

Numerical simulation of turbulent non-premixed combustion in diluted hot coflow using PaSR combustion model

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Abstract

Moderate and intense low oxygen dilution combustion is a new technology and concept to access high thermal efficiency and fuel savings while maintaining emission of pollutants at very low levels. It utilizes the concept of heat and exhaust gas recirculation to achieve combustion at a reduced temperature, a flat thermal field, and low turbulence fluctuations. In this paper, the aim is evaluation of PaSR combustion model for numerical simulation of turbulent non-premixed combustion in diluted hot coflow. The effects of oxygen concentration in a hot diluted oxidant stream on (H_2/CH_4) turbulent non-premixed flame under MILD condition are investigated. The modelling is performed for three co-flow O_2 levels, 3%, 6% and 9% O_2 , which is preheated to 1300 K. The distribution of species and temperature are investigated for different co-flow oxygen concentrations. The numerical simulation is performed by OpenFoam software, and the reduced kinetic mechanism DRM-22 is used in the current modelling. The combustion model is a Partially Stirred Reactor (PaSR) model, which has been used for turbulent non-premixed combustion. Moreover, the standard $k-\epsilon$ turbulence model with a modified constant ($C_{\epsilon_1}=1.6$) is used for turbulence modelling. It is found that the PaSR model with a detailed kinetic scheme, offers a practical and reasonably accurate tool for predicting the flow and flame characteristics of MILD combustion.

Introduction

MILD (moderate and intense low oxygen dilution) combustion can employ in nearly all combustion technology sectors; including gas turbines, boilers, furnaces, and etc. This regime of combustion has very low emissions and very high efficiency [1, 2]. Originally, the technology was named Excess Enthalpy Combustion while today it is called High Temperature Air Combustion (HiTAC) in Japan, Flameless Oxidation (FLOX) in Germany, Low NO_x Injection (LNI) in the USA, and MILD Combustion in Italy.

In a review paper, Wunning and his co-workers [1] showed Flameless combustion technique as highly efficient and with Low NO_x emission. They also showed that thermal NO_x which is a major source of NO_x formation in combustion systems can be reduced by reducing the peak temperature. Murer [3] conducted a series of experiments on a 30 kW laboratory scale combustor; equipped with an electrical air pre-heater, to study the effects of excess air and air preheat temperature on the flameless combustion characteristics. The results suggested significant effects of excess air and air preheat temperature on the location and shape of the combustion reaction zone and emission level. Dally [4] investigated the effect of concentration of oxygen in hot coflow on H_2/CH_4 turbulent non-premixed flame under MILD condition. An experimental burner is used in his study to simulate the heat and exhaust gas recirculation applied to a simple jet in a hot coflow. The results show that reducing the oxygen level in the hot coflow causes the flame becomes less luminous. While the peak temperature reduces considerably, the average temperature increases in the reaction zone by 100 K. Besides the levels of CO and OH concentration are lowered significantly. The level of

NO is also decreased with decreasing the oxygen levels, and at 3% O₂ by mass, the NO level is less than 5 ppm [4].

