15th Australasian Fluid Mechanics Conference
The University of Sydney, Sydney, Australia
13-17 December 2004

Application of Transport PDF Approach for Modelling MILD Combustion

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Abstract

A transport PDF (TPDF) approach was used for modelling turbulent non-premixed Methane/Hydrogen (1/1 by volume) flames issuing from a jet in hot, oxygen-diluted coflow. A comparison between the TPDF results and detailed experimental data of ξ, temperature, major species and OH is presented for flames with different oxygen level in the hot coflow (oxygen mass-fraction of 6%, and 3%). Results from a previous study using the eddy-dissipation concept (EDC) solver, is also presented. A comparison in performance between the TPDF and EDC models is presented.

Introduction

In moderate and intense low-oxygen dilution (MILD) Combustion [2,17], fuel is mixed with highly diluted and heated air to create a distributed reaction zone with a reduced peak temperature. Attractive features of these flames include a semi-uniform temperature field, higher radiation flux and low emission of pollutants. Whilst MILD combustion can be classified as non-premixed jet flames, studies of diffusion flames cannot be directly extended to characterise MILD combustion. This is because most studies of non-premixed flames are conducted in cold air surroundings. Although the concept of MILD combustion has been extensively studied experimentally [5,6,10,11], mathematical modelling of this regime has received relatively little attention [4,7,9]. At first glance this regime seems relatively straightforward to model as it does not feature high-density gradients and complex turbulence-chemistry interactions processes, which are prominent in conventional turbulent jet flames. However, the conditions of elevated and uniform temperature distribution and low oxygen concentration in MILD regime, lead to slower reaction rates and enhances the influence of molecular diffusion on flame characteristics. These two effects in particular challenge the applicability of simple combustion models that assume fast chemistry and neglect the effects of differential diffusion.

Motivation

In a previous study [3] the authors used Reynolds-Averaging Navier-Stokes (RANS) approach to model the flow, compositions and temperature fields of a fuel jet issuing into a hot, oxygen-diluted coflow. That study focused on modelling Jet in Hot Coflow (JHC) flames measured by Dally et al. [5], and examined the effects of various combustion and turbulence models, chemical kinetics mechanisms, thermal radiation and differential diffusion, on the accuracy of the predictions. It was shown [3] that the standard k-ε turbulence model with a modified dissipation equation constant ($C\varepsilon_1$) provided the best agreement with the experiment. Differential diffusion effects were found to have a strong influence on the accuracy of the predictions and therefore should always be accounted for. It was also found that conserved scalar based models, i.e. the ξ/PDF and flamelet models, are inadequate for modelling jet in hot coflow (JHC) flames. The representation of the chemistry in the model was also found to play an important role in accurately predicting flame characteristics. Using detailed chemical kinetics , rather than global or skeletal mechanisms, with the eddy-dissipation concept (EDC) model was found to improve the accuracy significantly. In general, the EDC model performed reasonably well for flames with higher O_2 concentration in the hot coflow, such as flames with 9% O_2 and 6% O_2. The agreement with the measurements however was poor for the 3% O_2 case. However, the largest discrepancy was noted at the 120mm axial location where the model did not perform well, particularly for 3% and 6% cases. This is due to the intermittent localised flame extinction that the EDC model could not capture. This paper is an extension of our previous study [3] and focuses on examining the performance of transport PDF (probability density function) approach in modelling JHC flames.

Model Description

The numerical model constructed for this study is based on the geometry and dimensions of the experimental JHC burner used by Dally et al. [5], which is designed to emulate the MILD combustion regime. The details of the burner geometry, computational domain, boundary and inlet conditions, and convergence criteria are presented in Ref. [3,5] and are not repeated here. The flames of interest that were modelled here composed of Methane/Hydrogen (1/1 by volume), issuing into a hot coflow with species composition as shown in Table1.

