Simulations of edge-flame propagation in turbulent non-premixed jets

E.S. Richardson , E. Mastorakos*

Cambridge University Engineering Department, UK

Abstract

Ignition, flame propagation and stabilisation have been simulated and analysed in a turbulent jet of non-premixed methane and air. The first order Conditional Moment Closure (CMC) turbulent combustion model was fully coupled with a Reynolds-Averaged Navier Stokes (RANS) flow simulation. A CMC model was developed to account for spark ignition. The over-prediction of turbulent flame propagation was attributed to the limitations of the first order reaction rate closure, and of the RANS description of the flow in the presence of thermal expansion around the flame front. A new model for the effects of counter gradient turbulent transport in partially premixed flows was implemented and the modification of the flame front was presented. The coupled CMC-CFD model successfully captures the physics necessary to represent unsteady flame evolution and hence may be used for simulation of ignition in practical combustor designs.

Introduction

Deeper understanding of forced ignition and flame propagation is needed by researchers developing modelling for the design of industrial burners. The ability to model ignition of non-premixed flow is of particular interest to manufacturers of aviation gas turbines who must satisfy certification bodies that their designs may be re-ignited at high altitude.

The numerical simulations in this paper were based on the experimental study of spark ignition and flame propagation in a partially premixed turbulent jet by Ahmed and Mastorakos [1]. This allowed comparison with a variety of measurements for the flame evolution in a well characterised flow. The configuration investigated is depicted in Fig. 1, and full details may be found in ref. [1]. The complete transient from spark ignition up to the stabilisation of a lifted flame was captured and the evolution of the mean position of the upstream flame front was reported.

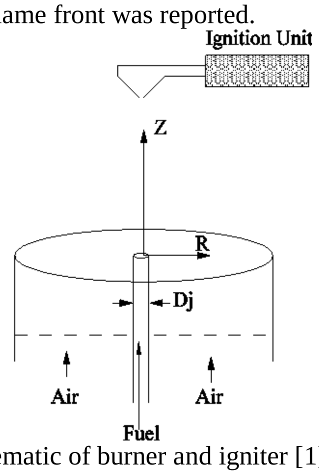

Fig. 1 Schematic of burner and igniter [1].

A number of studies have used the steady state turbulent lifted jet flame to examine models for partially premixed turbulent flame propagation [2,3]. The present configuration provides a somewhat more stringent test of the turbulent reacting flow model due to the variety of mixing and turbulence conditions experienced by the flame front during the ignition transient, and also due to the influence of thermal expansion on the fluid dynamics as the flame propagates.

The Conditional Moment Closure (CMC) is an advanced turbulent reacting flow model which accounts for the interaction of turbulence with chemical reaction schemes of arbitrary complexity. [4]. Modelled transport equations are solved for the conditional expectations of species and temperature. The primary advantage of solving the conditional moment closure is that due to the small size of conditional fluctuations compared to unconditional fluctuations, the conditional mean reaction rate may be given relatively accurately by a low order closure. In non-premixed flows the mixture fraction [4] is commonly used as the conditioning variable due to its physical significance in such flows and the small conditional fluctuations which may result.

The CMC has been applied to the solution of stabilised lifted turbulent jet flames [2,3]. These studies have highlighted the role played by conditional turbulent fluxes in the CMC description of the flame propagation, and a lack of validation for the usual modelling of this quantity. An *a priori* Direct Numerical Simulation (DNS) study of the CMC treatment of a non-premixed ignition kernel [5,6] indicated that the usual eddy diffusivity model for the conditional turbulent flux can be inaccurate, and in some circumstances it can give the incorrect sign. Furthermore it was noted that both first and second order closures gave poor predictions inside the flame propagating from the non-premixed spark kernel. It was concluded that a double conditioned closure may be beneficial for some ignition problems.

Formulation

Simulations have been conducted for mean jet velocities of 12.5ms^{-1} and 25.5ms^{-1} with a jet nozzle

* Corresponding author: em257@cam.ac.uk

Cambridge University Engineering Department, Trumpington Street, Cambridge CB2 1PZ, UK;

http://www.eng.cam.ac.uk/~em257/

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diameter of 5mm. The jet was composed of 70% methane mixed with 30% air by volume at room temperature. The jet issued into a co-flow of room temperature air, flowing at $0.1 ms^{-1}$.

