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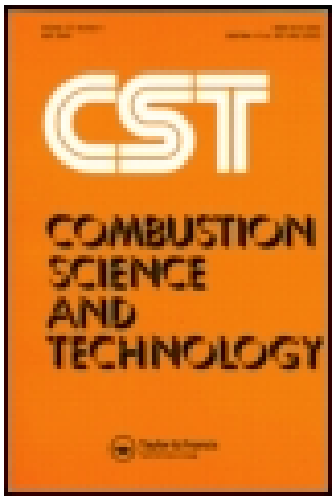

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Modelling Lifted Jet Flames in a Heated Coflow using an Optimised Eddy Dissipation Concept Model

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Abstract

Moderate or Intense Low oxygen Dilution (MILD) combustion has been established as a combustion regime with improved thermal efficiency and decreased pollutant emissions, including NO_x and soot. MILD combustion has been the subject of numerous experimental studies, and presents a challenge for computational modelling due to the strong turbulence-chemistry coupling within the homogeneous reaction zone. Models of flames in the Jet in Hot Coflow (JHC) burner have typically had limited success using the Eddy Dissipation Concept (EDC) combustion model, which incorporates finite-rate kinetics at low computational expense. A modified EDC model is presented which successfully simulates an ethylene-nitrogen flame in a 9% O_2 coflow. It is found by means of a systematic study that adjusting the parameters C_τ and C_ξ from the default 0.4082 and 2.1377 to 3.0 and 1.0 gives significantly improved performance of the EDC model under these conditions. This modified EDC model has

subsequently been applied to other ethylene-and methane-based fuel jets in a range of coflow oxidant stream conditions.

The modified EDC offers results comparable to the more sophisticated, and computationally expensive, transport probability density function (PDF) approach. The optimised EDC models gives better agreement with experimental measurements of temperature, hydroxyl (OH) and formaldehyde (CH_2O) profiles. The visual boundary of a chosen flame is subsequently defined using a kinetic mechanism for OH* and CH*, showing good agreement with experimental observations. This model also appears more robust to variations in the fuel jet inlet temperature and turbulence intensity than the standard EDC model trialled in previous studies. The sensitivity of the newly modified model to the chemical composition of the heated coflow boundary also demonstrates robustness and qualitative agreement with previous work. The presented modified EDC model offers improved agreement with experimental data profiles than has been achieved previously, and offers a viable alternative to significantly more computationally expensive modelling methods for lifted flames in a heated and vitiated coflow. Finally, the visually lifted flame behaviour observed experimentally in this configuration is replicated, a phenomenon which has not been successfully reproduced using the EDC model in the past.

Keywords: MILD Combustion, Turbulent Flames, Lifted Flames, JHC Burner, Eddy Dissipation Concept (EDC)

1. Introduction

The Moderate or Intense Low oxygen Dilution (MILD) combustion regime offers improved thermal efficiency and reduction of nitrogen oxides (NO_x) pollutants and soot, facilitating lower fuel consumption and cleaner exhaust gases (Cavaliere & de Joannon, 2004). A characteristic of the MILD regime is a distributed, homogeneous reaction zone, without flame temperature peaks and reduced pressure variations. Under these conditions, the Damköhler number (Da) is near unity in the reaction region (Galletti et al., 2007), indicating that both chemical and turbulence time scales are important in describing the MILD regime. A number of experimental studies into the mechanics of the MILD combustion regime have been performed using simplified jet flames in low oxygen, heated coflows. The Jet in Hot Coflow (JHC) burner, shown in Figure 1 and described by Medwell et al. (2007), consists of a central jet emanating into a coflow of combustion products. The 4.6 mm diameter central jet of the JHC burner, issues into an 82 mm diameter concentric coflow of combustion products from an up-stream secondary burner. The JHC burner has been used to provide experimental data for numerous fuel and Reynolds number combinations (Dally et al., 2002; Medwell et al., 2007, 2008; Medwell & Dally, 2012; Oldenhof et al., 2010, 2011, 2012), as has the similarly configured Vitiated Coflow Burner (VCB) (Cabra et al., 2002, 2005; Gordon et al., 2008).

Numerous computational studies of the JHC burner have been made using Reynolds averaged Navier-Stokes (RANS) modelling (Christo & Dally, 2005; Frassoldati et al., 2010; De et al., 2011; Aminian et al., 2011, 2012; Mar-dani et al., 2011, 2013; Gao et al., 2013; Wang et al., 2013) and large-eddy simulations (LES) (Ihme & See, 2011; Ihme et al., 2012; Afarin & Tabe-

jamaat, 2013; Kulkarni & Polifke, 2013), focussing on CH_4/H_2 fuel cases. Subsequent findings of these studies have been extended by recent modelling efforts of the more complex C_2H_4-based fuel experiments (Shabanian et al., 2013). This work, trialling a number of different turbulence and combustion models, found best agreement with the experimental results of Medwell et al. (2008) using the modified standard k - ε (SKE) turbulence model of Dally et al. (1998) and a modified eddy dissipation concept (EDC) finite-rate reaction model with the parameter C_τ increased from the default 0.4082 to 3 (Shaba-nian et al., 2013). The modified SKE and modified EDC model combination generally agreed well with the experimental data however, in most cases, the temperature distributions modelled downstream of the jet were in excess of those measured and the radial peaks in minor species distributions were not accurately predicted (Shabanian et al., 2013). These simulations also did not exhibit any lifted behaviour, in contrast to the C_2H_4-based flames measured by Medwell et al. (2008). The particle density function (PDF) modelling approach of Shabanian et al. (2013) was, however, in good agreement with this apparent lift-off phenomenon not captured by the computationally cheaper EDC model, especially in the C_2H_4/N_2 fuel case. The good agreement of PDF models with experimental measurements from the JHC is consistent with RANS modelling efforts of the VCB (Masri et al., 2003; Cabra et al., 2005; Cao et al., 2005; Gkagkas & Lindstedt, 2007; Gordon et al., 2007; Ren & Pope, 2009; Najafizadeh et al., 2013). In light of the limited success of the RANS-EDC models, the objective 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. The commercial FLUENT 14.0 code was adopted in the absence of any suitable alternative research code with similar capabilities, appropriate for

