Filtered turbulent flamelet model: analysis and numerical test

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1 Introduction

Because of unfordable mesh to resolve small scales in reactive turbulence, flame models are essentially important. In large eddy simulation (LES) for non-premixed turbulent combustion, scalar dissipation and scalar variance are critical modeling parameters. In the classical steady laminar flamelet models [1, 2], thermodynamic quantities and species are retrieved from a chemistry table generated through prescribed probability density functions (PDFs) of mixture fraction and scalar dissipation rate. Here, the filtered scalar variance for constructing the PDF of mixture fraction, and the filtered scalar dissipation rate for constructing its corresponding PDF are the main modeling parameters. Because of lack of universal closure model, it remains challenging to reasonably quantify these important parameters.
Generally flamelet models aim to map the dependent quantities to a low-dimensional parametric space to improve the numerical efficiency and model predictability. Especially the progress variable approach [2] implicitly provides an idea to eliminate the uncertainty in modeling the filtered scalar dissipation rate. In this method, the filtered scalar variance and progress variable are adopted as the entry parameters of the chemistry table. Here the filtered progress variable can be directly calculated from the filtered LES equations with a corresponding subgrid model without modeling the filtered scalar dissipation rate. The progress variable approach does show improvements [3]. However, modeling the filtered scalar variance still remains as an issue. In studying the filtered non-premixed turbulent flame structure at different filtering scales, Wang [4] derived a so-called filtered turbulent flamelet equation to relate directly the filtered species mass fractions and the filtered mixture fraction. Thus the models of scalar variance and scalar dissipation rate are not needed, which proposes a possible approach to eliminate the uncertainty of the prescribed PDFs of the scalar variance and scalar dissipation. In the following a tentative modeling idea is proposed along this line.

2 Modeling formulation

In non-premixed gaseous combustion, the governing equations for the mass balance, scalar (including the species and temperature) and the mixture fraction Z are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0, \tag{1}$$

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$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho \vec{u} Y_i) = -\nabla \cdot (\rho \alpha_i \nabla Y_i) + \rho \omega_i, \tag{2}$$

$$\frac{\partial \rho Z}{\partial t} + \nabla \cdot (\rho \vec{u} Z) = -\nabla \cdot (\rho D \nabla Z), \tag{3}$$

respectively. Here ρ is the fluid density, p is the pressure, μ is the dynamic viscosity, $\vec{u}$ is the flow velocity, $Y_i, (i = 1, ...n)$ represent the ith scalar (temperature or the species concentration) and α_i is the corresponding diffusion coefficient, respectively.
In LES, after the filtering operation at the resolved scale, together with the gradient transport models as

$$\bar{\rho}(\widetilde{\vec{u}}\widetilde{Z} - \widetilde{\vec{u}Z}) = \bar{\rho} D_T \nabla \widetilde{Z}, \tag{4}$$

$$\bar{\rho}(\widetilde{\vec{u}}\widetilde{Y_i} - \widetilde{\vec{u}Y_i}) = \bar{\rho} D_{T,i} \nabla \widetilde{Y_i}, \tag{5}$$

it finally yields the so called turbulent flamelet equation [4] as follows.

$$\begin{aligned} &\bar{\rho}\frac{\partial \widetilde{Y_i}}{\partial \tau} + \bar{\rho}(\widetilde{\vec{u}} \cdot \nabla_\perp \widetilde{Y_i} + \frac{\partial \widetilde{Y_i}}{\partial Z_2}\frac{\partial Z_2}{\partial t} + \frac{\partial \widetilde{Y_i}}{\partial Z_3}\frac{\partial Z_3}{\partial t}) \\ &= \frac{1}{2Le_{T,i}}\bar{\rho}\chi\frac{\partial^2 \widetilde{Y_i}}{\partial \widetilde{Z}^2} + \frac{\partial \widetilde{Y_i}}{\partial \widetilde{Z}}\nabla \cdot [\bar{\rho}(D_{T,i} - D_T)\vec{n}\frac{\partial \widetilde{Z}}{\partial n}] + \nabla \cdot (\bar{\rho} D_{T,i} \nabla_\perp \widetilde{Y_i}) + \overline{\omega_i}, \end{aligned} \tag{6}$$

where the turbulent scalar dissipation χ is defined as

$$\chi = 2D_T(\frac{\partial \tilde{Z}}{\partial n})^2$$

and the turbulent Lewis number $Le_{T,i} = D_T/D_{T,i}$.