Test Case	YO_2 %	YN_2 %	YH_2O %	YCO_2 %
1	3	85	6.5	5.5
2	6	82	6.5	5.5

Table 1. Species composition in the hot coflow. The jet Reynolds number is approximately 10,000 and the nominal fuel jet and coflow temperatures are 305K and 1300K, respectively.

Composition Transport PDF Model

In the RANS approach species equations are Reynolds-averaged, which leads to unknown terms for the turbulent scalar flux and the mean reaction rate. The turbulent scalar flux is modelled by gradient diffusion, treating turbulent convection as enhanced diffusion. The mean reaction rate is modelled by the finite-rate EDC model. Since the reaction rate is invariably highly non-linear, modelling the mean reaction rate in a turbulent flow is difficult and prone to error. An alternative to Reynolds-averaging the species and energy equations is to derive a transport equation for their single-point, joint PDF. This PDF, denoted by *P*, can be considered to be proportional to the fraction of the time that the fluid spends at each species, temperature, and pressure state. By solving this transport PDF equation, any thermochemical moment (e.g., mean or RMS temperature, mean reaction rate) can

be easily computed. The composition PDF transport equation [12] is derived from the Navier-Stokes equations as:

$$\frac{\partial}{\partial t}(\rho P)+\frac{\partial}{\partial x_i}(\rho u_i P)+\frac{\partial}{\partial \psi_k}(\rho S_k P)=-\frac{\partial}{\partial x_i}[\rho\langle u_i^{"}|\psi\rangle]+\frac{\partial}{\partial \psi_k}\left[\rho\left\langle\frac{1}{\rho}\frac{\partial J_{i,k}}{\partial x_i}\middle|\psi\right\rangle P\right] \quad (1)$$

where P is the Favre joint PDF of composition, ρ is the mean fluid density, u_i is the Favre mean fluid velocity vector, S_k is the chemical reaction rate for species k, ψ is the composition space vector, $u"_i$ is the fluid velocity fluctuation vector, and $J_{i,k}$ is the molecular diffusion flux vector. The notation of <...> denotes expectations, and <A|B> is the conditional probability of event A, given the event B occurs. In Equation (1), the terms on the left-hand side are closed, while those on the righthand side are not and require modelling. The first term on the left-hand side is the unsteady rate of change of the PDF, the second term is convection by the mean velocity field, and the third term is the reaction rate. The principal strength of the PDF transport approach is that the highly non-linear reaction term is completely closed and requires no modelling. The two terms on the right-hand side represent scalar convection by turbulence (turbulent scalar flux), and molecular mixing/diffusion, respectively.

Molecular mixing of species and heat was modelled using the Euclidean Minimum Spanning Tree (EMST) model [15]. Physically, mixing occurs between fluid particles that are adjacent to each other. The Modified Curl and IEM (interaction by exchange of momentum) mixing models take no account of this localness, which can be a source of error. The EMST model mixes particle pairs that are close to each other in composition space. The particle pairing is determined by an EMST, which is the minimum length of the set of edges connecting one particle to at least one other particle. The EMST mixing model is more accurate than the Modified Curl and IEM mixing models, but incurs a slightly greater computational expense.

The transport PDF (TPDF) equation is solved using a Monte Carlo method, which is ideal for high-dimensional equations since the computational cost increases linearly with the number of dimensions. The disadvantage is that statistical errors are introduced, and these must be carefully managed. The Monte Carlo algorithm involves notional particles that move randomly through physical space due to particle convection, and also through composition space due to molecular mixing and reaction. For the representation of the chemistry into the TPDF model, a GRI2.11-based augmented reduced mechanism (ARM) kinetics [16] is used. To reduce computational cost of time-integration of chemical reactions, the ISAT (*is-situ* adaptive tabulation) model of Pope [13], is used**.**

Results

Calculations were performed for the 6% and 3% O_2 flames using the FLUENT6 package [8]. For comparison purposes the modelling results obtained using the EDC model [3] are also presented here. It is worth noting that in the EDC model the GRI3.0[14] kinetics mechanism was used. This use of different mechanism is not expected to have any effect on the conclusions drawn from this study. The computational expense of using GRI3.0 with the TPDF is prohibitive. Due to space constraints only sample of the results are presented, and plotted against mixture fraction (ξ) computed using Bilger's formulation [1].