modelling turbulent flames in the MILD regime without requiring excessive customisation. The desire to develop the capabilities of RANS-EDC modelling of these flames is driven by the desire for reduced computational cost.

Flames in the transition to MILD combustion have been reported as appearing visually lifted in the JHC burner for ethylene (C_2H_4) based fuel streams (Medwell et al., 2008). Long exposure images of such flames, shown in Figure 2, demonstrate the apparent, visual lift-off of these transitional flames in comparison to MILD flames. Despite visually resembling lifted flames, laser diagnostic imaging has revealed the occurrence of reactions upstream of the apparent lift-off height, as evident by measurements of formaldehyde (CH_2O) and the hydroxyl radical (OH) (Medwell et al., 2008). This is the case for C_2H_4, C_2H_4/air and C_2H_4/N_2 fuelled jet flames with $\mathrm{Re}_{\mathrm{jet}} = 10,000$ in a 1100 K, 9% O_2 mol/mol coflow. Simplified one-dimensional modelling of these flames indicates that, despite the depleted oxygen concentration in the oxidant stream, under these conditions O_2 penetrates across the reaction zone to the fuel-rich side, which facilitates a radical pool build-up (Medwell et al., 2009). This observation is consistent with previous observations in similar lifted flames in a hot and vitiated coflow (Gordon et al., 2008). These flames present a particularly interesting test-case for investigating the finite-rate chemistry effects under depleted oxygen conditions. Such effects have been modelled using 2D PDF models (Masri et al., 2003; Cabra et al., 2005; Cao et al., 2005; Gkagkas & Lindstedt, 2007; Gordon et al., 2007; Ren & Pope, 2009; Najafizadeh et al., 2013) and 3D direct numerical simulations (DNS) (Yoo et al., 2011; Luo et al., 2012; Kerkemeier et al., 2013). The aim of this paper

is to improve the performance of the computationally cheaper RANS-EDC models for lifted flames in a heated and depleted oxygen environment.

2. Model Development

2.1. Domain and Boundary Conditions

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 computational domains previously employed in similar studies of the JHC burner (Frassoldati et al., 2010; Shabanian et al., 2013). The study of MILD combustion using the JHC burner is only valid where the fuel jet is entrained by the controlled coflow, up to ~100 mm (or ~22 jet diameters) downstream of the jet exit plane, after which the ambient air becomes influential. The near jet region is therefore the focus of the modelling effort for optimisation of the EDC model, with the focus of the work targeting the relationships between empirical parameters in the model and their effect on species reaction rates. The 400 mm (~85 jet diameters) downstream extent of the computational domain from the jet exit plane captures the experimental measurement locations of 30 mm (Dally et al., 2002) and 35 mm (Medwell et al., 2008) downstream of the jet exit plane. Although the radiation model has previously been shown to have negligible effect on these essentially soot-free flames (Frassoldati et al., 2010; Mardani et al., 2010; Aminian et al., 2011; Shabanian et al., 2013), the 'P1' radiation model was implemented to retain accuracy at a minimal computational cost. The simplest implementation of the 'P1' model assumes a basic grey-band model for gases with constant absorption and scattering coefficients.

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. Adiabatic, no-slip boundaries were used to describe the pipe walls in the JHC burner. 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 300 K. A coflowing wind tunnel velocity of 3.3 m/s was also included in models of the flames measured by Dally et al. (2002). The computational domain was divided into a structured, quadrilateral, computational mesh with 53610 elements based on mesh independence studies using the C_2H_4 and C_2H_4/H_2 fuel cases and additional meshes of 149060 and 251916 elements.

Previous attempts to model combustion in JHC burners have used experimentally measured inlet profiles (De et al., 2011), assumed constant velocity across the domain inlet (Frassoldati et al., 2010; Aminian et al., 2012; Sha-banian et al., 2013) or modelled the jet and coflow exit profiles (Christo & Dally, 2005; Mardani et al., 2011). Previous modelling of the C_2H_4-based JHC flames made the assumption of constant velocity profiles, although did not investigate any sensitivity to inlet boundary conditions (Shabanian et al., 2013). For this study the fuel pipe geometry was computationally modelled separately as a constant 4.6 mm diameter tube, 100 diameters in length, in order to ensure fully developed flow in the pipe. This was modified to 4.25 mm for the Dally et al. (2002) simulated cases. To determine the coflow velocity profile, an additional model of the secondary burner and outer annulus was generated, with the flow emanating with a uniform velocity of combustion products at the perforated plate 160 mm upstream of the coflow exit plane.

