially in the region near the wall and the shear layer. Also, more vortex can be captured in the LES, which play an important role in flame progress.

(2) The combustion progress is investigated by the DTF model with a modified wrinkling factor. The path of flame propagation can match with the experimental results. Firstly, the flame kernel moved to the bluff-body and spread in recirculation zone slowly. Then the mixture burns along the isosurface of the stoichiometric mixture fraction. The flame propagation velocity in the initial progress has a little difference for the neglect of strain rate. Moreover, the flame structure in different time is similar to the measurements. That is to say, the modified DTF model can predict the flame propagation more accurately.

NOMENCLATURE

F	thickening factor
C_p	specific heat of the mixture
E_{spark}	ignition energy of the spark
F_{max}	maximum value of thickening factor
S_l	unstrained laminar flame speed

E_a	activation energy
T_2	adiabatic flame temperature
T_1	temperature of the fresh reactants
u'_Δ	sub-grid-scale turbulent velocity
Re_Δ	sub-grid-scale turbulent Reynolds number
Ξ_Δ	sub-grid-scale wrinkling factor
Ω	flame sensor
Δ_{mesh}	mesh spacing
ξ_{st}	stoichiometric mixture fraction
ϕ	equivalence ratio
Ξ_Δ	wrinkling factor
α	model constant
β	model exponent
k_1	thermal conductivity
δ_l	unstrained laminar flame thickness
ρ_1	density of the gases
σ_t	ignition delay time
σ_r	initial spark radius
$\dot{\omega}_s$	heat release of the spark model
Γ	model constant (0.8 used here)
γ	model constant (0.5 used here)

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