Figure 1 shows comparison between measured and calculated mean temperature profiles at 120mm from the jet exit. The figure shows that for both the 3% and 6% O_2 flames, the TPDF model yields better agreement with the experiment than the EDC model. It predicts the peak temperature and its location (in ξ-space) more accurately than the EDC model. Similarly, the TPDF predictions of species e.g. OH and CO mass fraction are significantly closer to the experimental results than the EDC model, as shown respectively in Fig.2 and Fig.3. The figures also show that the EDC model tends to over-predict the peak values of temperature and mass fractions. This behaviour however is not erroneous; rather the EDC model tends to capture the peak values of the instantaneous measurements.

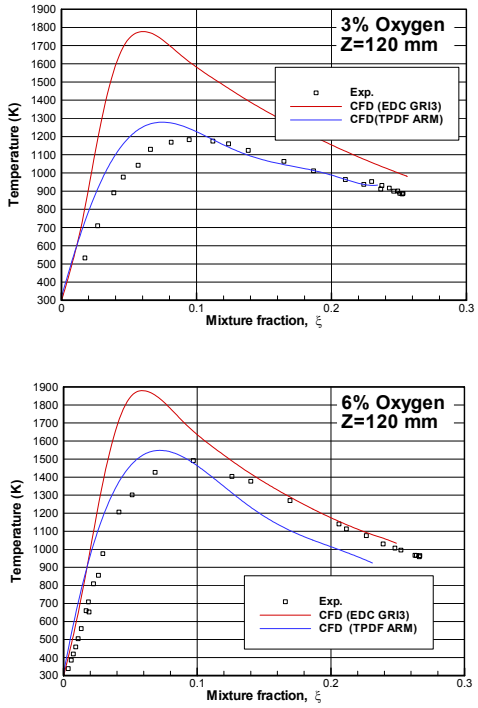

Fig. 1: A comparison between mean measured and calculated temperature at 120mm from the jet exit for 3% and 6% O2 flames.

It is worth mentioning that when using the Modified Curl or the IEM mixing models in the TPDF model, the flame has been completely blown off. A stable flame could only be achieved using a slightly adjusted EMST mixing model. It was necessary to increase the number of the randomly selected pairs of Monte Carlo particles at each iteration. The number of pairs (N_{pair}) is defined as

$$N_{pair}=\frac{1.5C_{\phi}N\Delta t}{\tau_t} \quad (2)$$

where N is the total number of particles in each computational cell, C_{ϕ} is an empirical mixing constant, and is τ_t is a turbulent time scale (for the k-ε turbulence model this is k/ε). It was necessary to increase the value of C_{ϕ} from the default value of 2 to 5 to stabilise the flame. Despite increasing the number of particles per cell from 20 to 40 particles, the solution was not significantly affected. To maintain low statistical error, 40 particles per cell were used in all the calculations (resulting of approximately 4 million particles been tracked at each iteration).

The results in Figs. 1-3 show that the 6% O_2 flame produces higher CO levels than the 3% O_2 flame. This is an unexpected behaviour since higher O_2 in the coflow stream is expected to yield higher conversion of CO into CO_2. Similar trends were also observed in laminar MILD flame measurements and calculations (not presented). It is believed that at MILD combustion conditions the current chemical pathways of CO conversion into

CO_2 do not hold, and a different kinetics mechanism might be required. This issue is beyond the scope of this paper.

