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Parametric study of EDC model constants for modelling lifted jet flames in a heated coflow

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Abstract

Moderate or Intense Low oxygen Dilution (MILD) combustion offers improved thermal efficiency and a reduction of NO_x pollutants and soot emissions compared to conventional combustion. Previously MILD combustion in the Jet in Hot Coflow (JHC) burner, using methane-based fuels, has been simulated with the Eddy Dissipation Concept (EDC) turbulence-chemistry interaction model. In this paper, the EDC model is used with a modified standard *k*-*ε* (SKE) turbulence model to simulate an ethylene-nitrogen flame in a hot, 9% O_2 coflow. Modifications to the parameters used in the EDC model are investigated and a parametric study of C_τ and C_ξ is undertaken. The combination of C_τ=3 and C_ξ=1, modified from the default C_τ=0.4082 and C_ξ=2.1377 used in the original model, shows better agreement with experimentally measured radial profiles than any previous implementation of the EDC model and replicates the visually lifted properties observed experimentally in this configuration which have not been modelled successfully in the past.

Keywords: RANS, EDC, Eddy Dissipation Concept, Combustion, Jet in Hot Coflow, JHC, MILD Combustion

1. Introduction

Moderate or Intense Low oxygen Dilution (MILD) combustion is a particular combustion regime which offers improved thermal efficiency and reduction of nitrogen oxides pollutants and soot [1]. This facilitates lower fuel consumption and cleaner exhaust gases. MILD combustion is achieved by recirculating hot combustion products back into the flame front. The result is a distributed, homogeneous reaction zone, minimising peak flame temperatures and reducing pressure variations. Under these conditions, the Damköhler number (Da) is near unity in the reaction region [2], such that both chemical and turbulence time scales are important.

A number of experimental studies into the mechanics of the MILD combustion regime have been performed by emulating hot, recirculated combustion products with the use of a secondary burner. Although for lifted flame studies rather than MILD combustion, the Vitiated Coflow Burner (VCB or, alternatively, the Cabra burner), features a central fuel jet emanating downstream of an unenclosed, concentric perforated plate burner [3]. Experimental data from 33%/67% CH_4/air mol/mol and 25%/75% H_2/N_2 mol/mol fuel mixtures in a 15% O_2 mol/mol coflow has been used for verification of numerous CFD models. These modelling efforts have utilised either Reynolds averaged Navier-Stokes (RANS) turbulence or large eddy simulations (LES) models and various chemistry-turbulence interaction models to understand the flows in the limited number of fuel cases.

The Jet in Hot Coflow (JHC) burner was developed independently of the VCB at the University of Adelaide specifically for achieving simplified MILD combustion conditions, and is described in [4]. The JHC features a 4.6mm diameter central jet, which is over 100 diameters long, ensuring fully-developed pipe flow. The jet issues into a 82mm diameter concentric coflow of combustion products from an upstream secondary burner and has been used to provide experimental data for numerous fuel and Reynolds number combinations [4-7]. Visually lifted flames have been observed in the JHC for ethylene (C_2H_4) based fuel streams with a jet Reynolds number of 10,000 in a 9% mol/mol hot coflow [7]. Although the C_2H_4, C_2H_4/air and C_2H_4/N_2 fuelled jet flames appear lifted under these conditions, reactions occur near the jet exit, with formaldehyde (CH_2O) and hydroxyl radicals (OH) species having been measured. This burner also provided the basis for the Delft JHC burner (DJHC), which has been subject to independent experimental and computational research.