As illustrated by Wang [4], for the filtrated turbulent flame fronts, the good alignment relations among the gradients of the species and mixture fraction are still valid. Therefore at the first attempt it is reasonable to simplify Eq. (6) as

$$\frac{1}{2Le_T}\bar{\rho}\chi\frac{\partial^2 \widetilde{Y_i}}{\partial \widetilde{Z}^2} + \overline{\omega_i(Y_1, Y_2, ..., T)} = 0, \tag{7}$$

by neglecting the time derivative and lateral derivative terms. The above equation has the same form as the steady laminar flamelet equation. However, the involved quantities have of different implications. The main challenge is the availability of the non-filtered species values Y_i to calculate the chemical source term $\overline{\omega_i(Y_1, Y_2, ...T)}$. According to Ref. [4], in the inertial range, the following scaling relation exists conditional on the stoichiometric Z isosurface:

$$\langle \tilde{Y}_i(\vec{r})_{,l} - Y_i(\vec{r}) \rangle \sim C_i l^{\alpha_i}, \tag{8}$$

where the two unknown parameters C_i and α_i can be determined if the filtering operation is performed at two different length scale l. Physically, Eq. (8) originates from the similarity of the scalar isosurface in the inertial range. In the above equation, the average operation $\langle \cdot \rangle$ is defined with respect to the entire flame surface. Numerically, C_i and α_i can thus be determined by filtering Y_i at several different scale l levels, from which at each flame surface point $\vec{r}$, $Y_i(\vec{r})$ can then be evaluated. Such relation provides an alternative approach (different from the existing ideas) to close the chemical sources. Therefore, combining Eq. (7) and Eq. (8), one obtains the turbulent flamelet solution.

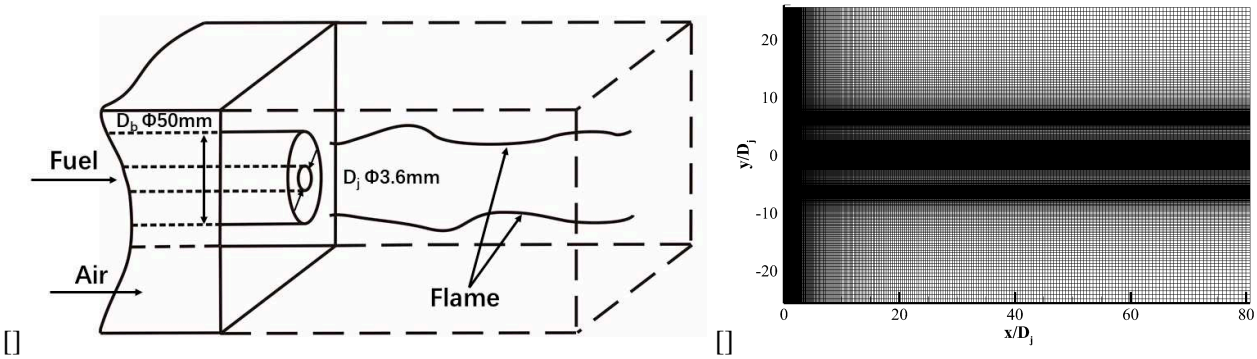

Figure 1: (a) Schematic of the bluff body burner. (b) Cross cut of the numerical mesh.

3 Numerical implementation

As shown in Fig 1 (a) the Sydney bluff-body burner investigated here consists of a cylindrical bluff-body with an orifice for the fuel jet and a co-flowing air stream. The bluff-body diameter is $D_b = 50mm$ and the fuel jet diameter is $D_j = 3.6mm$. The central nozzle fuel jet is composed of methane and hydrogen ($1:1$ by volume) with a stoichiometric mixture fraction $Z_{st} = 0.05$. The Reynolds number $Re = U_j D_j/\nu = 15800$, where U_j represents the bulk velocity of the turbulent fuel jet and ν is the gas kinematic viscosity. U_j and the ambient coflow bulk velocity U_e are set as $108m/s$ and $35m/s$, respectively [6].