2.2. Turbulence and Turbulence-Chemistry Interaction Models

The modified k - ε turbulence model is adjusted from the standard k - ε model by changing the common default value of $C_{1\varepsilon}$ from 1.44 to 1.6, as recommended and verified for 2D axisymmetric flows (Dally et al., 1998). The anisotropic Reynolds Stress Model (RSM), featuring the same modification to $C_{1\varepsilon}$, has been previously verified for non-reacting jets (Dally et al., 1998) and was also implemented in selected cases for comparison. In modelling the MILD regime in the JHC burner, simple global-chemistry and scalar-based combustion models are unable to provide the accuracy of the more sophisticated Eddy Dissipation Concept (EDC) combustion model (Christo & Dally, 2005; Shabanian et al., 2013). The EDC model allows for the implementation of finite-rate chemical kinetics mechanisms, such as GRI-Mech 3.0 (Smith et al., 2000). A reduced, 36 species, form of the GRI-Mech 3.0 kinetics mechanism, excluding N-O reactions, was used after a similar GRI-Mech 3.0 mechanism demonstrated success in CH_4-based fuels in the JHC (Christo & Dally, 2005) and good agreement with a separately reduced kinetics scheme for both CH_4- (Frassoldati et al., 2010) and C_2H_4-based fuels (Shabanian et al., 2013).

Analysis of excited, chemiluminescent species and the effect of minor species in the coflow required the use of additional kinetic mechanisms. Additional reactions for the excited species mechanism was implemented using a combination of kinetics rates and reactions (Hidaka et al., 1985; Tamura et al., 1998; Petersen et al., 2003; Hall & Petersen, 2006; Elsamra et al., 2005) and a 50 species modified GRI-Mech 3.0 mechanism was used for the inclusion of minor species in the coflow. CH* and OH* denote excited OH and CH molecules respectively, and emit light in

the blue and ultraviolet regions of the light spectrum upon de-excitation to their ground states. Concentrations of the excited CH* species therefore indicates a blue coloured flame and the lack of CH* in regions with OH species concentration may be interpreted as evidence of MILD (flameless) combustion. The distributions of these excited species were evaluated in post-processing using a combination of OH* excitation reactions by Petersen et al. (2003) and Hall & Petersen (2006), and CH* reactions by Elsamra et al. (2005) and quenching rates by Hidaka et al. (1985) and Tamura et al. (1998). The combined mechanism consisted of an additional 21 reactions which were chosen to be evaluated in post-processing rather than incorporated into the existing modified GRI-Mech 3.0 in the interest of brevity. Kinetics post-processing was employed with the expectation that the populations of OH and CH species would contain only a negligible fraction of excited molecules, which would therefore have little impact on the combustion chemistry. This assumption was later confirmed through inspection of the results. The effects of minor species were additionally investigated by adding equilibrium concentrations of OH and NO to the coflow composition, both separately and in simultaneously, using a further modified 50 species GRI-Mech 3.0 mechanism which included N-O reactions whilst excluding argon and C_3H_x species. The addition of 0.001% mol/mol OH and 0.03% mol/mol NO in the coflow, separately and simultaneously, were investigated for change of peak temperature and apparent lift-off height. The effects of a 1% concentration of OH in the coflow on the same parameters was similarly considered following recent work on the effect of minor species in reducing ignition delay (Medwell et al., 2014).

The mean reaction rate in the EDC combustion model, R_i, of species *i* is assumed to occur only within small turbulent structures, as described by Eq. 1 (Magnussen, 1981). Both the mean residence time (τ*) spent within fine structures with length fraction (ξ*), are scaled by C_τ and C_ξ, with default values originally derived from an extensive control volume analysis of isotropic turbulent structures (Magnussen, 1981). The equations defining τ* and ξ* are shown in Eq.s 2 and 3 respectively.

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

where ρ is density, Y_i the mass fraction of species *i* in a computational cell, Y_i^* within fine scales,

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

where $C_\tau = 0.4082$ (default), ν is the kinematic viscosity, ε the turbulent dissipation rate,

$$\xi^* = C_\xi \left(\frac{\nu\varepsilon}{k^2}\right)^{1/4} \quad (3)$$

where $C_\xi = 2.1377$ (default) and k is the turbulent kinetic energy. Finally, combining these equations, the mean reaction rate may be rewritten as:

$$R_i = \frac{C_\xi^2}{C_\tau}\left[1 - C_\xi^3\left(\frac{\nu\varepsilon}{k^2}\right)^{3/4}\right]^{-1}\frac{\rho\varepsilon}{k}(Y_i^* - Y_i), \quad (4)$$

Recent studies (Aminian et al., 2012; Shabanian et al., 2013), based on an earlier investigation on the Delft-Jet-in-Hot-Coflow burner (De et al., 2011), found that increasing C_τ in the EDC model to 1.5 (Aminian et al., 2012) or 3 (Aminian et al., 2012; Shabanian et al., 2013) provided better agreement to measurements from the JHC burner.

The results of the Delft-Jet-in-Hot-Coflow modelling (De et al., 2011) indicate that these variations of the standard EDC model act to improve the predictions of lift-off, although this was not particularly apparent by setting $C_\tau = 3$ for ethylene fuels in the JHC burner (Shabanian et al., 2013). This is in agreement with the observation that in the MILD combustion regime there is a decrease in chemical reaction rates (Galletti et al., 2007; Ihme & See, 2011). The modification of C_τ (inversely proportional to R_i, from Eq. 4) has been further justified 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 acts to compensate for this (Aminian et al., 2012). The near unity Damkohler number was similarly cited as a reason for unreliability of the EDC model for flows with low turbulence (De et al., 2011). It was shown that the standard value of C_ξ was unreliable for flows with $k^2/(\nu\varepsilon)$ less than 65 (De et al., 2011). Decreasing the C_ξ parameter decreases the reaction zone volume fraction in the fluid model, restricting interactions between species and slowing the reaction rates (De et al., 2011). In spite of this detailed discussion, the work of De et al. (2011), does not quantify the effects of changing

the parameter C_ξ on species profiles or rigorously investigate the effects of this empirical parameter on temperature profiles.

