Conditional Moment Closure for Turbulent Premixed Flames

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1 Introduction

The emission legislation is becoming more stringent to minimise the environmental impact of combustion, forcing us to develop efficient and less polluting combustion systems. Fuel lean premixed combustion has potential to meet these two demands simultaneously but it is susceptible to combustion oscillations and stability issues. Also, the interactions among turbulence, chemical reaction and diffusion are strong in lean flames. Thus, modelling turbulent lean premixed flames is challenging. Combustion models which are capable to address these interactions accurately with ability to predict emissions are required in the design and development of next generation of lean combustion systems.

The main objective of turbulent combustion modelling is to provide a closure for the mean reaction rate, $\overline{\dot{\omega}}_\alpha$, which appears in the mean species transport equation, for example. Since the reaction rate is a highly non-linear function of temperature and species concentration, evaluating its mean value using average temperature and scalar concentrations is known to be erroneous. Flamelet based methods are common for turbulent premixed flames [1]. Although the conditional moment closure (CMC) has been developed and successfully applied to various non-premixed combustion systems such as hood fires [2], lifted flames [3], bagasse-fired boiler [4], bluff-body fames [5], spray ignition [6] and soot formation [7], its application to premixed flames is not fully tested and validated yet. Despite some initial results reported in [8], the main difficulty in applying CMC to turbulent premixed flames is associated with modelling of conditional scalar dissipation rate, $\langle N|c=\zeta\rangle = \langle \mathcal{D}_c(\nabla c\cdot\nabla c)|\zeta\rangle$, for the progress variable c with molecular diffusivity $\mathcal{D}_c$. The progress variable is defined later and the conditional average is defined as the ensemble average subject to the condition $c=\zeta$. The aim of this work is two-fold; firstly to validate a simple model for the conditional scalar dissipation rate obtained using fundamental principles, secondly to perform CMC calculations and to validate the computed results using experimental data.

2 CMC Method

The CMC method is based on the hypothesis that the fluctuations of species mass fractions, temperature and enthalpy are associated only with the fluctuation of a key scalar [9]: mixture fraction Z in non-premixed and progress variable c in premixed combustion. The latter can be defined based on temperature or using fuel mass fraction [1]. An alternative definition using sensible enthalpy is also possible [9]. Here, it is defined as $c = Y_f/Y_f^u$ using the fuel mass fraction, where Y_f^u is the unburnt fuel mass fraction value. Actually this c is a regress variable, which is used as conditioning variable.

In CMC, the conditional average of scalar α is defined as $Q_\alpha(\zeta;\mathbf{x},t) \equiv \langle Y_\alpha(\mathbf{x},t)|c=\zeta(\mathbf{x},t)\rangle$, with angled brackets denoting ensemble averaging of samples satisfying the condition to the right of the vertical bar. Transport equations for conditional mean scalar values, Q_α, are derived by substituting $Y_\alpha(x,t) = Q_\alpha(\zeta;\mathbf{x},t) + y_\alpha(\mathbf{x},t)$ in the transport equation for the instantaneous scalar value Y_α [9]. An alternative approach using velocity-scalar joint probability density function (PDF) is also possible [9]. Both of these approaches essentially yield the same

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transport equation for the conditional mean, Q_α, which is written as [9, 10]

$$\langle\rho|\zeta\rangle\frac{\partial Q_\alpha}{\partial t}+\langle\rho u_i|\zeta\rangle\frac{\partial Q_\alpha}{\partial x_i}-\frac{\mathrm{Le}_c}{\mathrm{Le}_\alpha}\langle\rho N_c|\zeta\rangle\frac{\partial^2 Q_\alpha}{\partial\zeta^2}=\langle\dot{\omega}_\alpha|\zeta\rangle-\langle\dot{\omega}_c|\zeta\rangle\frac{\partial Q_\alpha}{\partial\zeta}$$
$$-\frac{1}{\widetilde{p}(\zeta)}\frac{\partial}{\partial x_i}[\langle\rho u_i^{''}Y_\alpha^{''}|\zeta\rangle\langle\rho|\zeta\rangle\widetilde{p}(\zeta)]+e_{Q_\alpha}, \quad (1)$$