Numerous efforts have been made to use RANS [8-11] and LES [12] models of the JHC and, to a lesser extent, the DJHC [13], focussing on fuel CH_4/H_2 cases. The findings of these studies have led to the recent modelling effort of the more complex C_2H_4-based fuel experiments [14]. This investigation found best agreement with the experimental results of [7] using the modified standard *k*-ε (SKE) turbulence model of [15]. This modification consists of adjusting the parameter $C_{1\varepsilon}$ from the FLUENT default value 1.44 to 1.6 to compensate for the cylindrical symmetry of the 2D computational domain [15]. The turbulence-chemistry interaction model found to be the most successful in [14], was a modified eddy dissipation concept (EDC) finite-rate reaction model with the parameter C_τ increased from 0.4082 to 3. The modification of C_τ was made in accordance with the findings of [8, 13], who found better agreement with higher values of C_τ compared to the default. The modified SKE and modified EDC model combination generally agreed well with the experimental data however, in most cases,

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the temperature distributions modelled downstream of the jet were in excess of those measured [14]. This modified EDC model was unable to predict the apparent lift-off height for any fuel case. The particle density function (PDF) modelling approach of [14] was, however, in good agreement with this apparent lift-off phenomenon, especially in the C_2H_4/N_2 fuel case.

Previous attempts to model combustion in JHC burners have used experimentally measured inlet profiles [13], assumed constant velocity across the inlet [8, 14] or modelled the jet and coflow exit profiles [9, 11]. Computationally modelled profiles used the internal dimensions of the JHC burner, in the absence of measured data. A previous set of simulations using CH_4/H_2 fuels in the JHC burner reported that the results of these models are insensitive to fuel boundary conditions. These flames did not, however, exhibit any lifted behaviour, in contrast to the C_2H_4/N_2 flames measured in [7]. The sole previous study modelling the C_2H_4 flames made the assumption of constant velocity profiles, although did not investigate any sensitivity to inlet boundary conditions [14].

In light of the above gaps, the aim of this paper is to systematically determine an approach for improving the performance of CFD modelling to capture lifted jet flame behaviour in a heated coflow using the ANSYS FLUENT 14.0 software package.

2. Model Development

2.1 Geometry

The computational domain for the JHC burner was chosen to be a two-dimensional rectangular region downstream of the jet plane exit. The geometry for this study was based on the computational domains of [10] and [14]. The 400mm (~85 jet diameters) downstream extent of this domain captures the entire MILD combustion regime, and sufficient flame length such that flame interaction with the domain exit will not influence the region of interest. The full length of the flame extends beyond the domain, however combustion in the downstream part of the flame is not in the MILD regime (because it is outside the potential core of the coflow) and thus not controlled. The computational domain was meshed with 53610 hex (quadrilateral) elements, following mesh independence studies for similar cases.

2.2 Boundary Conditions

The boundaries of the domain were a combination of walls, pressure outlets, velocity inlets and the axis of cylindrical symmetry through the centre of the coaxial jets. Pressure outlets specify the ambient surrounds to be simplified air, with 21% O_2 and 79% N_2 mol/mol, at zero gauge pressure and a temperature of 300K. Pressure outlets allow exchange between fluid in the domain and external air, conserving mass during simulations. The primary inlets in this domain are the fuel and coflow velocity inlets bounded by no-slip, adiabatic walls. The fuel stream enters the computational domain perpendicular to the velocity inlet boundary at 27.3m/s, 305K and zero gauge pressure was set to be 25% C_2H_4 and 75% mol/mol N_2, and the 2.3m/s, 1100K coflow was taken as 9% O_2, 3% CO_2, 78% N_2 and 10% H_2O mol/mol [7]. Inlet velocity profiles into the domain were assumed to take a uniform velocity, "top-hat" form across the inlets, with zero velocity at pipe walls. This was done for consistency with [14], numerical convergence speed [8] and a lack of information in the literature on the effects of inlet profiles on modelling C_2H_4/N_2 in MILD combustion.

2.3 The Standard k-ε Turbulence Model

The soot-free nature of MILD combustion [1] implies that radiation heat exchange between the region near the jet exit plane and the downstream flame is very low. The virtual independence of radiation model on the region near the jet exit has been confirmed by previous studies [9, 10, 14], and hence the most basic 'P1' radiation model was implemented to retain accuracy away from the jet at a minimal computational cost.