The effects of changing C_ξ on R_i are not immediately apparent due to the strong coupling of R_i, C_ξ and the flow variables ν, ε and k. The relationship can be seen by taking the partial derivative of R_i with respect to C_ξ, as shown in Eq. 5:

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

This highlights the complex interplay between R_i, C_ξ and the ratio $\nu\varepsilon / k^2$. In comparison, Eq. 6 shows the comparatively simple coupling between C_τ and the rate of change of R_i where:

$$\frac{\partial R_i}{\partial C_\tau} = -\frac{R_i}{C_\tau}, \tag{6}$$

It is hypothesised that decreasing R_i would result in a more accurate model, thus a parametric study using the combinations of C_ξ and C_τ summarised in Table 1, for the case of a C_2H_4/N_2 jet flame with Reynolds number (Re_{jet}) of 10,000 in a 1100 K, 9% O_2 mol/mol coflow. The C_ξ parameter was varied with both the default and most successful value of C_τ from previous studies of jet flames in the transition to the MILD regime (De et al., 2011; Aminian et al., 2012;

Shabanian et al., 2013) in order to gain an insight into the effect of each individual parameter on the accuracy of simulation results. The computational results of species and temperature distributions at 35 mm downstream from the jet exit and any apparent lift-off indicated from the CH and OH distributions were then compared to experimental measurements for each combination of parameters and the results of simulations using the more sophisticated, and computationally expensive, composition Probability Density Function (PDF) combustion model using an Euclidean Minimum Spanning Tree (EMST) mixing model.

The combination of EDC parameters and velocity boundary conditions which provided the best agreement to the measurements of the C_2H_4/N_2 flame in a 9% mol/mol O_2 coflow was then compared to other fuel cases, all summarised in Table 2. Note that coflow compositions specified by mass fraction (Y) correspond to methane based studies by Dally et al. (2002), with remaining cases measured experimentally by Medwell et al. (2008).

3. Results and Discussion

Results of the parametric study into the effects of C_ξ in the EDC combustion model were obtained for the C_2H_4/N_2 in a 9% mol/mol O_2 coflow. This produced a set of results from the previously listed parameter combinations for comparison against experimental temperature, OH and CH_2O profiles, in addition to visible lift-off behaviour. These results indicated best agreement using the modified SKE turbulence model (Dally et al., 1998) and a newly modified EDC model with the parameters $C_\tau = 3$ and $C_\xi = 1$, compared to the default $C_\tau = 0.4082$ and

$C_\xi = 2.1377$, and recently used modified values $C_\tau = 3$ and $C_\xi = 2.1377$ (Shabanian et al., 2013). The newly modified EDC model required approximately 1,500 CPU-hours for an individual computational case using ANSYS FLUENT 14.0. This lengthy time required for convergence highlights the complexity of using the EDC model with the modified GRI-Mech 3.0 and a simple, 2D geometry, whilst the PDF-EMST model simulations notably required an order of magnitude greater computational time. The profiles of temperature, hydroxyl (OH) and formaldehyde (CH_2O) concentrations of these selected EDC parameter combinations, and the results of simulation using the PDF-EMST model, are compared with the experimental data in Figure 3. Both the newly modified EDC and PDFEMST models show excellent agreement with the temperature distribution and the profile shapes of species distributions, despite a significant difference in peak magnitude. The best agreement with experimental data were found to require fully developed velocity profiles of the fuel jet at the jet exit. The combinations of developed velocity and uniform profiles were assessed for the most successful combination in the literature, $C_\tau = 3.0$ and $C_\xi = 2.1377$, in addition to $C_\tau = 3.0$ with $C_\xi = 1$ and $C_\tau = 0.4082$ with $C_\xi = 1.5$ which demonstrated the best agreement with experimental measurements among all the parameter combinations. The influence of the coflow profile, jet turbulent intensity (in contrast to previous findings for CH_4/H_2 jets (Christo & Dally, 2005)) and variations in jet temperature ~100 K were seen to have insignificant impact on the shape and magnitude of temperature and species distribution peaks. This could imply that the optimised EDC parameter combination of $C_\tau = 3$ and $C_\xi = 1$ offers a more robust model, or that the effects of turbulence intensity on the

axisymmetric C_2H_4-based jets are less significant than the effects on CH_4/H_2 when issuing into a heated coflow.

With apparent lift-off height an interest for investigation of flame stability and autoignition, the CH* distribution was compared to visual measurements by Medwell et al. (2008). The initial downstream formation locations of CH* then subsequently used to define the visible flame base for further analysis and comparison with experimental cases (Medwell et al., 2008). The combination of $C_\tau = 3$ and $C_\xi = 1$ demonstrated the best agreement with visual lift-off height whilst maintaining a reaction zone near the jet exit, and is shown using the developed jet and coflow profiles in Figure 4. The simulated number densities of OH and CH* species are shown for this case in Figure 4, showing both sets of results near the jet exit with a logarithmic scales in comparison to experimental observations. The logarithmic scale was chosen due to the proportional relationship between light intensity and the total light energy flux squared, and thus preserving a linear relationship between the log of the species concentrations and the intensity of the emitted light. Similar contours were produced using the PDF-EMST model, including the same general features clearly showing a difference of orders of magnitude between OH and excited species concentrations. A difference of several orders of magnitude between the excited and base CH and OH concetrations additionally justified the assumption that CH* and OH* reactions may be neglected in determining the overall structure of the flame, and that the time-saving post-processing stage is an effective means of defining a visible flame boundary. This figure clearly demonstrates a transitional flame with a jet flame visually detached from the jet exit (as indicated by CH*), yet showing evidence of minor species (OH) almost to the jet exit

plane. Such results, clearly replicating the visually lifted description of these flames, have not been previously demonstrated for this series of cases in the JHC burner using EDC combustion models, but are consistent with experimental measurements.