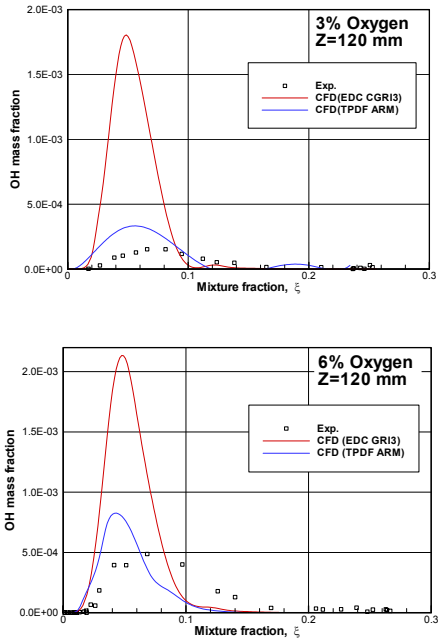

Fig. 2: A comparison between mean measured and calculated OH mass fraction at 120mm from the jet exit for 3% and 6% O2 flames.

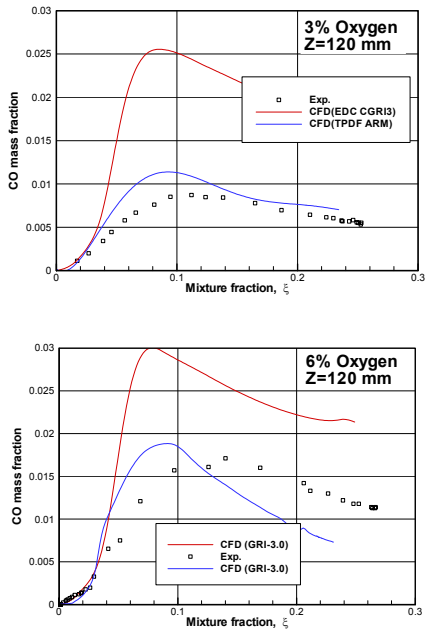

Fig. 3: A comparison between mean measured and calculated CO mass fraction at 120mm from the jet exit for 3% and 6% O2 flames.

Considering that the EDC model is based on Reynolds averaging and it does not resolve the fluctuations in mixture fraction, it cannot therefore account for the bias in mean profiles due to localised extinction or intermittency. The TPDF model on the other hand contains a complete statistical representation for each species (mean, RMS and higher moments), therefore it resolves scalar fluctuations and hence its mean predictions are closer to the measured values. Figure 4 illustrates this point clearly; showing the EDC biased tendency towards peak values while the TPDF model is closer to the (mean) measured values.

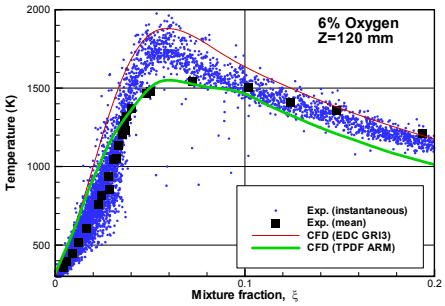

Fig. 4: A comparison between instantaneous and mean measured and calculated temperature at 120mm from the jet exit for 6% O2 flame.

Interestingly, the performance of the TPDF model at upstream axial locations of 30mm and 60mm from the jet exit was not accurate. The TPDF predictions at these locations were either comparable to or slightly better than the EDC model. The majority of the TPDF results at the upstream locations tend to under-predict the temperature and species concentration. This is clearly illustrated in Fig. 5, which shows profiles of H_2O mass fraction at 60mm for 3% and 6% O_2 flames.