The modified SKE turbulence model was chosen for this investigation, having been verified in both reacting [8-11, 15] and non-reacting (as a verification model and, previously, in [15]) flow cases. This model is modified from the standard model by changing the common default value of $C_{1\varepsilon}$, in equations for scalar dissipation rate, from 1.44 to 1.6 for 2D axisymmetric flows [15]. This modified SKE turbulence model was hence used throughout this study.

2.4 The Eddy Dissipation Concept

The standard EDC chemistry-turbulence interaction model implemented in FLUENT 14.0, based on [16], and the modified EDC model of [14] were used for initial model parameters. The EDC model of [16] assumes the mean residence time, τ^*, of species i in a fine structure with length fraction ξ^* where:

$$\tau^* = C_\tau \left(\frac{\nu}{\varepsilon}\right)^{1/2} \tag{1}$$

and

$$\xi^* = C_\xi \left(\frac{\nu\varepsilon}{k^2}\right)^{1/4}, \tag{2}$$

where ν is the kinematic viscosity, ε the turbulent dissipation rate and k the turbulent kinetic energy. These values are then used to calculate the mean reaction rate of i, R_i, as:

$$R_i = \frac{\rho(\xi^*)^2}{\tau^*\left[1-(\xi^*)^3\right]}\left(Y_i^* - Y_i\right), \tag{3}$$

where ρ is the density of the fluid, and Y_i^* and Y_i are the mass fractions of i in the fine structure and computational cell, respectively. It is readily seen from

(3) that R_i is simply inversely proportional to τ^* and, hence, C_τ. Substituting (1) into (3) differentiating with respect to C_τ:

$$\frac{\partial R_i}{\partial C_\tau} = \frac{-R_i}{C_\tau}. \quad (4)$$

Equation (4) clearly shows that an increase in C_τ results in a direct decrease of R_i and, hence, an immediate reduction in Da in accordance with experimental observations of MILD combustion. The dependency of R_i on C_ξ is, however, far more complicated. This is seen by substituting (2) into (3) and taking the partial derivative of R_i with respect to C_ξ as shown in (5):

$$\frac{\partial R_i}{\partial C_\xi} = \left(\frac{2}{C_\xi} + \frac{3C_\xi^2 \left(\frac{v\varepsilon}{k^2}\right)^{3/4}}{\left[1 - C_\xi^3 \left(\frac{v\varepsilon}{k^2}\right)^{3/4}\right]} \right) R_i. \quad (5)$$

Equation (5) highlights the complex interplay and strong coupling between R_i, C_ξ and the flow variables v, ε and k. Modification of the C_ξ parameter therefore offers a more dynamic adjustment of R_i throughout the flow field, as opposed to the linear change due to C_τ.

The modified EDC model of [14] globally decreased R_i by a factor of 7.35 compared to the standard EDC due to increasing C_τ from 0.4082 to 3. For subsequent models, the parameter C_ξ was given the values 0.5, 0.75, 1, 1.5, 2.1377 (FLUENT default value) and 2.5, in combination with C_τ of 0.4082 and 3. This systematic approach allowed for the analysis of the effects of C_ξ on the accuracy of the EDC model in the case of the C_2H_4/N_2 jet in the JHC.

