Coupling the Conditional Moment Closure Model to a Fully Compressible Large Eddy Simulation Algorithm

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Abstract
The Conditional Moment Closure (CMC) model provides a means of closing the subgrid terms for the reaction rates through the assumption that departures of the mean filtered reaction rate (conditional on a mixture fraction or progress variable) are small. Turbulent-chemistry interaction is incorporated through a conditional scalar dissipation. To date, all Large Eddy Simulation implementations of the CMC model are with incompressible solvers and for non-premixed flames. This paper presents a methodology of coupling the CMC model with a fully compressible solver, and resultant validation against DNS data. This methodology can be employed for both premixed and non-premixed flames. Several challenges associated with premixed modeling using this approach are outlined.

Introduction
Computational power now permits the application of time-accurate unsteady methods to problems of industrial interest [1-3]. A key challenge when using Large Eddy Simulation (LES) is to incorporate the effects of turbulence-chemistry interactions through a detailed subgrid model which permits the use of complex reaction mechanisms. The majority of combustion LES involve the coupling of the combustion subgrid model with a variable-density incompressible methodology via the continuity equation. However, this is not appropriate for flows which are influenced by compressible (acoustic) features. Examples of these types of flows include deflagrations, detonations, knock or ringing in homogeneous charge compression ignition engines at high load, knocking spark-ignition engines, combustion noise and acoustically driven instabilities in gas turbines.
The Conditional Moment Closure (CMC) model [4-6] has been thoroughly validated in RANS simulations of turbulent non-premixed flames and has recently been successfully extended to LES (denoted LES-CMC) of turbulent diffusion flames and bluff body flames [7-9]. This modelling approach has several advantages; most notably that it provides a simple means to integrate finite rate complex chemistry effects into an LES. Closure is achieved through assuming that the variations around conditional means are small. Several additional terms must be closed, including expressions for the conditional velocities, conditional scalar dissipation and the Filtered Probability Density Function (FDF). The closure of these terms is expected to be dependent on the combustion regime encountered.
This paper presents a new high-order accurate, fully compressible (shock capturing) implementation of the CMC modelling approach for lean premixed turbulent combustion. The CMC model is coupled through the energy and species equations using a fifth-order accurate in space modified Godunov method which has recently been derived specifically for problems including both compressible features and turbulent mixing [10-11]. In addition, the same

proposed algorithmic structure can be used for non-premixed combustion using LES-CMC where the chosen conditioning variable would then be the mixture fraction and not a progress variable based on a reacting scalar. The proposed algorithm is validated against the low Damköhler number slot flame DNS of Sankaran et al. [12].

Governing Equations and Numerical Methods

The governing equations chosen are the LES filtered equations for a compressible, reacting mixture [13-14]. This includes a single equation tracking the progress variable, the continuity, momentum and total energy equation. Using a direct numerical simulation database modelling a turbulent lean premixed methane slot flame due to Sankaran et al. [12], it has been shown in 'a-priori' tests [15] that the first order CMC closure assumption based on mass fraction of O_2 gives good results for the reaction rate of the major species. Hence the progress variable in this work is based on the mass fraction of O_2 and varies from 0 in the unburnt premixture to 1 in the burnt gases.

Following Vremen et al (1995) the subfilter contributions to the momentum and energy equations from unresolved fluctuations of the viscous stress tensor, and subfilter contributions from unresolved heat flux are neglected. In this paper, the novel reconstruction method proposed by Thornber et al. [10,11] is employed to model terms the unclosed Reynolds stress. This numerical method is not kinetic energy conserving. Rather, the reconstruction method is designed to give a leading order dissipation of turbulent kinetic energy proportional to the velocity increment at the cell interface cubed (Δu^3) as expected from Kolmogorov's analysis [16].

The improved interpolation approach helps overcome the typical poor high wavenumber performance of standard compressible Godunov methods [19, 20]. It acts as an implicit subgrid model [17,18] whilst naturally stabilising the numerical solution and retaining monotonicity. As with all LES models this relies on sufficient separation of the large scales from the scales where numerical dissipation acts strongly. In several previous test cases, this numerical method has demonstrated a good ability to represent the dissipation of turbulent kinetic energy [11, 21,22], most notably in flows requiring excellent resolution of turbulent scalar mixing parameters [23].