A complete discussion of the modelling and implementation used is given in Ref. [6]. The first order CMC has been fully coupled with a well validated RANS CFD solver [7], using a *k*-ε closure as in previous work [8]. The CMC was solved on either a one dimensional (axial) spatial grid as in Ref. [2], or a two dimensional axi-symmetric grid. In both cases adaptive refinement is employed to ensure adequate resolution of the conditional flame fronts. The CFD variables needed by the CMC solution were averaged over the relevant volume, weighted by the mixture fraction probability density function. A β-function PDF was presumed.

Conditional expectations are denoted $Q_\alpha \equiv \langle Y_\alpha | \eta = \xi \rangle$ where Y_α is the variable being averaged on the condition that the mixture fraction ξ equals the sample space variable η. Transport equations are solved for Q_α, the conditional expectation for the mass fraction of species α, and Q_T, the conditional expectation for the temperature.

The closed transport equation for the conditional temperature expectation is given by:

$$\frac{\partial Q_T}{\partial t} = -\langle u_i | \eta \rangle \frac{\partial Q_T}{\partial x_i} - \sum_{\alpha=1}^{n} h_\alpha \langle w_\alpha | \eta \rangle + \langle N | \eta \rangle \frac{\partial^2 Q_T}{\partial \eta^2}$$

$$\langle N | \eta \rangle \frac{1}{\langle c_p | \eta \rangle} \left(\frac{\partial \langle c_p | \eta \rangle}{\partial \eta} + \sum_{\alpha=1}^{n} c_{p\alpha} \frac{\partial Q_\alpha}{\partial \eta} \right) \frac{\partial Q_T}{\partial \eta}$$

$$+ \dot{T}_{spark}(\eta) - \frac{1}{\bar{\rho}\tilde{P}(\eta)} \frac{\partial}{\partial x_i} \left(-D_t \frac{\partial Q_T}{\partial x_i} \bar{\rho}\tilde{P}(\eta) \right)$$

$$- \frac{1}{\bar{\rho}\tilde{P}(\eta)} \frac{\partial}{\partial x_i} \left(F_{Ti} \bar{\rho}\tilde{P}(\eta) \right)$$

or in symbolic form,

$$\frac{\partial Q_T}{\partial t} = T_{cv} + T_c + T_{m1} + T_{m2} + T_{spark} + T_{tf} + T_{CGD} .$$

Thus the rate of change of Q_T is attributed to convection T_{cv}, with the conditional velocity $\langle u_i | \eta \rangle$ given by the linear model [4]. The remaining terms on the right hand side of the conditional averaged temperature equation refer to chemical reaction T_c, molecular mixing $T_m = T_{m1} + T_{m2}$, energy deposition due to spark ignition T_{spark}, and the turbulent flux transport T_{tf} and T_{CGD}.

In common with previous work [8], the conditional scalar dissipation rate $\langle N | \eta \rangle$ is modelled using the Amplitude Mapping Closure (AMC) model [9]. The conditional expectation of the chemical source term T_c was closed at first order using the expectations for the conditional temperature and mass fractions. The one step reaction model for partially premixed combustion by Tarrazo-Fernandez et al. [10] was used throughout this work. This one step model gives the correct premixed flame speed at all mixture fractions. It also displays the correct extinction behaviour in strained premixed and non-premixed flows, including oxygen leakage close to extinction. A skeletal mechanism [11] has also been used for comparison in specific cases.

The spark is modelled as an energy source whose volumetric power $\partial(\rho h)/\partial t$ is uniform in time and space within a specified ignition region and time period. A cylindrical volume aligned with the jet's axis, 2mm long and 2mm in diameter, and a 400μs duration are used to characterize those in the modelled flow. It should be noted that this does not constitute an attempt to fully describe the physics of the spark ignition, which would need to involve an accurate thermodynamic and electrical description of the compressible plasma kernel. Instead it is a procedure to arrive at a post spark condition which is comparable to that which would be observed in a real flow, in terms of enthalpy distribution, composition and velocity. Alternative spatial and temporal spark profiles might be considered however in the absence of data for the correct post spark condition no alternatives are presently pursued.

