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Sensitivity analysis of LES–CMC predictions of piloted jet flames

A. Garmory *, E. Mastorakos

Hopkinson Laboratory, Department of Engineering, University of Cambridge, Cambridge CB2 1PZ, United Kingdom

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ABSTRACT

The sensitivity of Large Eddy Simulation with Conditional Moment Closure (LES–CMC) simulations of the Sandia piloted jet Flames D and F to various parameters have been investigated. It was found that while an LES grid may sufficiently resolve velocity fields, the conditional scalar dissipation rate obtained may still be affected by grid size due to the calculation of sub-grid scalar dissipation rate, and this can affect the degree of localised extinction predicted. A study of the relative size of the terms in the CMC equation during an extinction/reignition event showed that transport, including in the cross stream direction, plays a key role. The results are sensitive to the choice of inlet boundary conditions as extinction is only observed when the inert-mixing distributions in mixture fraction space are used as inlet conditions for the CMC equation in the primary jet and air jets.

1. Introduction

Due to its superior ability to predict the details of turbulent mixing, large eddy simulation is increasingly being used to study turbulent combustion in a variety of industrial applications. Even with the greater spatial resolution of LES compared to RANS the combustion process still takes place on a scale which cannot be resolved by the grid, and as such some form of turbulent combustion modelling must be employed. These include steady (Di Mare et al., 2004) and unsteady (Pitsch and Steiner, 2000) flamelet models, the flamelet/progress variable (FPV) model (Pierce and Moin, 2004) and the stochastic fields or Eulerian Monte Carlo method (Mustata et al., 2006). The Conditional Moment Closure model, discussed later, is another advanced model that is being used for flames with strong turbulence-chemistry interactions.

In order for any such model to become a useful engineering tool it is important that they are validated against detailed measurements and that the models' sensitivity to modelling choices and parameters are investigated. The Sandia piloted jet flames (Barlow and Frank, 1998) provide detailed experimental data for both scalar and velocity fields and consequently have been widely used for this sort of validation work. Data is available for conditions ranging from a flame with very little local extinction (Flame D) to one that is close to global extinction (Flame F). RANS – Muliple Mapping Conditioning (MMC) simulations of Flame D have been performed by Vogiatzaki et al. (2011) in order to determine the value of modelling parameters which give the best agreement with conditional variance of temperature and various species mass fractions. Previous studies using transported PDF methods in RANS have produced good agreement with experiment (Lindstedt et al., 2000; Xu and Pope, 2000) for Flame F and also revealed the sensitivity of this Flame F to the chosen chemical mechanism (Cao and Pope, 2005). These studies were useful in determining the parameters needed in RANS–PDF modelling to give accurate results, a process that is now being undertaken for LES studies. The presence of localised extinction in Flame E has successfully been predicted in Ihme and Pitsch (2008) using the FPV model. The Eulerian stochastic fields PDF method has been used in Jones and Prasad (2010) to successfully predict the presence of localised extinctions in Flame F.

Conditional Moment Closure (CMC), which is the subject of this paper, has previously been used in an LES context for Sandia Flame D (Navarro-Martinez et al., 2005), bluff-body steady flames (Navarro-Martinez and Kronenburg, 2007), autoigniting jets (Navarro-Martinez and Kronenburg, 2009) and for spark ignition problems (Triantafyllidis et al., 2009). An LES–CMC formulation solving the CMC equations on a 3D grid (i.e. resolving variations of conditional average in three dimensions rather than using cross stream averaging) has been used to successfully predict the presence of localised extinction and reignition events in both Sandia Flame F (Garmory and Mastorakos, 2011) and the Delft III piloted jet flame (Ayache and Mastorakos, 2012). It was shown that the model can successfully predict the occurence of localised extinction, and the resulting statistics of species mass fractions and temperature.