The inflow velocity condition of the central fuel jet is obtained from a separated LES of a periodic pipe flow by enforcing the same bulk axial velocity and the Reynolds number. A plug flow with 2% turbulence intensity is set as the inlet condition of the annular air coflow. On the solid wall the no-slip condition is used for the velocity and Neumann conditions are used for all scalars and pressure. At the outlet the convection boundary conditions are adopted. The numerical mesh is locally refined with total $256 \times 165 \times 64$ grid points in axial, radial and circumferential directions, respectively. Specifically as shown in the mesh cross cut in Fig. 1 (b), the refined parts include the region near the inlet, the shear layer surrounding the fuel jet and the edge of bluff body.

A four-step global mechanism, suggested by Jones and Lindstedt [5], is used to solve the chemical species and temperature. Because of the implicit coupling between the flow field, the scaling relation and the turbulent flamelet equation, iteration needs to continue until quantities of interest, e.g. coefficients in Eq. (8) and the solution of Eq. (7), converge. Numerical tests show that basically two rounds iteration suffice to have satisfactory results. Fig. 2 shows the results for the temperature and CO (for the sake of brevity other scalars' results are not listed). It can be seen that the scaling relations do hold. Physically the scaling relation is attributed to the structure similarity at different scales on the flame front

Another issue related to the solution of Eq. (7) is the transition between reignition and extinction. For the flamelet/progress variable model, the reignition behavior can be reasonably captured by introducing the progress variable. As a first tentative test, a simplified steady turbulent flamelet model solution is used. From the following results it can be seen that even with such simplification the model predictability is still satisfactory.

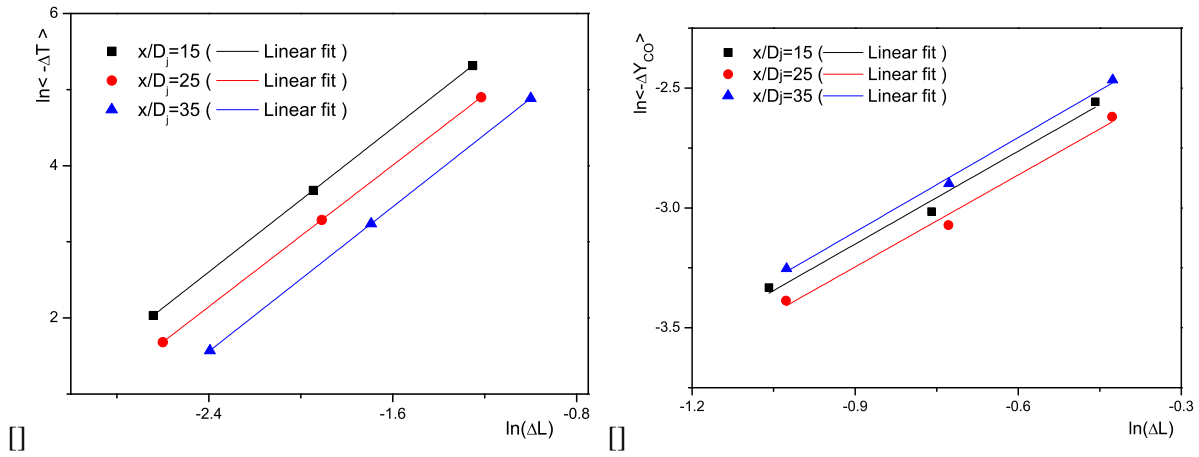

Figure 2: Numerical results of the scaling relation with respect to the filter size l for (a) $\langle -\Delta T \rangle = \langle -(\tilde{T}(\vec{r})_{,l} - T(\vec{r})) \rangle$ and (b) $\langle -\Delta Y_{CO} \rangle = \langle -(\tilde{Y_{CO}}(\vec{r})_{,l} - Y_{CO}(\vec{r})) \rangle$.

4 Case test and discussion

First the instantaneous contour plots of several representative field quantities at the statistically stationary state are presented in Fig. 3. Along the streamwise direction, larger scales develop and the circular shear layer and circular flame zone evolve gradually to converge with more fluctuation. The axial velocity decays more rapidly than the scalar quantities.