The CMC model requires that the energy source is expressed as a conditional temperature source. It is argued that the temperature attained by a fuel-air mixture inside the spark gap is largely prescribed by a balance between the electrical energy input and the heat lost to the electrodes and through radiation, as such the temperature would not be a strong function of mixture fraction. In the absence of chemical change at the η=0 and η=1 boundaries of mixture fraction, the following expression for the conditional temperature source gives equal temperature increments at η=0 and η=1, and maintains a linear variation of enthalpy between the two boundaries.

$$\dot{T}_{spark}(\eta) = \frac{1}{c_p} \frac{\partial h}{\partial t} \left[\frac{(1-\eta)\langle c_p | \eta = 0 \rangle + \eta \langle c_p | \eta = 1 \rangle}{\langle c_p | \eta \rangle} \right]$$

Terms T_{tf} and T_{CGD} arise from the modelling of the conditional turbulent flux:

$$\langle u_i'' T'' | \eta \rangle = -D_t \frac{\partial \langle T | \eta \rangle}{\partial x_i} + F_{Ti} .$$

The first term on the right hand side is the eddy diffusivity model which has become standard in elliptic CMC modelling. The second is a correction to account for the counter gradient transport effects, discussed in depth in Ref. [6]. The concept behind the model is similar to that of Bray and Libby's analysis for premixed turbulent flux [12,13,14]. It was noted that the PDF of a progress variable in a turbulent premixed flame can be close to bi-modal with peaks at the unburned and burned conditions, and arrived at an algebraic expression for the unconditional turbulent flux. The first step in the development of the correction for the conditional turbulent flux model is to define a progress variable for the non-premixed flow,

$$c = \frac{Y_{CH_4}^U(\eta) - \langle Y_{CH_4} | \eta \rangle}{Y_{CH_4}^U(\eta) - Y_{CH_4}^B(\eta)}$$

so that it varies between zero and one at all values of η (except η=0 and η=1 where it is not defined). The subscripts *u* and *b* refer to unburned and burned conditions. In the example of a steady lifted jet flame the burned condition has been taken as the conditional composition at the downstream boundary of the domain. It is not generally accurate to assume that the PDF of *c* is bi-modal [6] however use of this assumption is still interesting since it may be used to demonstrate one extreme of the possible behaviours.

The assumption of a bi-modal progress variable PDF results in the following expression for the conditional turbulent flux of the progress variable.

$$F_{ci} = \left(\langle u_i|\eta\rangle^b - \langle u_i|\eta\rangle^u\right)\langle c|\eta\rangle\left(1-\langle c|\eta\rangle\right).$$

The difference between the conditional velocity in the reactants and products is modeled as;

$$\langle u_i|\eta\rangle^b - \langle u_i|\eta\rangle^u \approx \tau(\eta)S_E$$

with the heat release parameter τ(η) given by;

$$\tau(\eta) = \left[\frac{\langle\rho|\eta\rangle^u}{\langle\rho|\eta\rangle^b} - 1\right],$$

and the propagation speed of the partially premixed (edge) flame denoted by S_E. S_E might be modeled using the estimate for the laminar triple flame speed, $S_E=\sqrt{\frac{\rho_u}{\rho_b}}S_L$, given by Ruetsch et al. [15]. It might also be useful to express S_E as a function of the scalar dissipation rate based on DNS data [16]. In this work $S_E=S_L$ was used.

The conditional, counter-gradient turbulent flux of the progress variable can then be scaled to give the flux of mass fractions or enthalpy.

$$F_{Y_\alpha i} = F_{ci}\frac{\langle Y_\alpha|\eta\rangle^B - \langle Y_\alpha|\eta\rangle^U}{\langle c|\eta\rangle^B - \langle c|\eta\rangle^U}$$

The counter gradient turbulent flux expression has been added to the gradient model as in previous algebraic models for the unconditional turbulent flux, eg. Ref. [17]. This gives the expected property that gradient transport processes dominate at high turbulence levels.

Results and Discussion

1) Validation

The predicted mean and variances of the inert velocity and mixing field resulting from the *k*-ε model with Pope's correction for round jets [18] closely matches empirical expressions [19, 20] for turbulent jets, see Ref. [6]. Grid and time step independence of the CMC solutions has also been demonstrated [6].

1D, fully coupled CMC solutions of the steady, lifted flame were evaluated with both the one-step and skeletal reaction mechanisms. The conditional temperature and heat release profiles computed are shown as a function of axial position in Fig. 2.