In an analysis of premixed and non-premixed methane air flames, Smooke and Giovangigli [24] demonstrated that the terms including enthalpy diffusion could be neglected by comparison to the other terms in the energy equation. Standard closures are employed for the remaining terms, utilising the Smagorinsky model [25] to provide an eddy viscosity type closure, with species and thermal diffusion given by a turbulent Schmidt number and the Prandtl analogy respectively.

The reaction rates are given by the filtered CMC equations,

$$\frac{\partial Q}{\partial t} + \widetilde{\mathbf{u}|\zeta} \cdot \nabla Q = \widetilde{\dot{w}_k|\zeta} - \widetilde{S_c|\zeta}\frac{\partial Q}{\partial \zeta} + \widetilde{N|\zeta}\frac{\partial^2 Q}{\partial \zeta} + e_Q, \qquad (1)$$

where the conditionally filtered averaged mass fractions $Q = Y_k|\zeta$, the filtered conditionally averaged scalar dissipation $N = D_c(\nabla c)^2$ and $.|\zeta$ refers to a mean conditional on $c = \zeta$ where c is the progress variable. $P(\zeta)$ is the Filtered Probability Density Function (FDF), $w_k|\zeta$ is the conditional filtered mass fraction production rate of species k, and the conditionally filtered density $\rho|\zeta$. S_c is the Favre averaged source term present in the equation for the progress variable, which in this paper is the scaled O_2 mass fraction production rate. $(\tilde{})$ indicates a Favre filtered quantity [26-28]. The reaction rates are thus computed in conditional space first, then integrated with the FDF to recover the filtered reaction rates required in the Navier-Stokes equations.

In order to reduce the computational cost incurred by effectively adding another dimension into the governing equations (progress variable space), the CMC equations are solved on a reduced grid, which could be any size from one-dimensional through to three dimensional. The means that there are several CFD cells for each CMC cell at the very least.
There are several terms in the CMC model which require closure. Firstly, the FDF is represented by a top hat distribution following Floyd et al. [29], where the variance of the progress variable required to construct the top hat is estimated using a gradient model. Quantities required on the CMC grid can then be computed by integrating over all CFD cells within a single CMC cell, i.e. for a function f

$$\widetilde{f^*|\zeta} = \frac{\int_{V_{CMC}} \bar{\rho}\widetilde{f|\zeta}\tilde{P}(\zeta)dV'}{\int_{V_{CMC}} \bar{\rho}\tilde{P}(\zeta)dV'} \tag{2}$$

Where (*) indicates that it is a function evaluated on the CMC grid. Thermodynamic quantities are required to compute the filtered conditional reaction rates. The conditional pressures are computed by averaging over all CFD points within a single CMC cell. Temperatures are computed in a similar manner from the conditionally averaged standardised enthalpy and conditional densities are then recovered from the ideal gas equation of state, where the thermodynamic properties of each species are defined using standard polynomial fits to the specific heats at constant pressure.
The conditional scalar dissipation represents the influence of turbulence providing mixing at the subgrid level. This paper employs a non-premixed type model for the scalar dissipation:

$$\tilde{N} = \overline{D_t}\frac{\tilde{c'^2}}{C_{c'}\Delta^2}. \tag{3}$$

For high Damköhler number flames this will not be physically correct, however the DNS simulated here is at a relatively low Damköhler number which permits this coarse approximation. In addition, it is employed here to demonstrate the stability and capability of the proposed numerical method. The turbulent diffusivity D_t is approximated using the eddy diffusivity approximation. To gain $N|\zeta$ the values of Favre filtered N computed on the CFD grid are conditionally filtered using the density weighted FDF.
Finally, the reaction model employed was developed for the lean premixed slot flame of Sankaran et al. [12] which has 72 elementary reactions with 17 species, 4 of which are steady state, hence requiring the simulation of 13 species.
The governing equations are solved using a fifth order accurate in space Godunov method which has been specifically modified to give dissipation which is uniform with Mach number [11]. This is a fully compressible method (shock capturing). Second order accurate explicit TVD Runge-Kutta time stepping has been employed, along with Strang time splitting for the terms involving scalar dissipation. Note that the same finite volume discretisation method has been employed for the LES and CMC equations, where non-conservative terms in the CMC equation have been treated using the approach of [30].