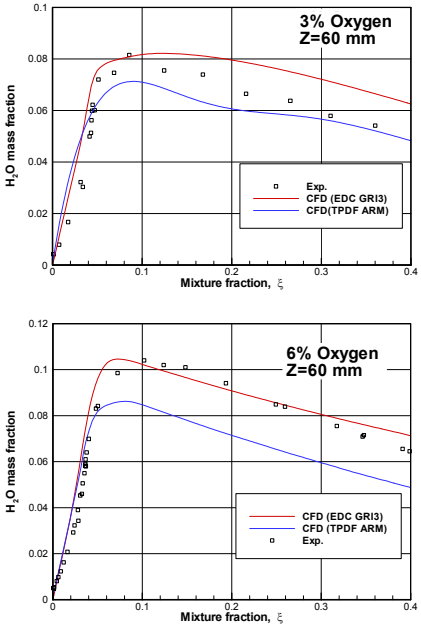

Fig. 5: A comparison between mean measured and calculated H_2O mass fraction at 60mm from the jet exit for 3% and 6% O2 flames.

Whilst the TPDF peak OH prediction is better than that of the EDC, it is still off by a factor of four from the peak-measured value for the 3% O_2 case. This is illustrated in Fig. 6, which indicates that the flame is not anchored close to the jet exit plane. Figure 7 is a contour plot of OH mass fraction for the 3%O_2 case, showing the flame-stabilisation location at approximately 120mm from the jet exit.

Although similar observation was noted in the experiment, neither model was accurate enough in predicting the flame-stabilisation distance. The experimentally observed distance was only of a few jet-diameters (~10mm), whilst the model shows a distance of ~30 jet-diameter.

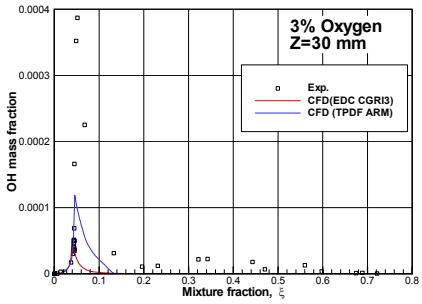

Fig. 6: Profiles of mean OH mass fraction at 30mm from the jet exit for 3% flame.

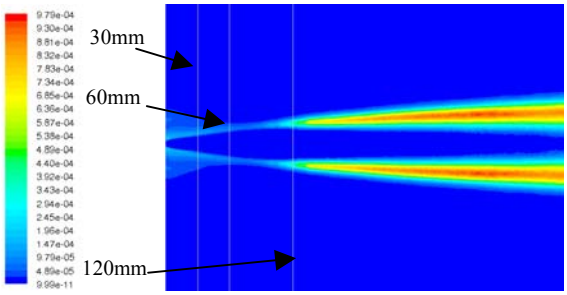

Fig. 7: Contours of mean OH mass fraction for the 3% flame showing the location of flame stabilisation above the jet exit plane.

Conclusions

For the 3% and 6% O_2 flames the TPDF model is proved more accurate than the EDC model, particularly at 120mm. This conclusion however does not extend to the TPDF performance at upstream locations of 30mm and 60mm, where both models have comparable accuracy. Considering that turbulent mixing is predicted accurately (see Ref [3]), and that oxidation of the fuel is represented in the TPDF model by the best available kinetics mechanism, we can only speculate (at this stage) on possible causes for these discrepancies. One possibility is that the TPDF model is highly sensitive to fluctuations in velocity field, which the current turbulence model may not be resolving accurately. One suggestion to assess this assumption is to model the JHC flames using a joint velocity-composition transport PDF approach. Another possible contributing factor is that for low-oxygen concentration flames the molecular mixing becomes extremely sensitive to composition fluctuations that even the EMST model is unable to reflect/capture accurately. This assumption is based on the fact that the TPDF prediction is reasonably accurate in the downstream location (120mm). 'Leakage' of high-concentration oxygen from the outer shroud air into the oxygen-diluted region, maybe reducing the sensitivity of molecular mixing to variations in compositions.

Accurately predicting flame-stabilisation location in JHC combustion remains a modelling challenge. Whilst the TPDF results are encouraging, establishing a model that can accurately predict JHC flames across the entire combustion domain remains a challenge.

Acknowledgement

The authors thank Dr Graham Goldin from Fluent Inc. for his valuable suggestions.

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