The combination of $C_\tau = 3$ and $C_\xi = 1$ results in better agreement with measured data than the default EDC parameters, and accordingly replicates the visual lift-off seen experimentally which had not previously been achieved for these jet flames using the EDC combustion model, or any other Reynolds averaged method. These parameters were then assessed for accuracy in modelling the remaining C_2H_4, C_2H_4/H_2 jet flames in identical coflow conditions and the CH_4/H_2 flames as listed in Table 2. These results are presented as Figs. 5–7, and demonstrate the good agreement between the $C_\tau = 3$ and $C_\xi = 1$ EDC model and the value of peak temperature in the C_2H_4 and both CH_4/H_2 flames, and in predicting the radial location of peak CH_2O species for all cases. The newly modified EDC with $C_\tau = 3$ and $C_\xi = 1$ offers improved temperature prediction compared to previously attempted parameter combinations with $C_\xi = 2.1377$ and varying C_τ (Aminian et al., 2012). In their comparison of fine-scale time constants, Aminian et al. (2012) found an 'optimal' value of $C_\xi = 1.5$ resulting in relative errors in peak temperatures (with respect to the experimental peak) of 2.0 and 3.7% for the CH_4/H_2 fuel flames in 9 and 3% O_2 coflows respectively (Aminian et al., 2012). In comparison, the new EDC parameter set offers an improved overall agreement with the two of these peak temperatures with relative errors of 2.7 and 1.7% for the same CH_4/H_2 fuel flames in 9 and 3% O_2 coflows respectively. These errors are shown, alongside other fuel cases, in Table 3 which shows significantly better

consistency in prediction of peak temperature for all flames in comparison to previously 'optimised' EDC parameters.

The effects of minor species in the coflow were investigated as a possible source of influence in modelling the visual lift-off of flames in the transition to the MILD regime. The effect of the alternate 50 species GRI-Mech 3.0 kinetics using the newly modified EDC, and inclusion of reactions involving nitrogen was a total peak temperature difference of 11.2 K, demonstrating the robustness of the solution to the inclusion of nitrogen reactions. Additionally the inclusion of equilibrium OH and NO did not significantly increase the peak temperatures 35 mm downstream or alter the apparent lift-off, resulting only 0.3 and 12.4 K increases respectively and 12.5 K when both were included. These results justify the removal of N-O reactions in the GRI-Mech 3.0 mechanism and the simplification of the chemical composition at the coflow boundary. The increased concentration of 1% OH, however, resulted in an increase in peak temperature of 65.5 K at 35 mm downstream of the jet exit plane, and resulted in the flame attaching to the jet exit plane, eliminating any form of lift-off. This is in accordance with previous findings where OH at similar concentrations was shown to significantly reduce ignition delay of jet flames in a hot environment (Medwell et al., 2014). The newly modified EDC model, in this sense, behaves as anticipated with altered inlet compositions and verifies the importance of OH in flame stabilisation.

The new, modified EDC under-predicts the number density of OH in all cases except the C_2H_4/N_2 fuel, where it is in good agreement with the PDFEMST model. The modelling deficiencies resulting in under-prediction of OH have previously been seen using the PDF-EMST

model for the C_2H_4/H_2 fuel case (Shabanian et al., 2013), and CH_4/H_2 cases (Christo & Dally, 2004; Aminian et al., 2012), reporting peak magnitudes reduced by a factor of four in the 3% O_2 coflow at the 30 mm measurement location with the PDF-EMST model and a factor of three assigning $C_\xi = 1.5$ (Aminian et al., 2012). These three- (Aminian et al., 2012) and four-fold errors (Christo & Dally, 2004) are significantly greater than the factor of two predicted by the newly modified EDC model in the same fuel case after optimisation of both the C_τ and C_ξ parameters. The normalised OH distribution, however, agrees very well with measurement for the C_2H_4/N_2 and both CH_4/H_2 flames. In comparison, the standard EDC model significantly over-predicts OH concentrations in both the C_2H_4/N_2 and CH_4/H_2 flames. The radial location of peak temperatures are over-predicted for all cases except the C_2H_4/N_2 fuel, however this location is very dependent on the choice of turbulence model. The combination of modified RSM and EDC with $C_\tau = 3$ and $C_\xi = 2.1377$ (not shown) shows excellent agreement with experimental measurements for the C_2H_4/H_2 fuel case, but results in significant discrepancies compared to the C_2H_4/N_2 case. This deficiency may therefore be attributed to the modified SKE model and hence implies the need for a more robust 2D turbulence model in order to accurately capture the detail of temperature and species distributions.

A possible explanation for the improvement of both modified EDC models may be due to the decreased fine structure sizes, for $C_\xi = 1$, and increased residence times more appropriately emulating the conditions of transitional jet flames in the JHC burner. This is consistent with reduced temperatures observed in MILD combustion (Cavaliere & de Joannon, 2004), which are indicative of reduced reaction rates resulting from the low oxygen dilution in the reaction zone.