where Le_α is the Lewis number of species α and $\widetilde{p}$ is the Favre PDF of c. The physical meaning of various terms in Eq. (1) is as follows. The first and second terms of Eq. (1) respectively denote the unsteady and convective changes of Q_α. The third term represents the diffusion of the conditional average in the sample space ζ. The fourth term is the chemical reaction rate for species α. Since c is a reactive scalar, its influence on the evolution of Q_α is given by the fifth term in Eq. (1). The sixth term represents the contribution of conditional fluctuation y_α to Q_α evolution. The last term represents contributions of molecular diffusion in the physical space and differential diffusion effects. This term is neglected in this study due to the high Reynolds number of the turbulent flames considered.

The quantities $\langle u_i^{''}Y_\alpha^{''}|\zeta\rangle$, $\widetilde{p}$, $\langle u_i|\zeta\rangle$, $\langle\dot{\omega}_\alpha|\zeta\rangle$ and $\langle N_c|\zeta\rangle$ require suitable models along with appropriate initial and boundary conditions to solve Eq. (1). The turbulent flux term is modelled using gradient transport hypothesis. The PDF of the progress variable is modelled by a presumed shape with a beta function. The conditional velocity is modelled using a linear model which showed good agreement with DNS results [10]. The conditional mean reaction rate is closed using a first order CMC closure [9]: $\langle\dot{\omega}_i(\rho,Y_i,T)|\zeta\rangle = \dot{\omega}_\alpha(\langle\rho|\zeta\rangle,\mathbf{Q}_i,Q_T)$, where T is the temperature.

The conditional mean scalar dissipation rate $\langle N_c|\zeta\rangle$ is related to the unconditional mean scalar dissipation rate $\widetilde{\epsilon}_c$ as

$$\langle N_c|\zeta\rangle=\frac{\widetilde{\epsilon}_c\, f(\zeta)}{\int_0^1 f(c)\,\widetilde{p}(c)\,\mathrm{d}c}, \quad (2)$$

where $f(c)$ is a known function obtained from laminar flame calculation [12]. The Favre mean scalar dissipation rate, $\widetilde{\epsilon}_c$, is modelled using a simple algebraic model developed in [13] and it is given by

$$\widetilde{\epsilon}_c=\frac{1}{\beta'}\left[(2K_c^*-\tau C_4)\,\frac{S_L^0}{\delta_L^0}+C_3\frac{\tilde{\varepsilon}}{\tilde{k}}\right]\widetilde{c^{''2}}, \quad (3)$$

where, $\beta'=6.7$, $K_c^*=0.85\tau$, $C_4=1.1/(1+\mathrm{Ka})^{0.4}$, $C_3=1.5\sqrt{\mathrm{Ka}}/(1+\sqrt{\mathrm{Ka}})$. The Karlovitz number is $\mathrm{Ka}=[(u'/S_L^o)^3(0.5(1+\tau)^{0.7}/(\delta_L^o/\Lambda)]^{0.5}$ using turbulence rms velocity u' and its integral length scale Λ. The unstrained laminar flame speed is S_L^o, its thermal thickness is δ_L^o and the heat release parameter is $\tau=(T_b-T_u)/T_u$ with the subscripts b and u respectively denoting burnt and unburnt mixtures. The Favre averaged turbulent kinetic energy and its dissipation rate are denoted by $\widetilde{k}$ and $\widetilde{\varepsilon}$ respectively. After solving the CMC equations along with other governing and modelling equations for turbulent reacting flows, the unconditional means can be obtained using $\widetilde{Y}_\alpha=\int_0^1 Q_\alpha\,\widetilde{p}(\zeta)\;\,d\zeta$.