3. Results and Discussion

3.1 EDC Parametric Study

Numerical solutions were obtained for different combination of the EDC parameters C_τ and C_ξ using the ANSYS FLUENT 14.0 software package. The modelled flow fields were then simultaneously compared to radial profiles measured experimentally in [7], at a distance 35mm downstream of the jet exit plane. The plots, shown in Fig. **1**, indicate the effects of changing the EDC parameters on the resulting temperature and species profiles. It is clear from the radial temperature profile in Fig. **1**a) that the combination of C_τ=3 and C_ξ=1 (pink dashed line) best match the experimental measurements for peak temperature location and magnitude. The available experimental data does not describe absolute concentrations of formaldehyde, and thus all curves were normalised to the concentration given by the combination of C_τ=3 and C_ξ=1, having the best agreement in temperature distribution. These results in Fig. **1**b) show good agreement between the experimental profile of formaldehyde and that predicted with C_τ=3 and C_ξ=1, in both peak location and distribution beyond the peak. Similarly, Fig. **1**c) shows good prediction of the OH peak location: although the magnitude of the peak is over-predicted by a factor of three, this in fact represents a significant improvement on the standard EDC model. None of the C_τ, C_ξ combinations accurately captured the averaged OH distribution at the 35mm downstream location. It should be noted that the C_2H_4/N_2 flame in 9% O_2 coflow appears visually lifted 34mm downstream of the jet exit [7]. Within this region between the base of the blue flame and the jet exit plane, however, is a reaction zone featuring both formaldehyde and hydroxyl species in 'flameless' combustion [7] which has not previously been accurately modelled using RANS simulations. To describe the visible blue flame, characteristic of excited CH radicals [17], the visible flame was defined by the presence of CH in post-processing.

The computational results using each combination of C_τ and C_ξ were investigated for comparison with these experimental measurements of visual lift-off height. Of these cases, only the combinations of C_τ=3 and C_ξ=1, which showed the best agreement with profiles in Fig. **1**, and C_τ=0.4082 and C_ξ=1.5 (solid black line) exhibited apparent lift-off with a reaction region below the CH-defined, visible flame base. The C_τ=0.4082 and C_ξ=1.5 combination, however, significantly over-predicted the peak temperature and did not accurately model the radial peak location of either formaldehyde or hydroxyl species. The contours presented in Fig. 2 present the differences between the default

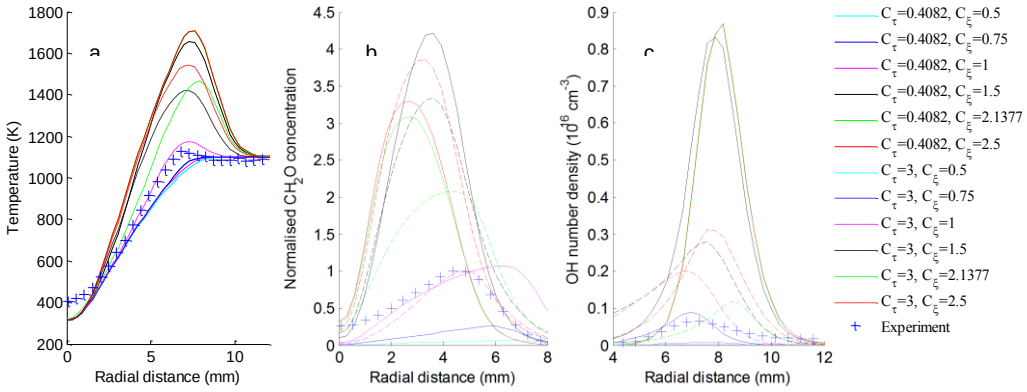

Fig. 1. Mean radial profiles of a) temperature (units K), b) normalised CH2O concentration and c) OH number density (units 10^{16}/cm^3) from a parametric EDC study results 35mm downstream of the jet exit plane for a C_2H_4/N_2 flame in a 9% O_2 coflow compared to experimental results [7].

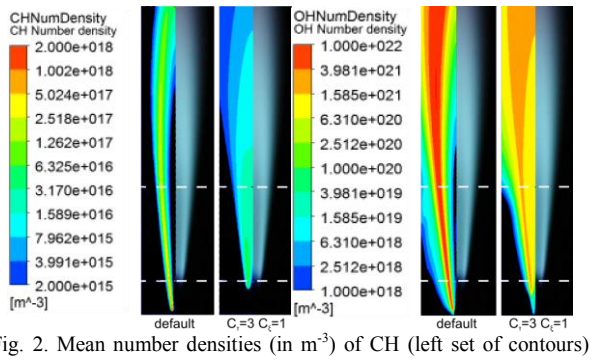

Fig. 2. Mean number densities (in m^{-3}) of CH (left set of contours) and OH (right set of contours) species near the jet exit, with a logarithmic scale spanning three and four decades respectively, alongside flame photographs [7]. Modelled using the EDC combustion model with default EDC parameters (left contours) and C_τ = 3 and C_ξ = 1 (right contours) for C_2H_4/N_2 fuel in a 9% O_2 coflow.

