Available online at www.sciencedirect.com
SCIENCE DIRECT®
Proceedings of the Combustion Institute 30 (2005) 911–918
Proceedings of the Combustion Institute
www.elsevier.com/locate/proci

Simulations of turbulent lifted jet flames with two-dimensional conditional moment closure

I.S. Kim, E. Mastorakos*

Hopkinson Laboratory, Department of Engineering, University of Cambridge, Trumpington Street, Cambridge, CB2 1PZ, UK

Abstract

Simulations of H_2 air lifted jet flames are presented, obtained in terms of two-dimensional, first-order conditional moment closure (CMC). The unsteady CMC equation with detailed chemistry is solved without the need for operator splitting, while the accompanying flow field is determined using commercial CFD software employing a $k - \varepsilon$ turbulence model. Computed lift-off heights and Favre-averaged species mole fractions are found to be very close to values obtained experimentally for a wide range of jet velocities and fuel–air mixtures. Simulations for which the initial condition is an attached flame and the jet velocity gradually increased do not result in lift-off, a result fully consistent with experimental observation and capturing the hysteresis behaviour of lifted flames. The stabilisation mechanism is explored by quantifying the balance of terms comprising the CMC in the lift-off region. In line with experimental data, it is found that the scalar dissipation rate at the stabilisation height is well below the extinction value, and that axial transport and molecular diffusion play a major role. The radial components of spatial convection and diffusion are always small, fully justifying the alternative approach of employing a cross-stream averaged CMC.

Keywords: Conditional moment closure; Lifted turbulent flames; Stabilisation

1. Introduction

Turbulent lifted jet flames involve a complex balance between convection, diffusion, and chemistry, and hence present a considerable challenge to combustion models. Many experimental and numerical results have aimed to clarify the stabilisation mechanism of the lifted flame [1–3]. The premixed flame propagation model by Vanquickenborne and van Tiggelen [4] assumes that there is a fully premixed mixture before burning and that the flame is stabilised at a position where the mean flow velocity along the stoichiometric contour is equal to the turbulent burning velocity. Peters and Williams [5] argued that the amount of premixing at the molecular level is not sufficient and proposed that flamelet extinction by excessive strain rate occurred close to the nozzle. In another approach, the strain rate in large-scale turbulent structures caused extinction of the flame, and a Damköhler number criterion was used to predict lift-off height [6].

More detailed modelling, originally using non-premixed flamelets only [7], and later including partial premixing [8,9] and detailed chemistry, showed an increasingly good agreement with experimental data. Bradley et al. [10] used a

* Corresponding author. Fax: +44 (0)1223 332662.
E-mail address: em257@eng.cam.ac.uk (E. Mastorakos).

1540-7489/$ - see front matter
doi:10.1016/j.proci.2004.08.039

mixedness–reactedness model and accurately predicted lift-off heights of hydrocarbon flames, while Ma et al. [11] extended the modelling to include radiation, which was found to be important. Direct numerical and large eddy simulations support the concept that a triple flame exists at the base of the lifted flame [12–14], consistent with experimental data [15,16]. It is evident therefore that significant advances have been made in our capability to model lifted flames.

Recently, lifted turbulent flames have also been examined by Devaud and Bray [17] with the conditional moment closure (CMC) model. In this work, the first-order CMC approach included the spatial convection and diffusion terms, but cross-stream averaging was performed following [18], so that the conditional averages were predicted to depend only on the axial distance. A very good agreement with experimental data was found. In attached turbulent non-premixed jet flames, the homogeneous version of CMC (i.e., without any spatial transport terms) has produced very accurate results [19–21]. Two-dimensional first-order CMC calculations have been performed for autoignition problems [22–24] and bluff-body flames [25]. Devaud et al. [26] developed a two-dimensional formulation for methane flames, but no detailed analysis of the differences between cross-stream averaged CMC and two-dimensional CMC was given. Second-order effects are thought to be important for extinction and ignition [27–30], and should, in principle, be included for lifted flame stabilisation. Double-conditioning could also be used, but has not been tested yet for realistic problems [31], while a formulation including premixed flames could also be developed [32]. In practice, it is important to examine the degree of success of the simpler and computationally faster first-order conventional CMC model, but with multi-dimensional spatial transport.

In the present paper, we revisit the problems simulated by Devaud and Bray [17]. Two-dimensional CMC simulations of turbulent lifted jet flames of hydrogen with a wide range of jet velocities and dilutions are performed to explore lift-off height and to understand better the stabilisation mechanism. In the next section, the model and numerical methods are presented, which is followed by a detailed discussion of the results. The paper ends with a summary of the main conclusions.