The computational tool with standard $k-\varepsilon$ turbulence model used in this study has been validated in previous CMC studies for non-premixed flames [4] and this computer code has been modified for premixed flames by including transport equations for the Favre averaged progress variable, its variance and the extra source/sink terms in the CMC equations for reactive scalars.

3 Test Flames

The test flames used in this study are the pilot stabilised turbulent Bunsen flames of Chen et al. [14]. Stoichiometric methane-air flames with a fuel nozzle diameter $D=12$ mm and a pilot diameter $d_p=68$ mm were considered. Three flames, F1, F2, and F3, were investigated in the experiments. In the current study the flame F1 is computed using the RANS-CMC approach. The bulk mean velocity at the exit of the fuel nozzle U_o and the turbulent kinetic energy $\widetilde{k}_o$ at the centre line of the fuel nozzle are 65 m/s and 12.7 $\mathrm{m^2/s^2}$ respectively. The Reynolds number, Re, based on D and U_o is 52000. The hot stoichiometric products from the pilot flames were flowing with a uniform velocity of 0.2 m/s at the burner exit. A small uniform velocity of 0.2 m/s is specified to account for the ambient air

entrainment. The effect of ambient air on the mixture is taken into account by solving the mean mixture fraction equation and its variance. A computational domain of size 1000 mm in the axial direction x and 270 mm in the radial direction r is used with refined grid near the fuel exit. The smallest cells size is 0.5×1.0 (in mm) and the CFD computational domain has $80 \times 80 \times 120$ cells in $x,\ y,\ z$ directions, for turbulence and mean quantities. For CMC, 500 non-uniform cells are used in ζ space which were required to resolve the strong gradients, and two cells in each direction of the main grid are combined to create the CMC physical grid. The value of $C_{\epsilon 1}$ in the standard k-ε model is changed from 1.44 to 1.52 to account for round jet anomaly. The combustion chemical kinetics are simulated using Smooke's mechanism [15]. A steady flamelet solution is specified as initial condition for the CMC equation, and gives appropriate boundary conditions for Q_α.

4 Results and Discussion

Figure 1 shows the conditional mean scalar dissipation rate obtained using Eq. (2) and from Direct Numerical Simulation (DNS) data of a V-flame [16]. The results are normalised using S_L^o and δ_L^o and are shown for two locations inside the flame brush of the V-flame. The DNS flame conditions correspond to lean methane-air flames with reactant preheated to 600 K having equivalence ratio, ϕ, of about 0.58. The results is shown in Fig. 1 are typical and show a very good agreement between the model and DNS. Thus, this model is used for the CMC calculations reported in this study.

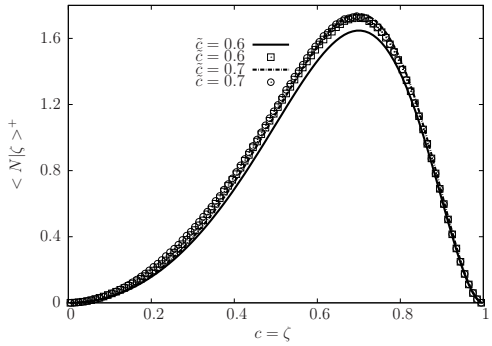

Figure 1: Comparison of modelled, Eq. (2) (lines), conditional mean scalar dissipation rate and DNS (symbols) results. The values are non-dimensionalised using S_L^o and δ_L^o.

Simulations of the non-reacting flow were carried out first, in order to assess the turbulence models and the flow boundary conditions used. Figure 2a shows the results for non-reacting flow. The normalised mean axial velocity $\overline{U}/U_o$ and turbulent kinetic energy $\overline{k}/k_o$ are compared to the experimental data at five axial locations in the flame. It is apparent that the computational results agree well with the measurements of the mean axial velocities at all axial locations. The computed radial variation is also in good agreement with the measurements. The normalised kinetic energy at the centre line is in excellent agreement with the measurements and in the radial direction they are slightly over predicted at all axial locations. However in general the results from the cold flow are satisfactory and acceptable.