Validation

The chosen validation case is a comparison to the recent DNS of a lean premixed methane Bunsen burner of Sankaran et al. [12]. Case 'C' is run here, with a Reynolds number of 2100 based on slot width, a turbulent Reynolds number Ret = 250 and a Karlovitz number of 225. The premixed fuel/air inlet has an equivalence ratio of 0.7, and is introduced into the domain at a temperature of 800K and mean inflow velocity of 100m/s (rms turbulent fluctuations ≈ 35% of the mean inflow velocity) with a slot width of 1.8mm. The laminar coflow velocity is 25m/s.

In the following simulations a three dimensional CFD grid is employed along with a one-, two and three dimensional CMC grid (in space), where only data from the one-dimensional CMC grid are presented here. Interestingly, the results employing two- and three-dimensional CMC grids were only marginally better than those with a simple one dimensional axial grid. The CFD grids from coarse to fine have 75 × 25 × 144, 100 × 32 × 192 and 150 × 50 × 288 and 200 × 64 × 384 points, where x is the cross-stream coordinate, y the homogeneous direction, and z the axial direction. The one-dimensional CMC grid has the same number of points in the axial (z) direction as the CFD grid, but only one cell in the y and z direction respectively.
The inflow boundary conditions and reaction model employed are the same as those used for the DNS. Figure 1 shows an instantaneous flow visualisation of Favre filtered $|\nabla c|$ on the finest grid, and three dimensional isosurfaces of Favre averaged progress variable of 0.65 for the highest resolution grid. The instantaneous flame structure is physically correct, with a clear preheat zone at intermediate progress variables due to turbulent mixing, and steep gradients in the with the heat release zone.