Both solutions are within one jet diameter of the observed lift off height. Additionally little difference is seen between the conditional temperature profiles. Both models predict the co-existence of rich, lean and stoichiometric flame elements at the flame tip, and a trail of diffusion flame. It must be emphasised that the CMC is a statistical model which does not infer any particular flame structure. The observations of Fig. 2 are consistent with the presence of a triple flame but such a structure is not necessarily implied. The use of simplified combustion schemes appears appropriate for ignition calculations since the main quantity needed from the combustion model is the heat release.

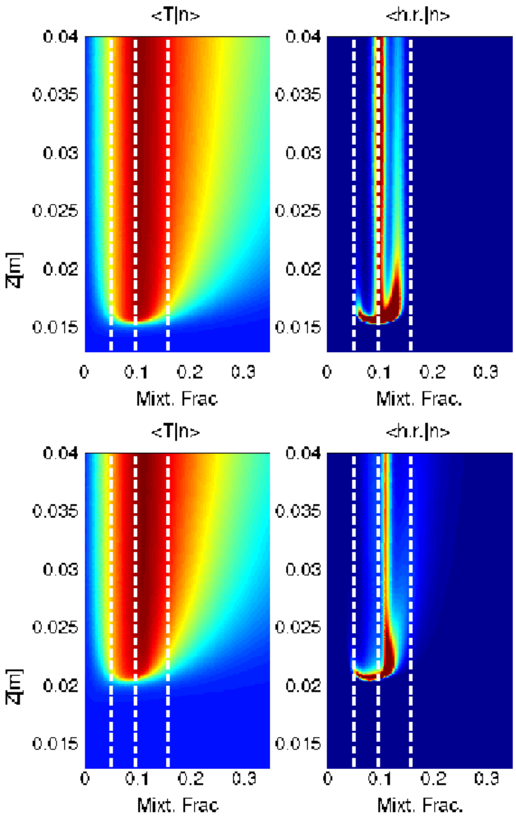

Fig. 2 Conditional temperature, K (left) and heat release, Ks^{-1} (right), using the 1-step (top) and skeletal (bottom) reaction schemes in coupled, 1D solutions for the stabilised lifted flame, W_j=12.5ms^{-1}. The lower (blue) and upper (red) bounds of the colour scale were 293-2200K for temperature and 0-$10^6$$Ks^{-1}$ for the heat release rate.

2) Edge Flame Propagation

Simulations of flame propagation and stabilisation in the turbulent jets W_j=12.5ms^{-1} and W_j=25.5ms^{-1} were performed, neglecting F_{Ti} and $F_{Y\alpha i}$, using the following model configurations:

i)1-dimensional CMC, using an inert CFD solution.
ii)1-dimensional CMC, fully coupled to the CFD.
iii)2-dimensional axi-symmetric CMC, fully coupled.

The position of the upstream flame front (given by $\langle T|\eta_{st}\rangle$=1200K) is plotted for the various model configurations and from experimental measurements [1] in Fig. 3.

The simulated flame front positions vary significantly depending on the model configuration, and always reached the final lift-off height at an earlier time than in the experiment. In particular, introducing the effect of heat release into the flow field calculations has a very large effect on the predictions, accelerating the propagation process and reducing the expected lift off height. The difference between the 1D and 2D coupled calculations is also significant resulting in differing final lift off heights.

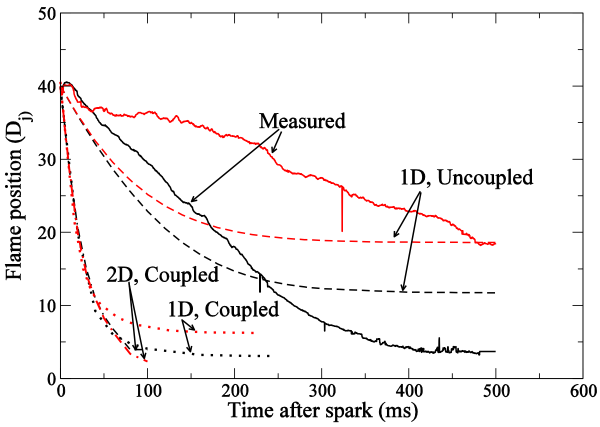

Fig. 3 Temporal evolution of the upstream flame front's position for W_j=12.5ms^{-1} (black) and W_j=25.5ms^{-1} (red).