Results for the reacting case are shown in Fig. 2b. The comparison of normalised mean axial velocity and turbulent kinetic energy with the measurements is shown for five axial locations. The values of mean axial velocities are well-predicted at axial locations 6.5 and 8.5 and slightly over-predicted at other axial locations shown. The results are typical of $k - \epsilon$ modelling and the comparisons are reasonable.

Figure 3 shows the computed conditional mean values for major and minor species mass fractions for $\tilde{c}$ = 0.5. This flame structure in ζ space is similar to unstrained laminar flames. Furthermore, the conditional mean shows a weak dependence on the location inside the flame brush. This seems to support the CMC hypothesis of a weak spatial dependence of Q_α. These values will be averaged using the pdf to obtain the mean quantities.

Figure 4a compares the computed mean mass fraction of CH_4 (left side) and the mean temperature $\overline{T}$ (right side) with the experimental measurements (symbols). In Fig. 4a $\overline{T} = (\overline{T} - T_u)/(T_b - T_u)$, the Reynolds mean is obtained from the calculated Favre mean as explained in [12]. The computed values of CH_4 mass fraction is in reasonable agreement with the measurements. In the mean temperature $\overline{T}$, there are some discrepancies

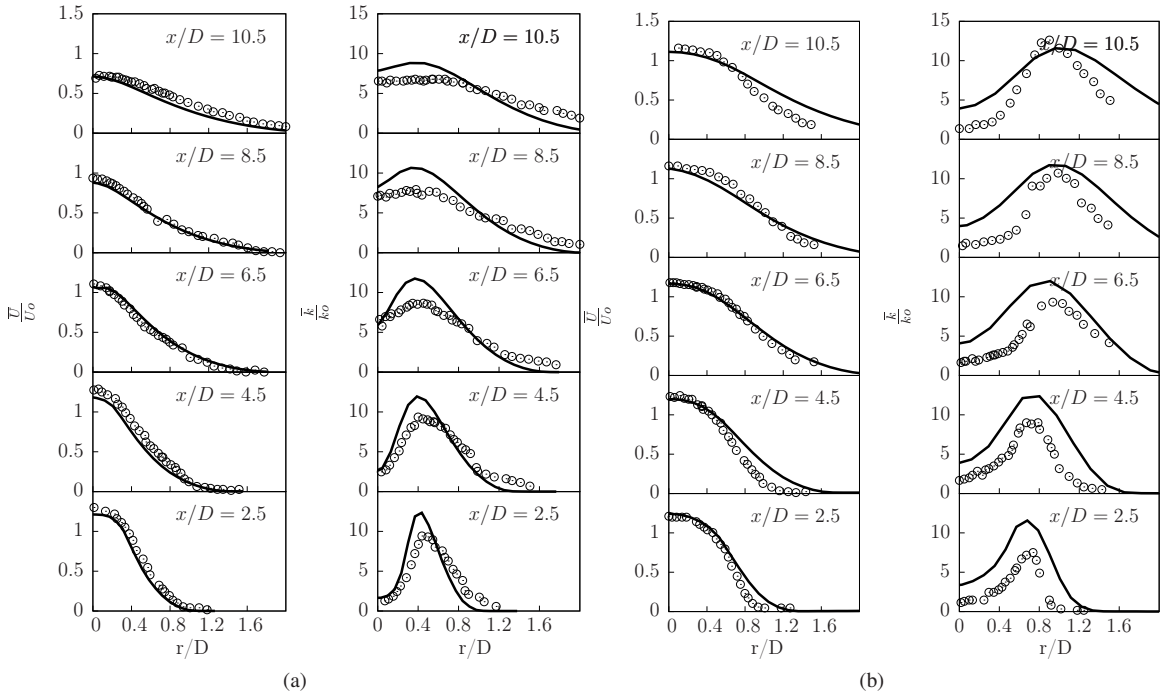

Figure 2: The calculated (lines) normalised mean axial velocity and turbulent kinetic energy from (a) non-reacting and (b) reacting flows are compared to the the measurements (symbols).

between the computed and measured values. The simulated flame tends to have higher temperature compared to the experiment at all axial locations.