The purpose of this paper is to revisit the simulations of Sandia Flames D and F in order to investigate the sensitivity of the results to the modelling choices used. This will build confidence to the use of the LES–CMC approach for more complex flames of practical

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* Corresponding author. Present address: Department of Aeronautical and Automotive Engineering, Loughborough University, Loughborough LE11 3TU, United Kingdom.

E-mail address: A.Garmory@lboro.ac.uk (A. Garmory).

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significance. An extended discussion of how the CMC method predicts extinction/reignition and how this may influence its accuracy is also presented. In the next section the formulation of the LES–CMC method is briefly covered and its numerical implementation is discussed. Particular emphasis is placed on modelling choices where more than one option is employed here. This is followed by results obtained using these choices with a discussion of them. The conclusions of this work are summarised in the last section of the paper.

2. Formulation

2.1. LES with CMC

In the CMC method the assumption is made that while reactive scalar values might fluctuate strongly, their fluctuations about a value conditionally averaged on the value of some conserved scalar will be small. Hence the fluctuations of all reactive scalars can be related to that of a conserved scalar, usually mixture fraction in non-premixed combustion. Transport equations for the conditional averages are solved on a grid considerably coarser than that used for the LES. The required scalars for the LES code are then found by using their conditional average and a local mixture fraction PDF. In this paper we examine the ability of LES–CMC to predict localised transient extinction and re-ignition events within a turbulent non-premixed flame.

The LES–CMC code developed in Triantafyllidis et al. (2009) and Triantafyllidis and Mastorakos (2010) and used in Garmory and Mastorakos (2011) and Ayache and Mastorakos (2012) has been employed here. Filtering the governing equations for the flow yields equations for filtered mass

$$\frac{\partial \bar\rho}{\partial t} + \frac{\partial(\bar\rho\tilde u_i)}{\partial x_i} = 0 \tag{1}$$

momentum

$$\frac{\partial(\bar\rho\tilde u_i)}{\partial t} + \frac{(\bar\rho\tilde u_i\tilde u_j)}{\partial x_i} = -\frac{\partial\bar p}{\partial x_j} + \frac{\partial\tilde\tau_{ij}}{\partial x_i} - \frac{\partial\left(\bar\rho\tau^r_{ij}\right)}{\partial x_i} \tag{2}$$

and a conserved scalar, mixture fraction, ξ,

$$\frac{\partial(\bar\rho\tilde\xi)}{\partial t} + \frac{(\bar\rho\tilde\xi\tilde u_i)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\bar\rho(D+D_t)\frac{\partial\tilde\xi}{\partial x_i}\right) \tag{3}$$

The term τ^r_{ij} in Eq. (1) is the sub-grid scale stress tensor and is modelled by the dynamic Smagorinsky (Germano et al., 1991). In Eq. (3) a gradient model has been used to model the sub-grid scale flux $\widetilde{u_i\xi} - \tilde u_i\tilde\xi = -D_t\partial\tilde\xi/\partial x_i$. $D_t = \nu_t/\mathrm{Sc}_t$ is the turbulent diffusivity, and $\mathrm{Sc}_t = 0.7$ is the turbulent Schmidt number, assumed here to be constant (Branley and Jones, 2001). It is also necessary to obtain the sub-grid scale variance of the mixture fraction. Here this has been done by assuming a gradient type model:

$$\widetilde{\xi''^2} = C_V\Delta^2\frac{\partial\tilde\xi}{\partial x_i}\frac{\partial\tilde\xi}{\partial x_i} \tag{4}$$

C_V is a constant whose value is determined dynamically according to Cook and Riley (1994) and Pierce and Moin (1998). Δ represents the grid spacing or filter width.

When the CMC model (Klimenko and Bilger, 1999) is used, equations are solved for the conditionally filtered reactive scalars, in a non-premixed case it is natural that the conditioning be done on ξ. The filtered value of the variable f can then be obtained by integration over η-space (Triantafyllidis et al., 2009):

$$\tilde f = \int_0^1 \widetilde{f|\eta}\;\widetilde{\mathcal{P}}(\eta)\,d\eta \tag{5}$$

Table 1
Summary of LES grids.