The uncoupled calculations are closest to the measured propagation rates however their initial propagation speeds are above that observed experimentally. In Ref. [5] the first order reaction rate closure was seen to over-predict the actual heat release from turbulent propagating flames, which may play a part in the over prediction of the propagation speed observed here.

The mean dilatation at the upstream flame front acts to reduce the z-direction velocity, allowing a higher propagation speed. Additionally the expansion intensifies the turbulence at the flame front, for example increasing the predicted stoichiometric conditional turbulent diffusivity from 1.1x10^{-3}m^{2}s^{-1} to 3.8x10^{-3}m^{2}s^{-1} as the flame front passes through 20Dj in the W_j=12.5ms^{-1} case. The relative turbulent intensification falls as the flame approaches the higher velocity flow close to the nozzle. Provided the flame is far from extinction, both processes may be expected to increase the modelled turbulent burning rate, potentially feeding back into a further increase in the propagation speed. Thus the propagation and stabilisation model may be particularly sensitive to the accuracy of the fluid dynamic and turbulent combustion models. Given the role that specific large scale structures are thought to play in the stabilisation of a lifted, round turbulent jet, Ref. [21], it may be questioned whether a *k*-ε RANS solution encapsulates enough of the flow physics to form the basis for a simulation of propagation and stabilisation.

The complete ignition process is illustrated by the evolution of the Favre averaged (unconditional) temperature and mean mixture fraction field shown in Fig. 4 for W_j=12.5ms^{-1}. The mean velocity and mixing patterns undergo significant modification caused by thermal expansion during, and for some time after ignition and stabilisation of a lifted flame. The lateral expansion around the spark location and subsequent development of a thin, tubular flame agrees qualitatively with experimental observations [1].

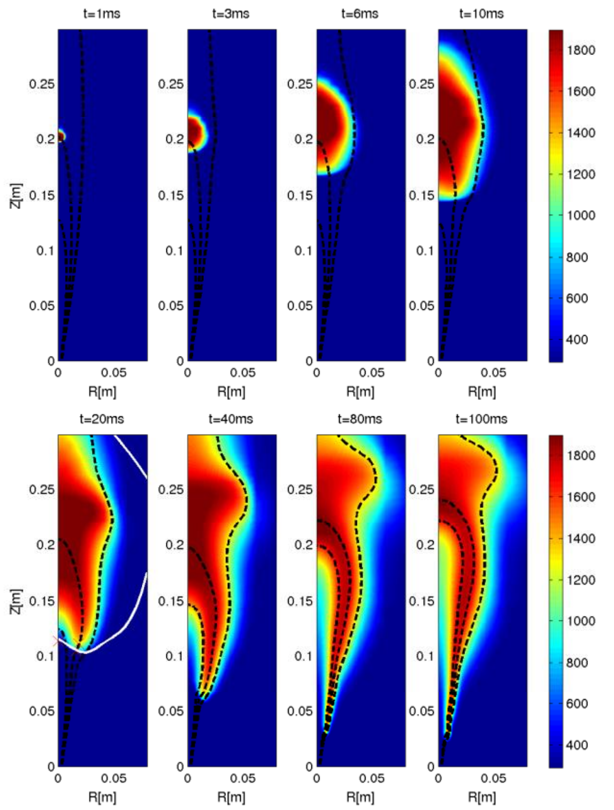

Fig. 4 Unconditional temperature contours, coloured from blue = 293K to red = 1900K for W_j=12.5ms^{-1} at 1, 3, 6, 10, 20, 40, 80 and 100ms after inception of the spark. Iso-lines of mean mixture fraction are plotted in black for the lean flammability limit ξ=0.0502 (inner), stoichiometry ξ=0.0976 (middle), and the rich flammability limit ξ=0.158 (outer). The plot for 20ms contains a white contour at $\langle T|\eta_{st}\rangle=0.8(T_{ad}-T_0)+T_0$.

The CMC representation of the propagating front is explored in Figs. 5-7at 20ms after the spark. Figure 5 shows the component of the CMC terms parallel to the mean stoichiometric mixture fraction iso-surface through the flame front. The conditional temperature gradients are far greater than the unconditional temperature gradient observed in Fig. 4, with the conditional flame front being approximately 2mm thick at stoichiometry.