Figure 4b compares the computed mean major (right side) and minor (left side) species mass fractions to the measurements (symbols) at different axial locations. The overall comparison of the major species mass fractions are reasonable. Also the simulation captures the influence of air entrainment on the flame. However, there are under-prediction of O_2, CO_2 and H_2O at all axial locations. The comparison of the minor species OH and H_2 are under-predicted while the CO is over-predicted compared to the experimental data. The level of comparisons shown here for normalised temperature and scalar mass fractions will duly be influenced by the chemical kinetics mechanism used in the simulations. This is being explored currently.

5 Conclusion

In premixed CMC, the conditional scalar dissipation rate is a key quantity and an accurate model is required for this. The conditional scalar dissipation rate values obtained using the model in Eq. (2) is compared with the DNS results of V-flame and this comparison is good. This model is used to compute a pilot stabilised Bunsen flame, F1, of Chen $et\ al.$ [14] using the RANS-CMC method. A first order closure is used for the conditional mean reaction rate along with a standard k-ε turbulence model.

The turbulence models and the flow boundary conditions are assessed by first simulating the non-reacting flow and the computed mean velocity and kinetic energy agree reasonably well with the measurements. The pdf of the progress variable is obtained using a presumed shape with a beta function. The computed $\widetilde{Y}_{\mathrm{CH_4}}$ is in reasonable agreement with measurements. The normalised mean temperature $\overline{T}$ is over predicted at all axial locations but the calculated axial and radial trends are acceptable. The predicted major and minor species mass fractions are also in reasonable agreement with the experimental data. However, the chemical kinetics mechanism and turbulence models used will have some influence on the computed results and this will be addressed using the GRI mechanism in future work. Also differential diffusion $e_{Q_\alpha} \simeq (1 - \mathrm{Le}_\alpha)\partial Q_\alpha/\partial\zeta\langle(\nabla \cdot \rho\mathcal{D}_\alpha\nabla c)|\zeta\rangle$ effects will be included in future simulations to assess their influence on the computed values.

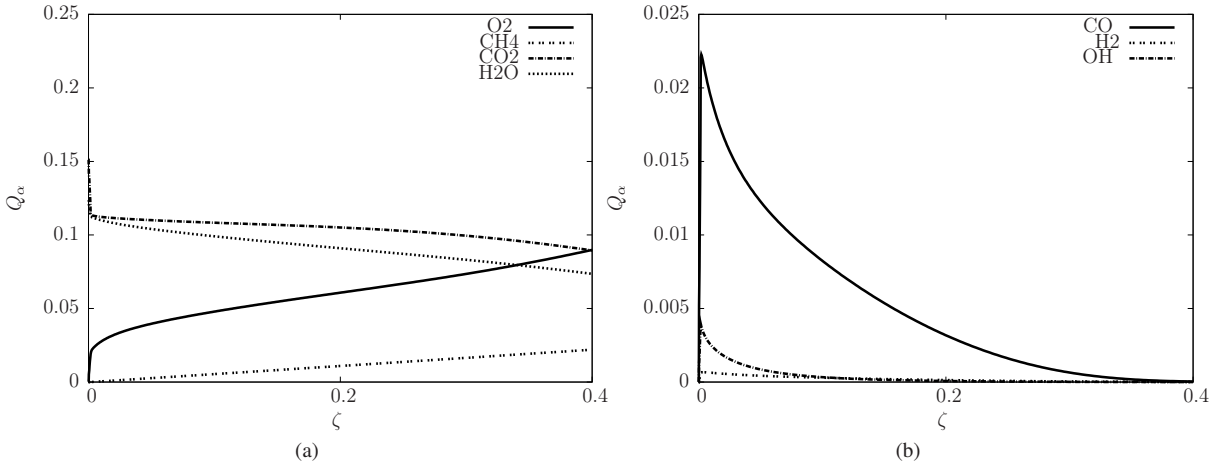

Figure 3: The variation of conditional mean mass fractions with ζ for (a) major and (b) minor species.