FLUENT EDC parameters, C_τ=0.4082 and C_ξ=2.1377, and the combination of C_τ=3 and C_ξ=1. This figure clearly shows the good agreement between the CH profile computed using C_τ=3 and C_ξ=1 and the optical measurement of apparent lift-off. Reactions are also evident below the visible flame base with low concentration of OH being produced, consistent with experimental measurements [7].

A previous modelling effort of the JHC justifies the modification of C_τ (inversely proportional to R_i from (1) and (3)) by stating that the homogeneity of the MILD reaction region invalidates the assumption that species do not react beyond the confines of fine structures, and that increasing residence times (through an increase in C_τ) acts to compensate for this [8]. Conceptually, decreasing the C_ξ parameter decreases the size of the fine structure reactions zones in the fluid model. Numerically, however, the fine structure volume fraction, ξ^{*3}, is inherently limited as it must be contained within a control volume, but is not a function of any variables specific to cell size. To ensure this, the fine structure volume fraction is limited to 0.755 of the cell volume by ANSYS FLUENT 14.0 as seen in Fig. 3. This represents a flaw in the EDC model of [16] in

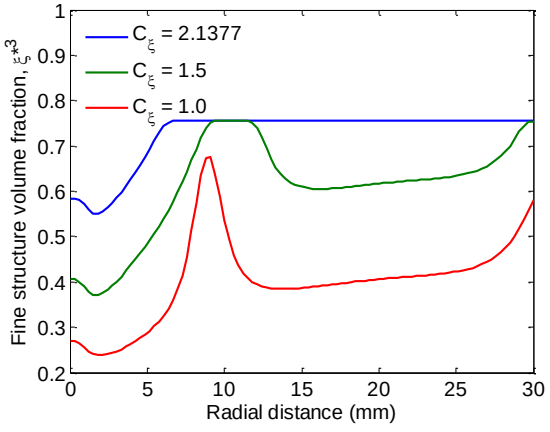

Fig. 3. Radial profiles of ξ^{*3}, 35mm downstream of the jet exit plane for three different values of C_ξ, with C_τ = 0.4082.

simulating flames for $v\varepsilon \sim k^2$ where the volume fraction is close to, or exceeds, one. This deficiency strengthens the argument of [8] that the analysis of fine structures in MILD jet flames using the same approach for conventional flames may be inappropriate.

The accuracy of simulations modelled with smaller interaction regions between species in the JHC, may be explained by viscous shear effects between the high Re jet and slow coflow streams limiting the interaction regions between the fuel and oxidiser. These limited interactions, combined with the low Da associated with the MILD combustion, could also justify longer time scales for fluid species encapsulated within these smaller fine structures. These attributes of the JHC may therefore explain the increased accuracy of the EDC model with the modifications of changing C_τ=0.4082 and C_ξ=2.1377 to C_τ=3 and C_ξ=1.

4. Conclusions

This paper has presented RANS CFD results of a lifted C_2H_4/N_2 jet flame issuing into a 9% O2 and 1100K coflow. The modification of the EDC model parameters C_τ and C_ξ from their default C_τ=0.4082 and C_ξ=2.1377 to C_τ=3 and C_ξ=1 results in better agreement between simulated and experimental results of OH, CH_2O and temperature profiles 35mm downstream of the fuel jet exit plane. Additionally, this combination of parameters predicts the visual lift-off, flameless combustion region which has been reported experimentally, but not successfully modelled in the past.

5. References

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