Although experimental studies of MILD combustion, such as those reported in [3, 4], provide important data that can also be used for calibrating numerical models, the information is prevalently limited to specific burner design and is connected to the measured properties. Numerical modelling of MILD combustion offers more flexibility for predicting complex combustion systems and provides insight on the flow and flame characteristics. In a numerical study, Christo and Dally [5] were found that conserved scalar-based models, i.e., the ζ /PDF and flamelet models, are not suitable for modelling flames under MILD condition. They also found that the eddy-dissipation concept (EDC) model with detailed chemical kinetics, rather than global or skeletal mechanisms, can improve the accuracy significantly [5]. In general, they noticed that the EDC model performed reasonably well for the 9% O₂ and 6% O₂ flames, but not for the 3% O₂ case. For the 3% O₂ case, the model over predicted the flame liftoff height. In addition, due to some drawbacks of EDC model, the model did not predict flame characteristics (e.g., temperature and species concentration) at 120-mm above the jet exit, [5, 6]. In addition to Dally, Frassoldati [7] and Mardani [8] also simulated the JHC (Jet in Hot Co-flow) flame with using EDC model. Frassoldati [6] described a methodology for computing pollutant formations in steady turbulent flows for MILD combustion. He also investigated the effect of boundary conditions for the turbulent kinetic energy. Mardani and Tabejamaat [8] investigated the Effect of hydrogen on hydrogen-methane turbulent non-premixed flame under MILD condition using the EDC model and k - ϵ turbulence model. In their work, it was observed that the EDC model is suitable for predicting the characteristics of MILD Combustion. However, the accuracy of this model was limited to regions close to the jet exit. Moreover, Mardani [8] used the DRM-22 kinetic mechanism to model the MILD combustion and compared the results with the results of GRI1.2 mechanism. He found that there is a good agreement between the results of these two sets of kinetic mechanisms. Kazakov [9] showed better performance of the DRM-22 in comparison with the DRM-19 mechanism (both DRM-19 and DRM-22 are reduced version of the GRI1.2.) to predict ignition delay time and laminar flame speed in atmospheric pressure.

Generally, mixing in MILD combustion controls both chemical kinetics and fluid motion. Hence, the partially stirred reactor (PaSR) model can be a good candidate to assess the extent of turbulence-kinetics interaction in MILD combustion. The PaSR combustion model was developed by Golovitchev [10] in 2000 to simulate of the Diesel engines. This model is an extension of the Eddy Dissipation Concept (EDC) combustion model that is capable of using a detailed kinetics. Golovichev et al. [11] applied detailed kinetics and the Partially Stirred Reactor concept (PaSR) to correctly describe the turbulence/chemistry interaction in Flameless combustion. His methodology has been integrated into KIVA-3V code modified for gaseous fuel injection. His Simulation results clearly illustrate that the flame structure is significantly affected by oxygen concentration [11]. D'Errico [12] compared the EDM (Eddy dissipation model) and the PaSR combustion models for diesel engines. He showed the flame structure computed by PaSR model is more accurate than EDM model [12].

The aim of this work is evaluation of PaSR model for MILD combustion. The distribution of species and temperature are investigated for different co-flow oxygen concentrations. The study focuses on experiments reported by Dally et al. [4] since it provides the most comprehensive set of data with well-defined initial and boundary conditions.

Model Description

The numerical model proposed for this study is based on the geometry and dimensions of the experimental jet in hot coflow (JHC) burner used by Dally [4], which is designed to emulate the MILD combustion regime. The experimental burner consists of an insulated and cooled

central jet (i.d. = 4.25 mm) and an annulus (i.d.= 82 mm) with a secondary burner mounted upstream of the exit plane. The secondary burner provides hot combustion products which are mixed with air and nitrogen via two side inlets at the bottom of the annulus to control the O₂ levels in the mixture. The cold mixture of air and nitrogen also assists in cooling the secondary burner. The cold mixture of air and nitrogen is composed of 23% O₂ and 77% N₂ (mass basis). Mean inlet velocities of hot (combustion products) co-flow and wind tunnel air are fixed at 3.2 m/s and mean inlet velocity of fuel jet is set at 58 m/s. Table 1 lists the experimental conditions. The fuel jet consists of 80% methane and 20% hydrogen (mass basis). The investigations are performed for three mass fractions of O₂ (i.e., 9, 6, and 3%) in the hot co-flow. The mean temperature of fuel jet, co-flow, and shroud air temperatures are approximately 305, 1300, and 294 °K, respectively. Due to the symmetry of the burner, a geometrically simplified axisymmetric computational model was constructed to simulate the burner. The computational domain started at the exit plane of the burner, and extended 400 mm downstream across the axial direction and 170 mm across the radial direction. The equivalent axisymmetric constructed computational model is shown in Fig. 1.

Table 1. Operating conditions for cases studied [4].