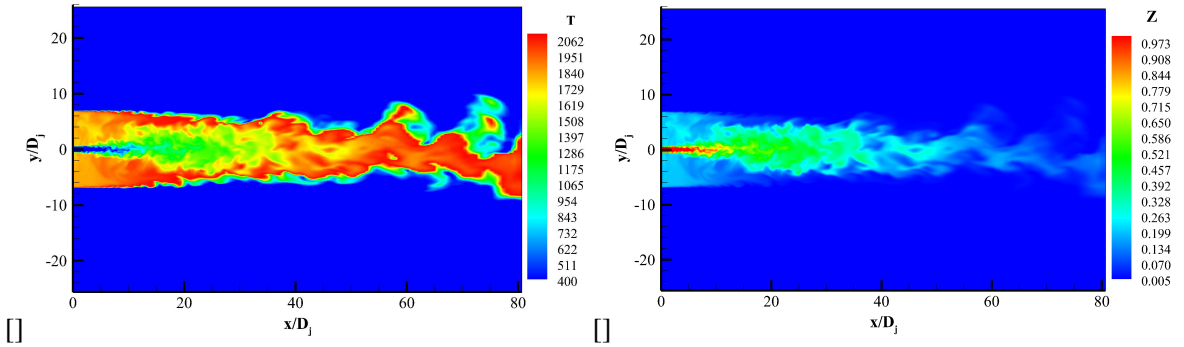

Figure 3: Instantaneous contour plots for: (a) temperature and (b) mixture fraction.

For comparison, we list the simulation results from the present turbulent flamelet method using the JL mechanism (TFM-JL), the experimental measurements (Exp.), the flamelet/progress variable approach using the JL mechanism (FPV-JL), and the literature results from other methods as well, including the steady flamelet/progress variable approach [3] using detailed chemical mechanism of GRI-Mech 2.11 [7] (FPV-GRIMech) and the steady laminar flamelet model using detailed chemical mechanism with 97 species and 629 chemical reactions(LFM) [8].

The mixture fraction profiles in Fig. 4 from TFM-JL and FPV-GRIMech are almost identical, showing a satisfactory match with the experiment data, which hence implies that the present model can effectively capture the thickness of the mixing layer, while FPV-JL and LFM show clearly large deviation. In the

recirculation zone, the mixture fraction remains larger than the stoichiometric ratio, which means fuel-enriched combustion there. Considering the mean temperature in Fig. 5, the current turbulent flamelet

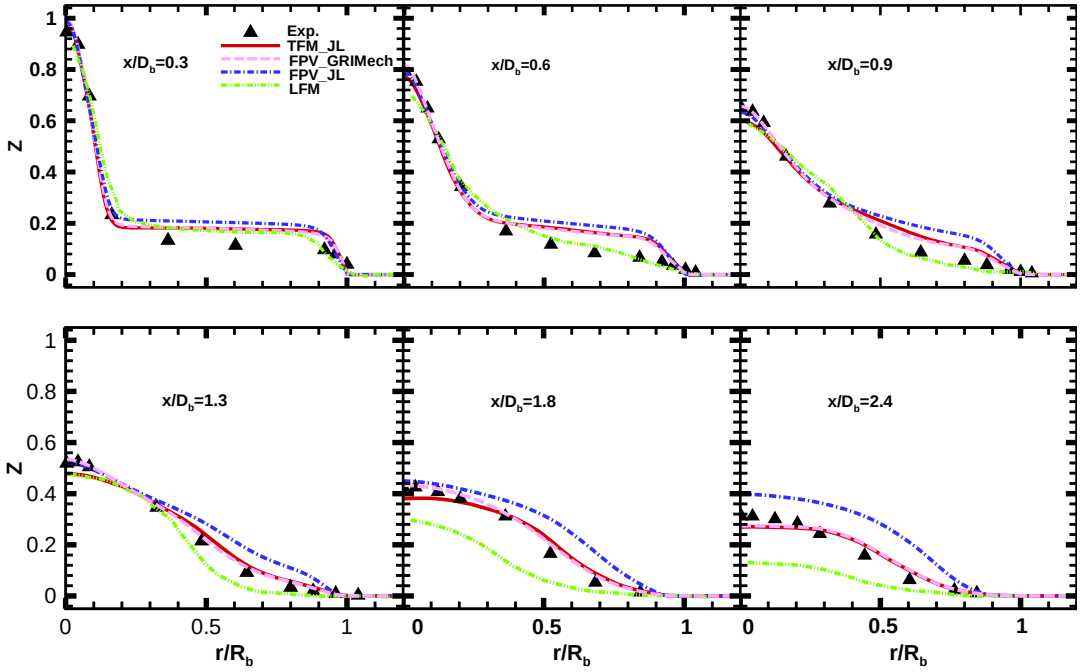

Figure 4: Results comparison for the mixture fraction $\tilde{Z}$.