In contrast to conventional combustion, the MILD and, similarly transitional, regimes may be categorised such that fluid and chemical time scales are similar and turbulent time scales are reduced compared to conventional combustion. Similarly, Eq. 3 shows that C_ξ is a monotonically decreasing function of the ratio $k^2/(\nu\varepsilon)$ which is, in turn, proportional to the square of the turbulent kinetic energy of the fluid. This relationship implies that reacting fine structure scales increase in size with less energetic fluids, resulting in extended residence times in larger fine structures, serving to decrease the chemical time scale. In such circumstances, the combustion regime of a large control volume, such as a furnace, would tend towards emulating a well-stirred reactor where all products are completely mixed. The JHC burner, however, drives fluid motion downstream of the jet exit and dictates mixing between the ambient temperature, fast moving jet and heated, slow, low oxygen coflow. The laminarising, viscous shear effects between these streams may result in limited interaction regions between the fuel and oxidiser, reducing the boundaries for interactions between species whilst simultaneously increasing the time a fluid particle is encapsulated within a fine structure. Such viscous fluid effects may not be captured accurately by the EDC model due its assumption of isotropic Reynolds averaging (Magnussen, 2005), and numerical unreliability at low turbulence (De et al., 2011). Turbulent fine scales within the flow therefore need to be adjusted, through the parameters C_τ and C_ξ, in order to account for these viscous effects to better predict the mixing and chemical interactions between species in this region.

4. Conclusion

Lifted jet flames in a heated and depleted oxygen coflow stream in the transition to MILD combustion present an interesting test case for models. The use of RANS-based EDC models is particularly attractive due to the low computation cost yet retaining the capacity to model finite-rate chemical kinetics. However, previous RANS-EDC modelling efforts of the JHC burner have failed to accurately predict the experimental observations of transitional flames. These flames are characterised by measurements of combustion reactions in a region which visually appears lifted. Through a parametric investigation it has been demonstrated that adopting the EDC constants $C_\tau = 3$ and $C_\xi = 1$ enable the behaviour of these transitional flames to be recreated as shown through CH* contours of a visually lifted flame. It is also shown that this pair of constants similarly improves the EDC model capabilities in predicting peak temperatures, OH, CH_2O and temperature profiles measured experimentally across a range of operating conditions and fuels. Importantly, the optimised EDC model also shows less sensitivity to boundary conditions, such as jet inlet turbulence intensity and jet temperature and robustness to the chemical composition of boundary conditions. The modification of the EDC parameters is physically justifiable due to the distributed reaction zone associated with MILD combustion, explaining these improvements in the accuracy of results. These results demonstrate the capabilities of simplified RANS-based models for the modelling of flames in hot and vitiated oxidant streams, including visually lifted flames in the transition to MILD combustion which have not been reproduced previously using an EDC model.

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Table 1. Parameters and values chosen for parametric study, with combinations of six different C_ξ using both the default (0.4082) and previously most successful value of C_τ (3.0).

C_τ	C_ξ
	0.5
0.4082[a]	0.75
	1
	1.5
3.0	2.1377[a]
	2.5

[a]default parameter value.

Table 2. Fuel jet and coflow stream operating conditions (Dally et al., 2002; Medwell et al., 2008).

Composition Description *Fuel (Temperature)*	Mean Inlet Velocity (m/s)	Composition (% vol/vol)			
		C_2H_4	CH_4	N_2	H_2
C_2H_4 (305 K)	17.7	100	0	0	0
C_2H_4/H_2 (305 K)	30.6	50	0	0	50
C_2H_4/N_2 (305 K)	27.3	25	0	75	0
CH_4/H_2 (305 K)	58.7	0	50	0	50
Coflow (Temperature)		O_2	CO_2	N_2	H_2O
Y = 3% O_2 coflow (1300 K)[a]	3.2	2.6	3.5	83.9	10
Y = 9% O_2 coflow (1300 K)[a]	3.2	7.8	3.5	78.7	10
X = 9% O_2 coflow (1100 K)	2.3	9	3	78	10

[a]within a coflowing wind tunnel with air velocity of 3.2 m/s, and temperature assumed to be 300 K.

Table 3. Comparison of relative error in peak temperatures at 30 (CH_4/H_2 flames only) or 35 mm downstream of jet exit plane, as a percentage of experimental peak temperature (Dally et al., 2002; Medwell et al., 2008), coflows contain 9% mol/mol O_2 unless stated otherwise (Aminian et al., 2012; Shabanian et al., 2013). Dashes indicate no available CFD results.

EDC parameters	Relative error (%)				
	CH_4/H_2 (3%)[b]	CH_4/H_2 (9%)[b]	C_2H_4	C_2H_4/H_2	C_2H_4/N_2
$C_\tau = 1.5$[a]	3.7	2.0	–	–	–
$C_\tau = 3$[a]	–	7.9	14.9	9.2	28.6
$C_\tau = 3$, $C_\xi = 1$[c]	1.7	2.7	2.7	9.6	3.3
PDF-EMST[a]	–	–	10.3	9.6	0.5[c]

[a]CFD results for CH_4/H_2 flames by Aminian et al. (2012), otherwise Shabanian et al. (2013).

[b]percentage coflow O_2 by mass.

[c]current study.