Case	Oxidant coflow			
	Y _{O₂} %	Y _{CO₂} %	Y _{N₂} %	Y _{H₂O} %
1	3	5.5	85	6.5
2	6	5.5	82	6.5
3	9	5.5	79	6.5

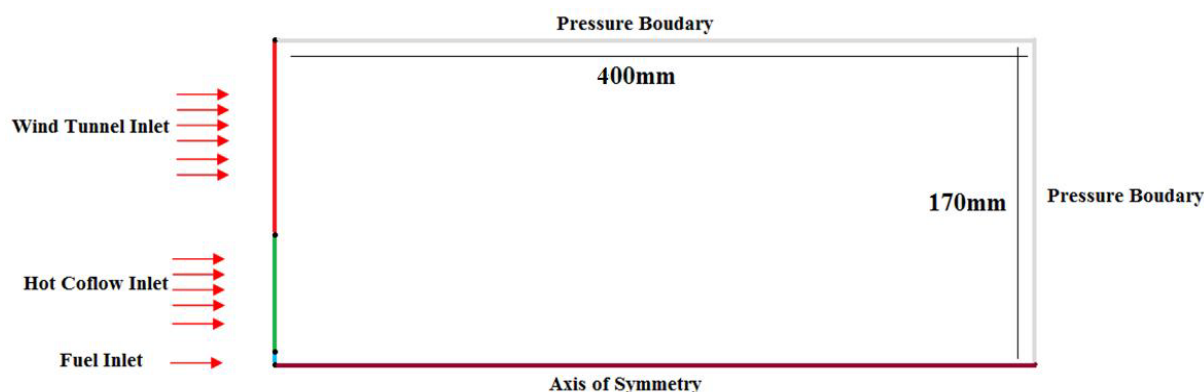


Figure 1. Computational model of JHC burner and boundary conditions.

The numerical simulation of the flow field includes the solution of the governing equations which consists of Favre-averaged form of continuity, momentum, energy, species conservation, and modified standard k- ϵ equations. For this study, C++ library OpenFoam was used for numerical simulation. The flow solver of OpenFoam is based on the PISO algorithm [13]. Boundary conditions at upstream consists of velocity profiles, inlet temperature, species mass fractions. The other boundary conditions are shown in Fig. 1. The velocity profiles at the inlets are assumed to be uniform. The DRM-22 [9] is used for chemical kinetics modelling. The DRM-22 is a reduced version of the GRI1.2. [13] It consists of 22 species and 104 reversible reactions.

Government Equations

Balance equations for the mean quantities in RANS simulations are obtained by averaging the instantaneous governing equations. This averaging procedure introduces unclosed quantities

that have to be modelled by using turbulent combustion models. Using the Favre averages formalism, the averaged balance equations become [14, 15]:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i) = 0. \quad (1)$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i \tilde{u}_j) + \frac{\partial \bar{p}}{\partial x_j} = \frac{\partial}{\partial x_i} (\bar{\tau}_{ij} - \bar{\rho} \overline{u_i'' u_j''}) + \bar{\rho} g. \quad (2)$$

$$\frac{\partial \bar{\rho} \tilde{Y}_k}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i \tilde{Y}_k) = \frac{\partial}{\partial x_i} \left(\frac{\mu}{Sc_k} \frac{\partial \tilde{Y}_k}{\partial x_i} - \bar{\rho} \overline{u_i'' Y_k''} \right) + \bar{\omega}_k \quad k = 1, \dots, N. \quad (3)$$

$$\frac{\partial \bar{\rho} \tilde{h}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i \tilde{h}) = \frac{Dp}{Dt} + \frac{\partial}{\partial x_i} \left(\frac{\mu}{Pr} \frac{\partial \tilde{h}}{\partial x_i} - \bar{\rho} \overline{u_i'' h''} \right). \quad (4)$$

In Eq. 3, the thermal diffusion (Soret effect) and the pressure diffusion are neglected. In this work it is assumed that Sc_k (Schmidt number) is unity which means that the effective specie diffusivity is equal to the viscosity. In Eq. 4, h , the enthalpy consists of both sensible enthalpy and enthalpy of formation. Moreover, the results of Christo and Dally [5, 6] demonstrated that for the JHC configuration, thermal radiation did not have noticeable effect on the solution; so, it is not considered here. In addition, it is assumed that Lewis number is equal unity.