LES grid	Overall dimension (radial × axial)	Total cells
Coarse	20D × 80D	1.3 M
Fine	20D × 40D	2 M

We assume here that $\widetilde{\mathcal{P}}(\eta)$ has a β-function shape, which can be calculated based on the $\tilde\xi$ and $\widetilde{\xi''^2}$.

The CMC equations can be derived by filtering the transport equations for the reactive scalars Y_α (Navarro-Martinez et al., 2005). Using the primary closure assumption, the CMC equation becomes

$$\frac{\partial Q_\alpha}{\partial t} + \widetilde{u_i|\eta}\frac{\partial Q_\alpha}{\partial x_i} = \widetilde{N|\eta}\frac{\partial^2 Q_\alpha}{\partial\eta^2} + \widetilde{\omega_\alpha|\eta} + e_f \tag{6}$$

where $Q_\alpha = \widetilde{Y_\alpha|\eta}$ is the conditionally filtered reactive scalar, $\widetilde{u_i|\eta}$ is the conditionally filtered velocity, $\widetilde{N|\eta}$ is the conditionally filtered scalar dissipation rate, $\widetilde{\omega_\alpha|\eta}$ is the conditionally filtered reaction rate, while the term

$$e_f = -\frac{1}{\bar\rho\;\widetilde{\mathcal{P}}(\eta)}\frac{\partial}{\partial x_i}\left[\bar\rho\widetilde{\mathcal{P}}(\eta)\;\left(\widetilde{u_iY_\alpha|\eta} - \widetilde{u_i|\eta}Q_\alpha\right)\right] \tag{7}$$

is the sub-grid scale conditional flux and accounts for the conditional transport in physical space.

In this work the conditional scalars are the mass fractions of chemical species plus absolute enthalpy. This means a conditional temperature equation does not need to be solved as it can be determined from absolute enthalpy and species composition. All the species are assumed to have equal diffusivities and the Lewis number is assumed to be equal to one. A gradient model is used for the sub-grid scale conditional flux $\widetilde{u_iY_\alpha|\eta} - \widetilde{u_i|\eta}Q_\alpha = -D_t\frac{\partial Q_\alpha}{\partial x_i}$ (Navarro-Martinez et al., 2005). This model has given reasonable results in problems with significant spatial gradients of the conditional averages in LES of ignition (Triantafyllidis et al., 2009). Eq. (6) without spatial transport terms and with a prescribed $\widetilde{N|\eta}$ has also been solved to give reference “laminar flamelet” solutions, denoted as “0D-CMC”, and for initialisation.

The terms $\widetilde{u_i|\eta}$ and $\widetilde{N|\eta}$ are unclosed and require modelling. The simple assumption that the conditional velocity is equal to the unconditional is made here, $\widetilde{u_i|\eta} = \tilde u_i$. The accuracy of this assumption is clearly open to question, however there appears to be no

Table 2
Summary of CMC grids.

CMC grid	Cross jet cells	Axial spacing
CMC 1	23 × 23	3 mm Until 3 jet diameter then successive ratio of 1.3.
CMC 2	23 × 23	Constant spacing of 7.2 mm. (y/D = 1) up to y/D = 15

Table 3
Modelling choices for simulations. For CMC boundary, ‘standard’ refers to burning flamelets only in the pilot and inert in jet and co-flow, ‘Option’ refers to burning flamelets at all inlet nodes.

Case	D1	D2	F1	F2	F3	F4	F5
Flame	D	D	F	F	F	F	F
LES grid	C	F	C	C	C	C	C
Convection	TVD	TVD	TVD	UDS	TVD	UDS	UDS
CMC grid	1	1	1	1	2	1	1
CMC boundary	S	S	S	S	S	O	S
Velocity (m/s)	99	99	99	99	99	99	119