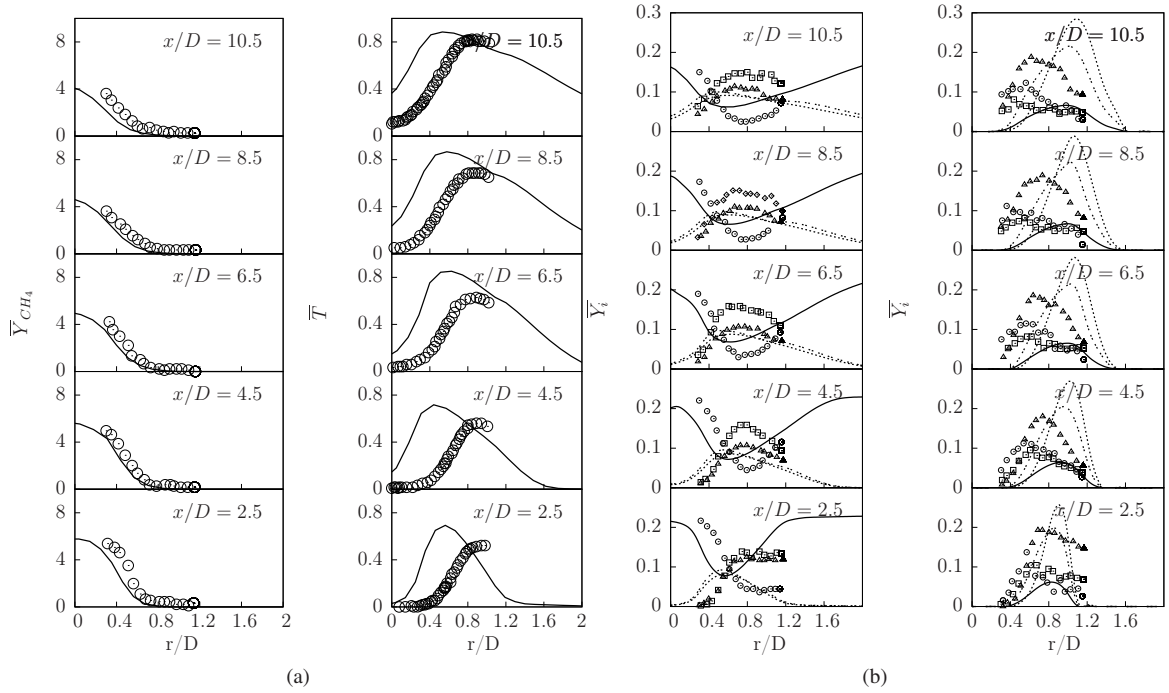

Figure 4: The mean $100 \times CH_4$ mass fraction: ($\circ$,$-$) (left side) (a) and the mean temperature $\overline{T}$: ($\circ$,$-$) (right side) (a). The major species mass fractions: O_2 ($\circ$,$-$), CO_2 ($\square$,$\ldots$) and H_2O ($\triangle$,$\cdot\ \cdot\ \cdot$) (left side) (b) and the minor species mass fractions $10 \times$ CO ($\circ$,$\cdot\ \cdot\ \cdot$), $100 \times H_2$ ($\square$,$-$) and $75 \times$ OH ($\triangle$,$\ldots$) (right side) (b). Solid lines represent CMC calculations and symbols represent experimental data of Chen $et\ al.$ [14]..

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