The CMC terms contribute as may be expected. Chemical heat release, T_c, is exothermic, peaking at the hot side of the flame, where it is also most strongly opposed by molecular "micro-mixing", T_m. The conditional convection, T_{cv} term provides a weak cooling effect on the hot side of the flame, however the flow stagnates somewhere near the cold edge of the flame and a very weak heating effect is seen at the cold edge. The turbulent flux, T_{tf} is treated using the eddy diffusivity model, therefore it is seen to move heat down the mean temperature gradient from the products to the reactants.

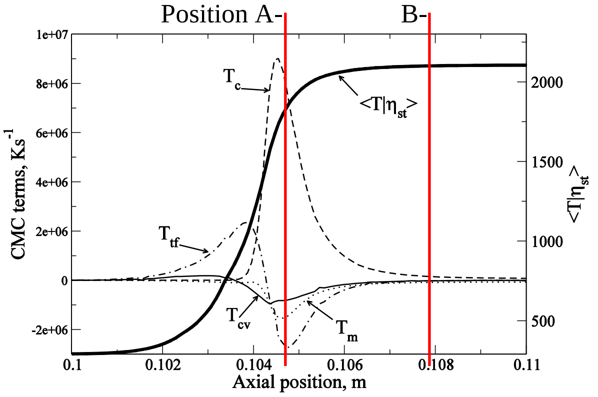

Fig. 5 The temperature and terms of the CMC equation conditioned on stoichiometry, along the mean stoichiometric contour.

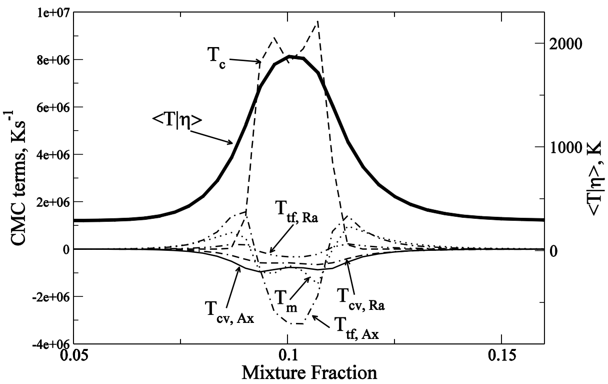

Fig. 6 Mixture fraction space profiles for CMC terms and conditional temperature expectation at position A shown in Fig. 5.

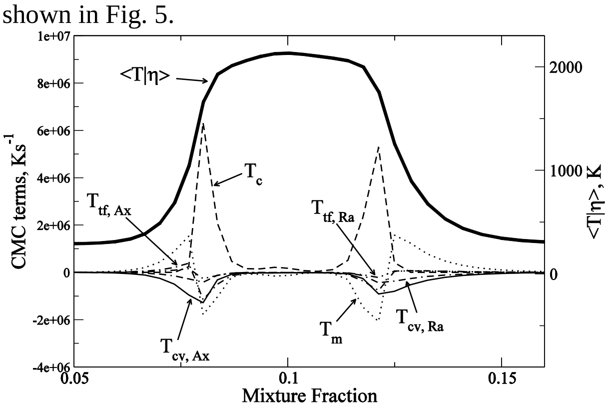

Fig. 7 Mixture fraction space profiles for CMC terms and conditional temperature expectation at position B shown in Fig. 5.

Figures 6 and 7 show the mixture fraction space profiles of the conditional source terms at selected points in the upstream flame front. Figure 6 is positioned at the intersection of the mean stoichiometric iso-line and the white line in Fig. 4 representing the conditional, stoichiometric flame front. The furthest upstream position of the conditional flame front is found at a slightly greater radius, where the mean flow is leaner and slower moving. In Fig. 6 the narrowness of the flame does not allow a clear distinction between rich and lean premixed fronts or of a diffusion flame and as such it may correspond to the triple point of a tri-brachial flame. After the chemistry, the next largest term is the axial turbulent flux, which acts to cool the hotter stoichiometric region and heat the cooler rich and lean areas. This may be explained by the differing positions of the conditional flame front at different mixture fraction, since the rich and lean conditional flames do not propagate as fast. Figure 7 is also positioned on the mean stoichiometric iso-surface, at z=0.108m. At this position the stoichiometric temperature is close to its adiabatic value, however the flame is still developing at richer and leaner mixture fractions. The presence of distinct reaction fronts is seen in mixture fraction space with the scalar dissipation term T_m playing an important role in the transport of heat to the unburned reactants.