Turbulence Model

Closure for the Reynolds stress terms in the government equations were achieved using the $k-\varepsilon$ turbulence model [14, 15]. Dally [5] showed that the standard $k-\varepsilon$ model with a modified constant $C_{\varepsilon 1}$ from 1.44 to 1.6 in the dissipation equation is the best model among the $k-\varepsilon$ models for numerical simulation of MILD combustion. Therefore, in this research, it is used as turbulence model. In this work, it is assumed that Sc_{kt} (turbulent Schmidt number), and Pr_t (turbulent Prandtl number) are unity.

Combustion Model

The Partially Stirred Reactor (PaSR) model is used in this work as the combustion model. Since the main contribution of the present work is using the PaSR model to study the MILD combustion, the model is described in this section with some details.

In the PaSR approach, a computational cell is split into two different zones: in one zone all reactions occur, while in the other one there are no reactions (Fig. 2). Therefore, the composition changes due to mass exchange with the reacting zone. In addition, the reaction zone is treated as a perfectly stirred reactor (PSR), in which all reactants are assumed to be perfectly mixed with each other. This allows us to neglect any fluctuations when calculating the chemical source terms. Three average concentrations are presented in the reactor, the mean mixture concentration of the feed c^0 , the mixture concentration in the reaction zone c , the mixture concentration at the exit of the reactor c^1 .



Figure 2. Conceptual diagram of PaSR reactor (the reaction zone is painted) [16].

The whole combustion process is regarded as two processes. In the first process initial concentration in the reaction zone changes from c^0 to c ; in the second process the reacted mixture (with concentration c) is mixed with the un-reacted mixture (with concentration c^0 by turbulence), the results is the averaged concentration c^1 . The reaction rate of this computational cell is determined by the fraction of the reactor in this cell. It seems quite clear that it should be proportional to the ratio of the chemical reaction time τ_c to the total conversion time in the reactor, i.e. the sum of the micro-mixing time τ_{mix} and reaction time τ_c [11, 12, 16],

$$\kappa_k = \frac{\tau_c}{\tau_c + \tau_{mix}}. \quad (5)$$

The micro-mixing time τ_{mix} characterizes the exchange process between reactant mixture and unburnt mixture. In this study the micro-mixing time τ_{mix} was obtained from the k- ϵ equation, $\tau_{mix} = C_{mix} \sqrt{(\mu + \mu t) / \rho \epsilon}$, the model constant C_{mix} was set to 1. The reaction time τ_c was derived from the laminar reaction rate. Thus, the overall reaction rate $\bar{\dot{\omega}}$ and the homogenous reaction rate $\dot{\omega}$ of this computational cell ($\dot{\omega}$ represents the reaction rate of the species according to the used kinetic mechanism) have the following relationship,

$$\frac{c_k^1 - c_k^0}{dt} = \bar{\dot{\omega}}_k = \kappa_k \dot{\omega}_k \quad (6)$$

Results and Discussions

The results of the present research illustrate that the solution is not sensitive to the turbulence intensity at the hot co-flow and wind tunnel inlets, which are also reported by Christo and Dally [5, 6] and Frassoldati [7], while the turbulence intensity at the fuel inlet is important. Christo and Dally [5, 6] reported the experimentally assessed mean turbulent kinetic energy of $16\text{m}^2/\text{s}^2$ at the fuel inlet. In the present study, the turbulent kinetic energy at the fuel jet inlet is adjusted to $16\text{m}^2/\text{s}^2$. The grid used to simulate the flame is a structured non uniform grid with about 17500 cells. Mesh refinement is found to improve convergence rate and ensured adequate grid resolution for smooth representation of flow and scalar properties. Fig. 3 shows the mesh independency for z-velocity in $Z=30\text{mm}$.