2. Model formulation and method of solution

2.1. CMC model

A conservation equation for the conditional mean of a reactive scalar is given in [18,33,34] and for the temperature (rather than enthalpy) in [23]. The conditionally averaged mass fraction of species α and the temperature T are defined as $Q_\alpha(\eta,x,t) = \langle Y_\alpha(x,t)|\xi(x,t)=\eta\rangle$ and $Q_T(\eta,x,t) = \langle Y_T(x,t)|\xi(x,t)=\eta\rangle$, where ξ is the mixture fraction, η is the sample space variable for the conserved scalar, and $\langle\cdot|\xi=\eta\rangle$ denotes the ensemble averaging subject to the condition that $\xi=\eta$; in short $Q_\alpha = \langle Y_\alpha|\eta\rangle$. The governing equation for the conditional species mass fractions and temperature can be written as

$$\frac{\partial Q_\alpha}{\partial t} = -\langle u_i|\eta\rangle\frac{\partial Q_\alpha}{\partial x_i} + \langle N|n\rangle\frac{\partial^2 Q_\alpha}{\partial \eta^2} - \frac{1}{\bar{\rho}\tilde{P}(\eta)}\frac{\partial}{\partial x_i}\left(\langle u_i'' y_\alpha''|\eta\rangle\bar{\rho}\tilde{P}(\eta)\right) + \langle \dot{w}_\alpha|\eta\rangle \quad (1)$$

and

$$\frac{\partial Q_T}{\partial t} = \underbrace{-\langle u_i|\eta\rangle\frac{\partial Q_T}{\partial x_i}}_{T_{cv}} + \underbrace{\langle N|n\rangle\frac{\partial^2 Q_T}{\partial \eta^2}}_{T_{m_1}} + \underbrace{\langle N|n\rangle\left[\frac{1}{\langle C_P|\eta\rangle}\left(\frac{\partial\langle C_P|\eta\rangle}{\partial\eta} + \sum_{\alpha=1}^{n} C_{P,\alpha}\frac{\partial Q_\alpha}{\partial\eta}\right)\right]\frac{\partial Q_\alpha}{\partial\eta^2}}_{T_{m_2}} \times \underbrace{\frac{1}{\bar{\rho}\tilde{P}(\eta)}\frac{\partial}{\partial x_i}\left(\langle u_i'' T''|\eta\rangle\bar{\rho}\tilde{P}(\eta)\right)}_{T_d} + \underbrace{\frac{\langle\dot{w}_H|\eta\rangle}{\langle\rho|\eta\rangle\langle C_P|\eta\rangle}}_{T_c}, \quad (2)$$

respectively. In Eq. (2), the T_{cv} and T_d terms are for spatial convection and diffusion, and T_{m_1} and T_{m_2} correspond to molecular diffusion (i.e., mixing in mixture fraction space). Pressure is assumed constant, and hence the pressure work term is neglected. The chemical source terms in Eqs. (1) and (2) are closed at first-order, i.e.,

$$\langle\dot{w}_\alpha|\eta\rangle = \dot{w}(Q_\alpha, Q_T, P); \quad \langle\dot{w}_H|\eta\rangle = -\sum_{\alpha=1}^{N} h_\alpha\langle\dot{w}_\alpha|\eta\rangle \quad (3)$$

with h_α the absolute enthalpy. The conditionally averaged specific heat capacity and density are given by $\langle C_P|\eta\rangle\sum_{\alpha=1}^{N} C_{P,\alpha}Q_\alpha$ and $\langle\rho|\eta\rangle = (P\overline{M})/(RQ_T)$ with $\overline{M}$ the mean molecular mass. The conditional turbulent fluxes and conditional velocity are important in the present 2-D formulation, as they are expected to affect the stabilisation height where the gradients of the conditional averages are strong. Here, we used the conventional modelling from [18] that gives:

$$\langle u_i''\phi''|\eta\rangle = -D_t\frac{\partial Q_\phi}{\partial x_i}$$
$$\langle u_i|\eta\rangle = \tilde{u}_i - \frac{D_t}{\widetilde{\xi''^2}}\frac{\partial\tilde{\xi}}{\partial x_i}(\eta - \tilde{\xi}) \quad (4)$$

with the turbulent diffusivity defined as $D_t = \nu_t/Sc_t$, where ν_t and Sc_t denote, respectively, the turbulent viscosity coming from the $k-\varepsilon$ model and the turbulent Schmidt number taken as 0.7.