Figure 1 Schematic of the JHC burner used for MILD combustion experiments

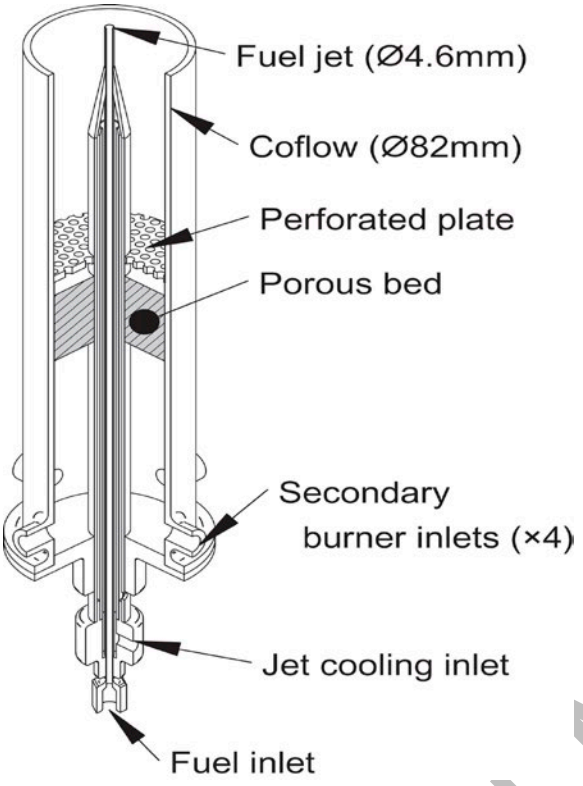

Figure 2 Visual comparison of different C_2H_4 based flames at Re_{jet} = 10, 000 in the JHC burner up to 300 mm above jet exit plane, showing heights in millimetres; labelled with exposure times and O_2 coflow conditions

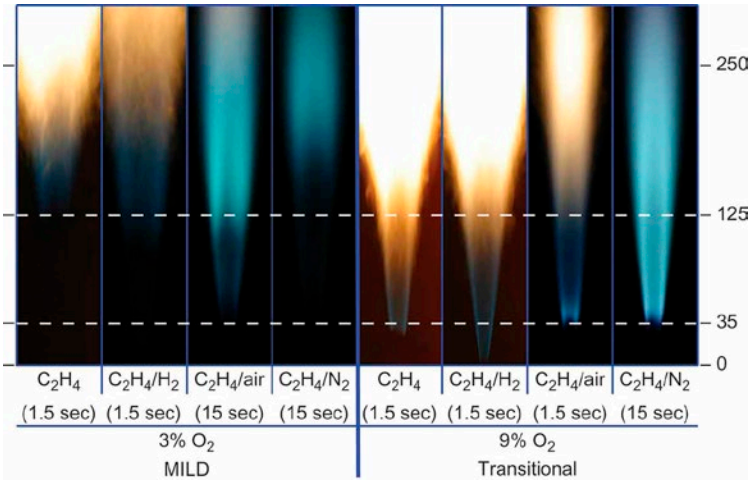

Figure 3 Temperature and species profiles 35 mm downstream from jet exit for C_2H_4/N_2 fuel in a 9% mol/mol O_2 coflow, showing two modified EDC models, PDF with EMST model and experimental measurements (experimental data from Medwell et al., 2008)