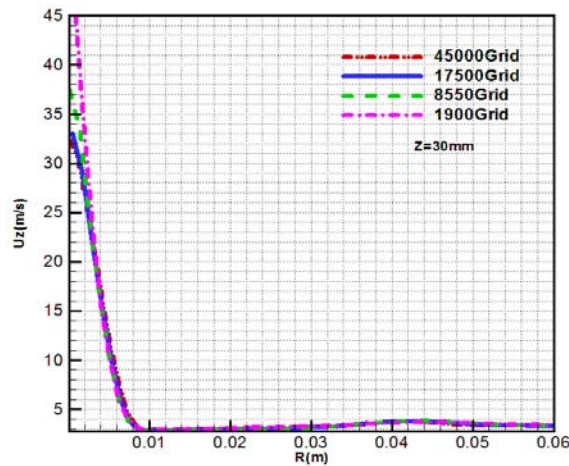


Figure 3. mesh independency for U_z in $z=30\text{mm}$.

In Fig. 4, the radial profiles of mean temperature at 30 mm above the jet exit for the 3% O_2 are shown. In this figure the calculated temperature using the PaSR model is compared with the temperature predicted by PDF and EDC models.

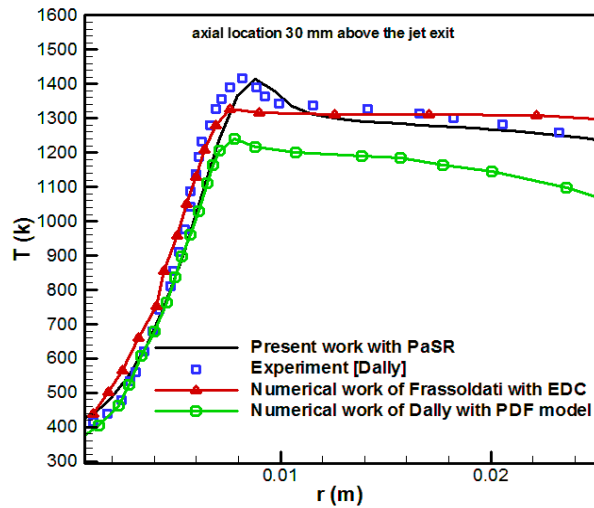


Figure 4. Temperature plots at axial location 30mm above the jet exit- comparison of PaSR, PDF [6], and EDC [7] models with experimental measurement [4].

It is seen that the temperature profiles predicted by PaSR model is closer to the experimental data than the predictions of PDF and EDC models. Specifically, the predicted peak temperature by the PaSR model is in very good agreement with the experimental value.

Fig. 5 shows radial profiles of mean temperature and mass fractions of O_2 for 3% O_2 , at axial location 30 mm above the jet exit. The temperature distribution is in reasonable agreement with measurement up to $r = 25$ mm. However, the temperature is over-predicted for $r > 20$ mm. This agreement shows that the PaSR model with standard $k-\epsilon$ model offers an acceptable tool for predicting the flow and flame characteristics under MILD condition.