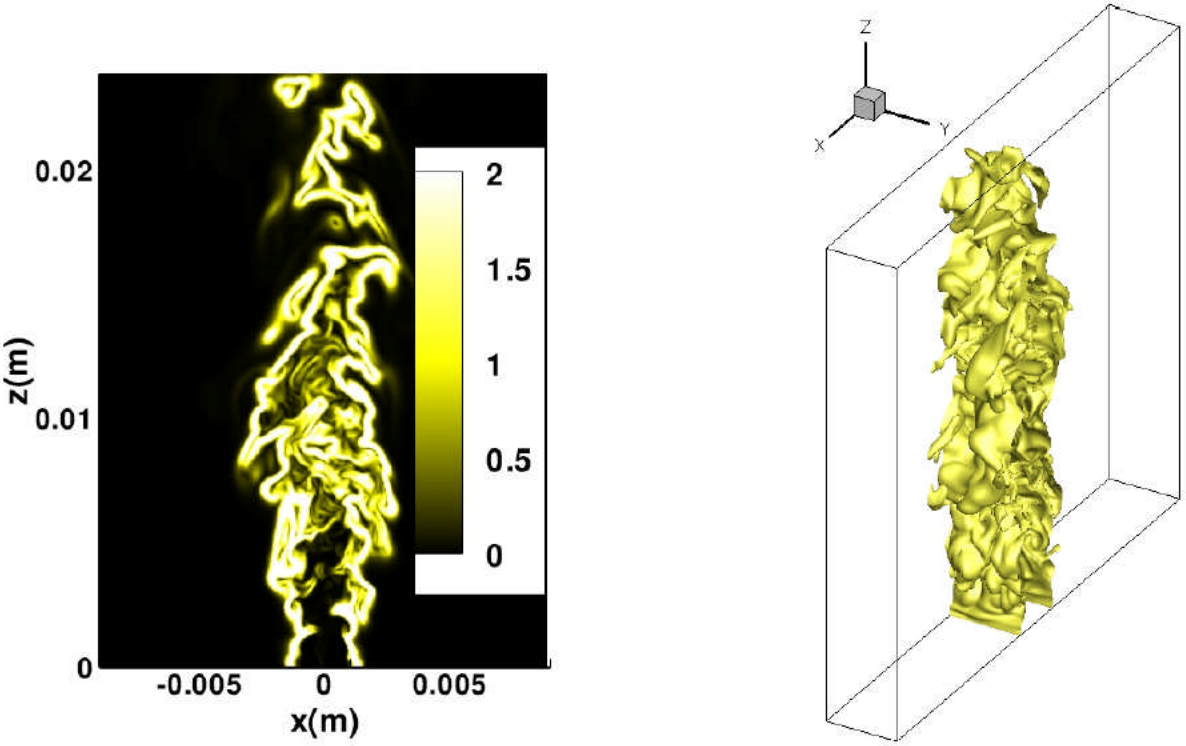

Figure 1. Instantaneous visualisation of absolute progress variable gradient (left) and isosurface of Favre filtered progress variable 0:65 (right).

Cross-stream quantitative data have been extracted along z = 0.005m ($z/L_f \approx 26\%$). and z=0.015 ($z/L_f \approx 80\%$). Figure 2 shows the mean density, temperature and axial velocities along each of these lines (averaged in the homogenous y direction). Comparisons of density and temperature show excellent agreement with DNS, with a maximum error of 9% in density and 3% in temperature in the core at the downstream position. The axial velocity profile indicates that the flame width is slightly narrower than that predicted by DNS.
Figure 3 shows the predicted CH_4, OH and CO mass fractions along both lines. The mass fractions of CH_4, O_2, H_2O, and CO_2 are in very good agreement with DNS, with a small overestimation of CO_2 and H_2O on the boundary of the flame. CO is underestimated by ~19%, but matches the DNS data qualitatively. A comparison of the mass fraction of OH show that there is a significant difference in form at z = 0.005m. There is a peak in the DNS

data at x ~ 0.0026m which is not present in the LES data at any grid resolution. At z = 0.015m the match with DNS is qualitatively good with an underestimation of OH levels by 24%.