3) Conditional Turbulent Flux Modelling

The steady lifted jet flame, W_j=12.5ms^{-1}, was simulated using the 1D-CMC model with and without the new modelling for the turbulent flux term, F_{Ti} and $F_{Y\alpha i}$. The resulting profiles of the stoichiometric CMC terms along the axial direction are shown in Fig. 8. The roles of the CMC terms in Fig. 8 are the same as those observed in the upstream flame front throughout the propagation phase, for example in Fig. 5. The inclusion of counter gradient effects into the model resulted in a slight increase in lift off height and a notable reduction in the flame thickness. The counter gradient term acts to take heat and products away from the upstream side of the lifted flame front and move it back towards the burned, product rich side of the flame. The resulting reduction in flame thickness leads to an increase of the gradient diffusion component in the turbulent flux model.

In isolation the counter gradient component of the turbulent flux model is unstable. The gradient diffusion component combined with the scalar dissipation term in the CMC equation act in a stabilising way and can make the model workable in partially premixed flames, as in the present study. However, some initial conditions resulted in numerical problems. A more complete discussion of the numerical properties of this model is given in Ref. [6]. This model requires extensive development and validation. This might be achieved through comparison with detailed experimental measurements, or further turbulent DNS data. In the first instance though, the model may be improved through experience of its application to a broader range of flows and conditions.

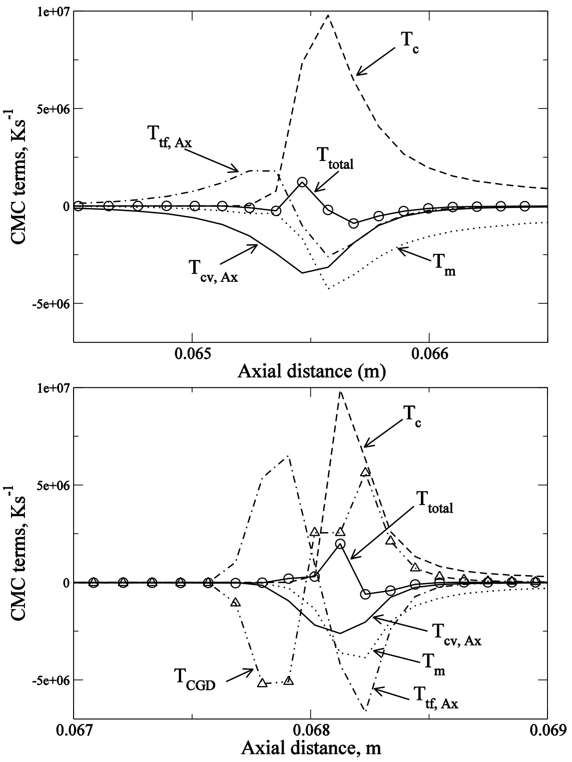

Fig. 8 Budget of CMC temperature equation terms with the standard eddy diffusivity model (top) and the additional counter gradient model (bottom), in stable 1D CMC solutions of the W_j=12.5ms^{-1} lifted flame.

Conclusions

The CMC has been implemented for the solution of flame ignition, propagation and stabilisation in a methane jet. An axi-symmetric formulation of the first order CMC model has been fully coupled with a RANS flow field solution.

Study of the transient flame propagation phase shows the expansion across the flame having a strong effect on the propagation speed. Therefore a full coupling of the flow field and the combustion processes needs to be included in predictive calculations. The over prediction of flame propagation rates was attributed to possible over statement of the conditional reaction rate due to its first order closure, and the use of the RANS turbulence closure. Alternative CMC closures which account for fluctuations around the conditional averages, and turbulence models where the large scale motions are resolved may be needed.

A one-step reaction model with variable model parameters produced excellent results for this problem compared to a skeletal mechanism for methane combustion. The use of similar reaction models may prove valuable in intensive industrial simulations of partially premixed propagation where the heat release rate is of primary interest.

A new modelling approach which incorporates counter gradient transport effects into the conditional turbulent flux model has been demonstrated. The model results in a modification to the structure of the conditional flame profiles, however it does not change the prediction of the lift off height greatly

This study represents a new and challenging test of the CMC model and provides a first step towards the application of the CMC to industrial ignition simulations.

Acknowledgements

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