model and FPV-GRIMech perform much better than LFM and FPV-JL. The TFM-JL results fit better the peak values and the corresponding locations, while the FPV-GRIMech results predict more accurately the temperature at the jet center with $r = 0$. A probable reason of the over predication of the temperature by TFM-JL is that the extinction-reignition behavior can not be sufficiently accounted for with the simplified JL mechanism and the simplified steady turbulent flamelet model solution. In principle the steady flamelet solution implies that the chemical reaction is at all times in balance with the rate at which reactants diffuse into the flame. Thus under this assumption the chemical reaction and heat release rate will be sightly faster than the real cases to lead to some overprediction.

5 Conclusions

Directly from the filtered governing equations in the context of large eddy simulation (LES), a so called filtered turbulent flamelet equation can be derived. The filtered scalar dissipation, which can be calculated numerically instead of modeling, functions as one of the entry parameters of the chemistry table. Meanwhile, the strongly nonlinear chemical sources are closed using scaling relations, as suggested by Eq. (8). Overall, results from the present model and the flamelet/progress variable approach with detailed chemistry (FPV-GRIMech) are comparable, while the laminar flamelet model with detailed chemistry (LFM), the flamelet/progress variable approach with simplified JL chemistry mechanism (FPV-JL) show much larger deviation. Considering the simplified JL mechanism and much reduced calculation time, the present turbulent flamelet model shows promising predictability.

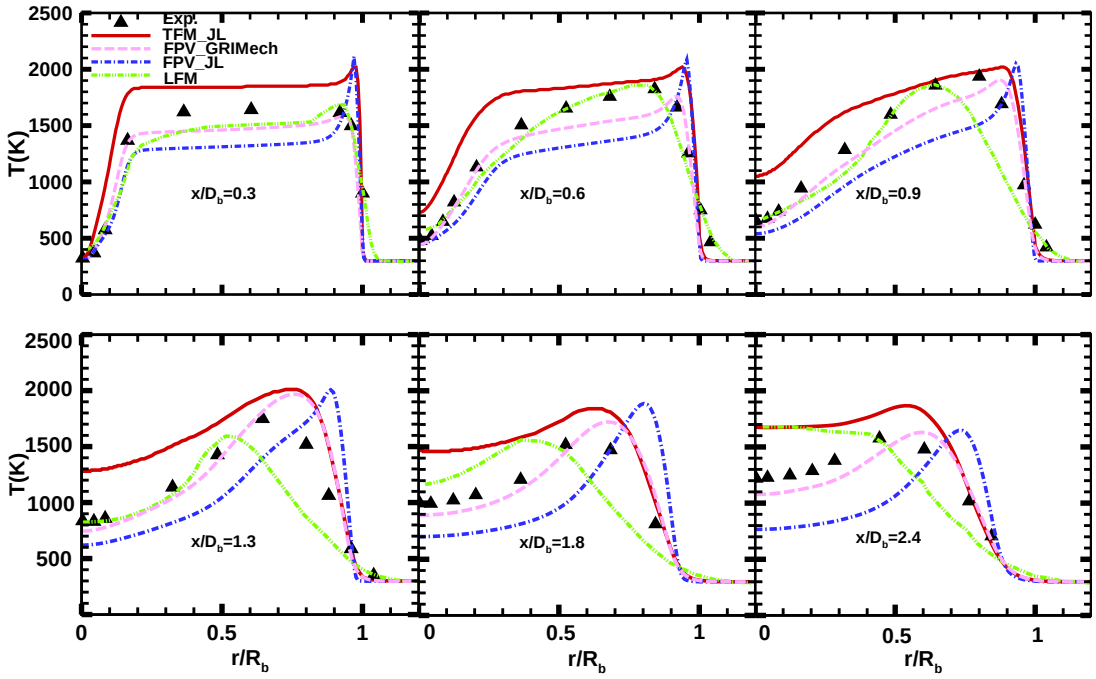

Figure 5: Results comparison for the temperature $\tilde{T}$.

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