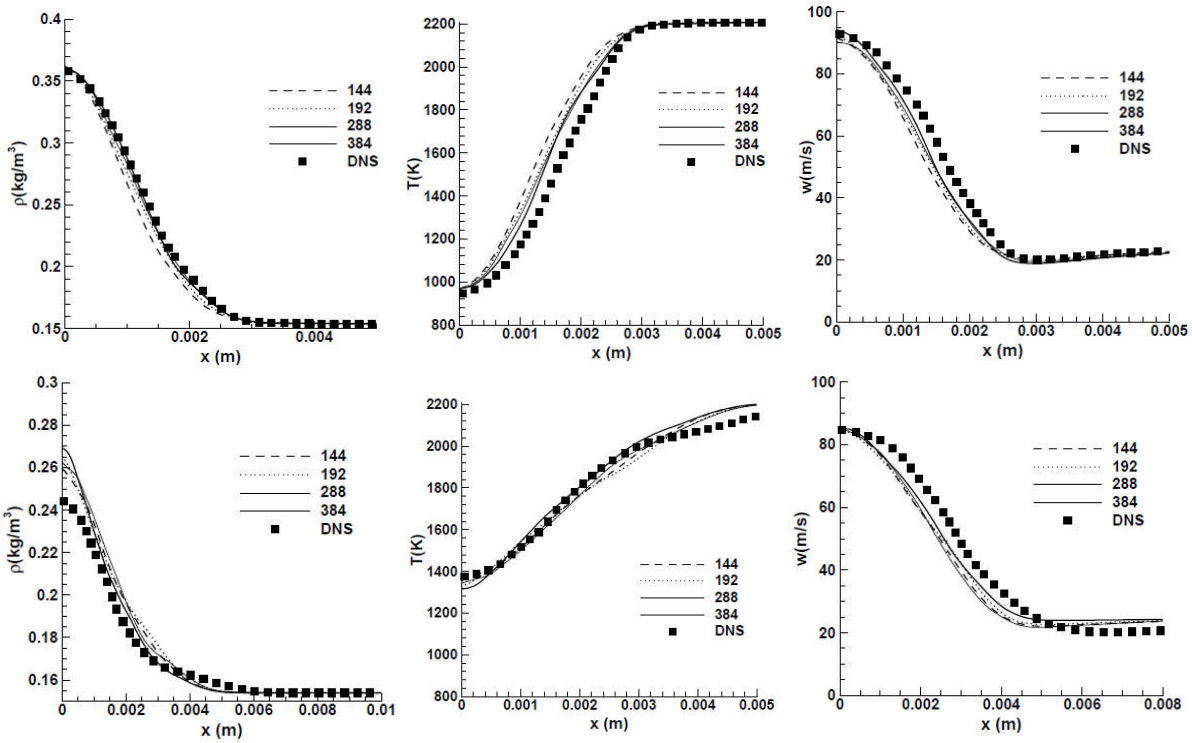

Figure 2. Mean density, temperature and axial velocities measured at z=0.005m (top) and z=0.015m (bottom)

A comparison of conditional mass fractions of OH can be seen in Figure 4. The LES match very well the DNS data both qualitatively and quantitatively. Initially very high levels of conditional scalar dissipation lead a rapid decrease in gradients in conditional space. It appears that the modelled conditional scalar dissipation rate in the LES overestimates that present in the actual DNS, or that the conditional reaction rates close to the jet inlet are lower. These results are promising for the further application of CMC in the closure premixed reaction rates in turbulent flows.

Conclusions

This paper has presented an outline of a fully compressible LES-CMC method which is validated against simulations of a lean premixed methane slot burner. It shows very good agreement with DNS data, particularly in the response of the conditionally averaged species mass fractions. Future work will focus on the extension of these methods to more complex geometries and industrially relevant applications, and use of the base numerical scheme to investigate potential premixed flame closures.

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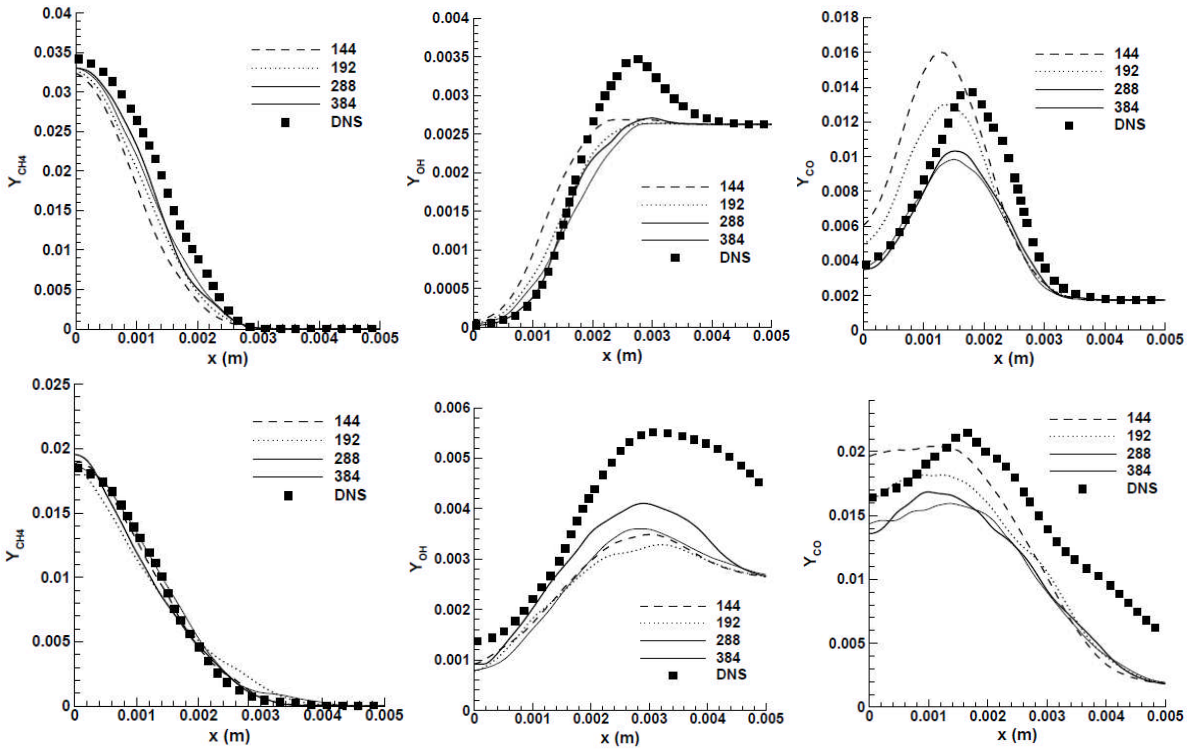