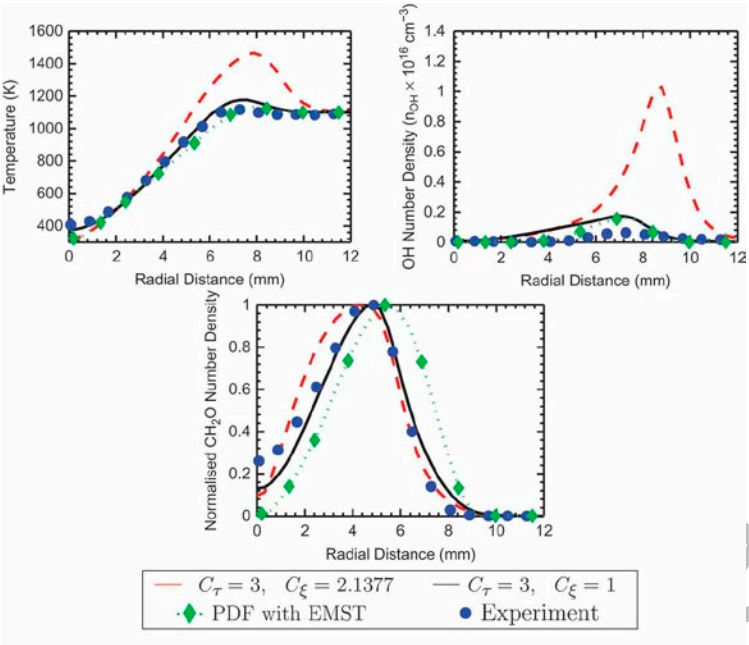

Figure 4 Number densities of OH and chemiluminescent species near the jet exit

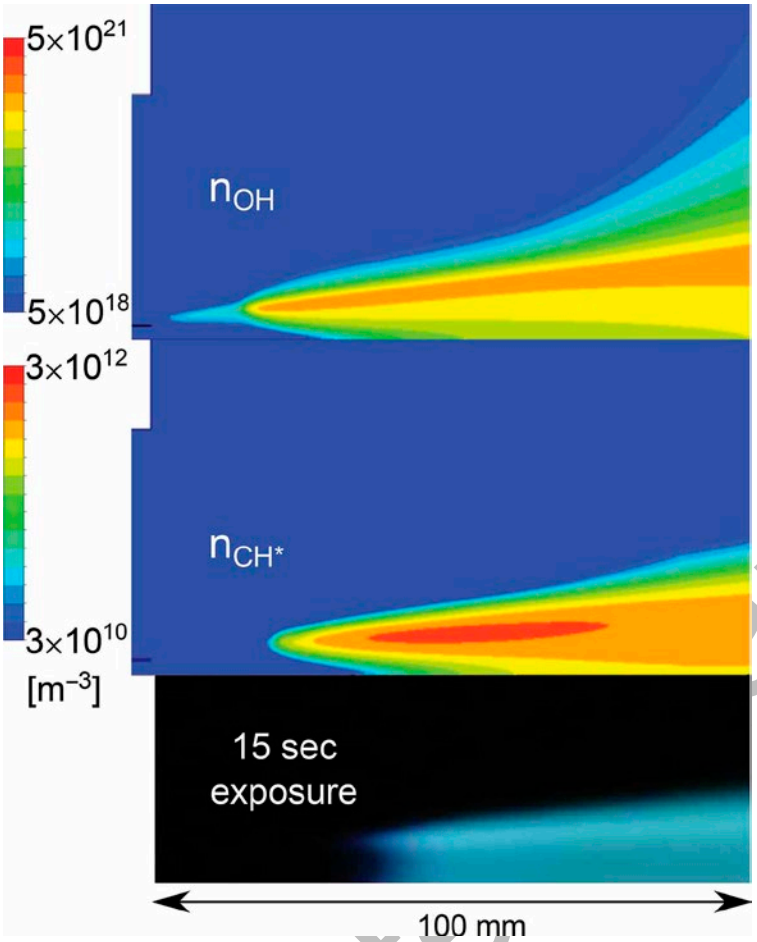

Figure 5 Temperature and species profiles 35 mm downstream from jet exit for C_2H_4 fuel in a 9% mol/mol O_2 coflow, showing two modified EDC models and experimental measurements (experimental data from Medwell et al., 2008).

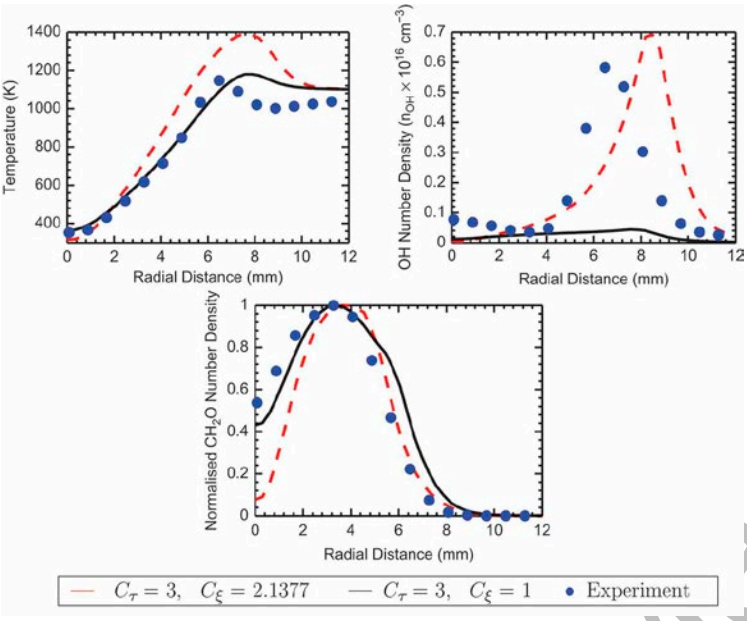

Figure 6 Temperature and species profiles 35 mm downstream from jet exit for C_2H_4/H_2 fuel in a 9% mol/mol O_2 coflow, showing two modified EDC models and experimental measurements (experimental data from Medwell et al., 2008)

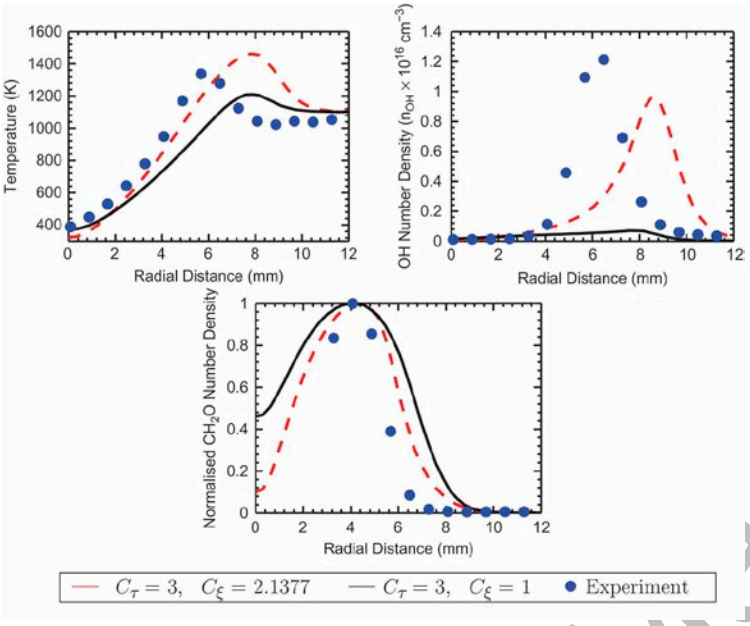

Figure 7 Temperature and species profiles 30 mm downstream from jet exit for CH_4/H_2 fuel, showing modified EDC models with $C_\tau = 3$ and $C_\xi = 1$ (lines), and experimental measurements (markers) for 3% and 9% mass O_2 coflows (experimental data from Dally et al., 2002).