Figure 3. Averaged mass fractions measured at z=0.005m (top) and z=0.015m (bottom)

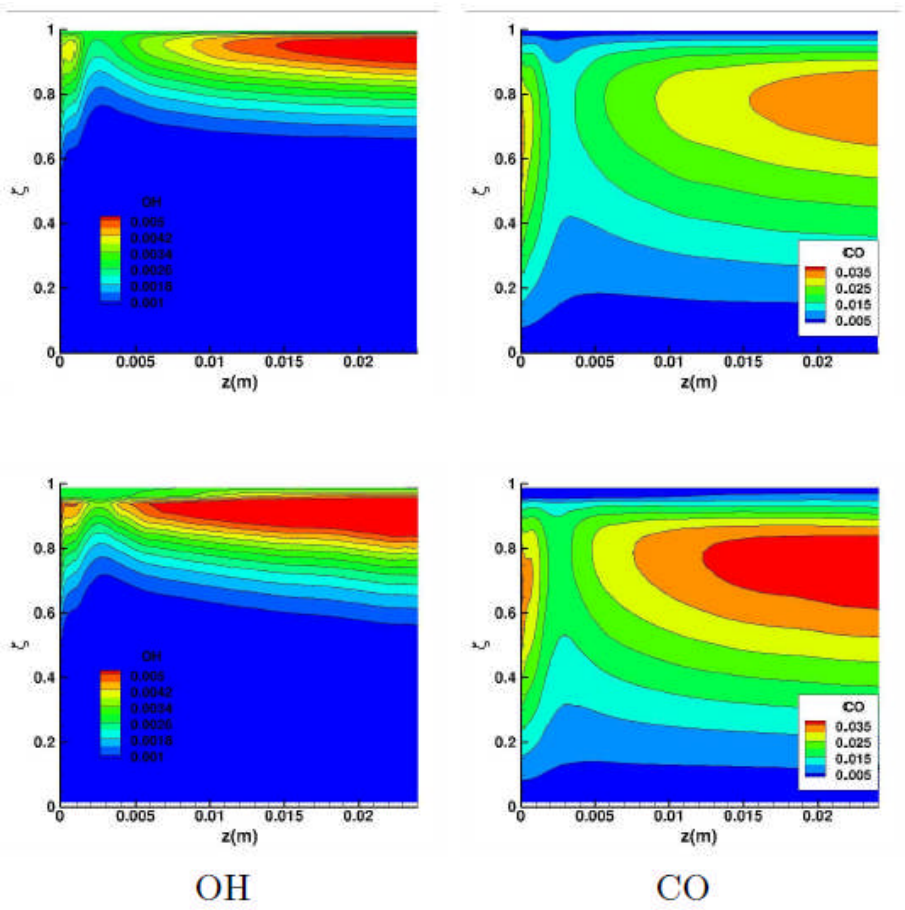

Figure 4. Conditionally averaged mass fractions as a function of axial distance computed from the LES (top) and the DNS (bottom)

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