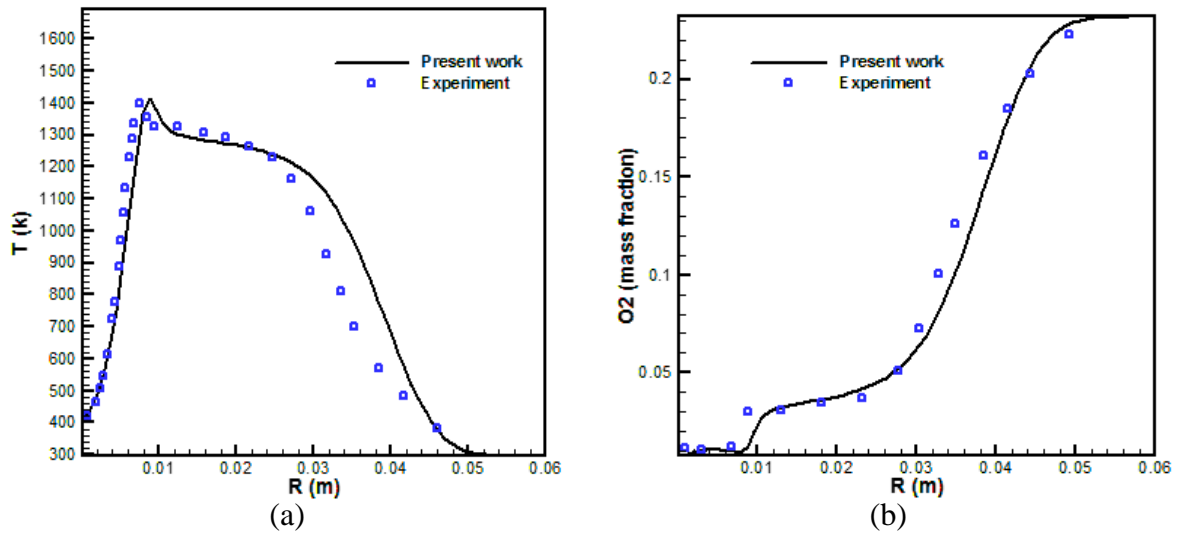


Figure 5. the radial distribution of temperature (a) and O₂ mass fraction (b) and comparing of them with experiment for 3% O₂ in z=30mm.

Fig. 6 shows the distribution of the same data as Fig. 5 for axial location 120 mm above the jet exit.

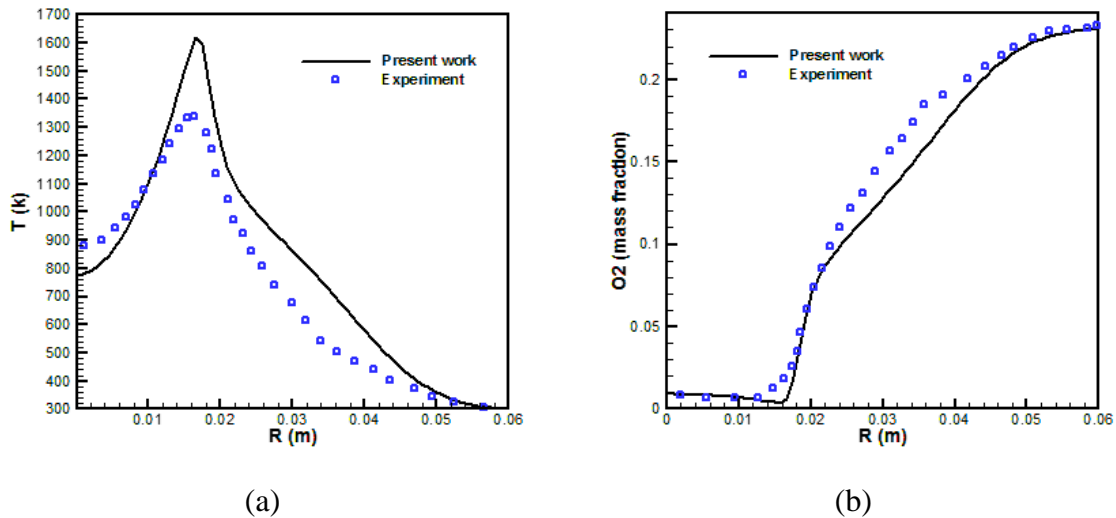


Figure 6. The radial distribution of temperature (a) and O₂ mass fraction (b) and comparing of them with experiment for 3% O₂ in z=120mm.

It is observed that the temperature is over-predicted. This discrepancy was also observed by Dally [5, 6] and Frassoldati [7]. A possible explanation for this discrepancy can be found in the oxygen radial profile. The O₂ plot shows the predicted consumption of O₂ is more than the experimental value. The higher availability of oxygen increases the combustion intensity and directly affects the temperature levels.

The same discrepancy between numerical data and experimental measurements far from the jet exit was previously reported by Christo and Dally [5], utilizing the EDC as the combustion model. They showed that their simulation tended to capture the maximum values of the instantaneous measurements. They argued that since their simulation was based on RANS approach, it could not resolve the fluctuations in the mixture fraction, as a result, their simulation could not account for the bias in mean profiles due to localized extinction.

Figs. 7 and 8 illustrate temperature and distributions of CO for three different oxygen levels in the hot coflow (oxygen mass fractions of 9, 6, and 3%) at Z= 30 mm and Z=120mm.

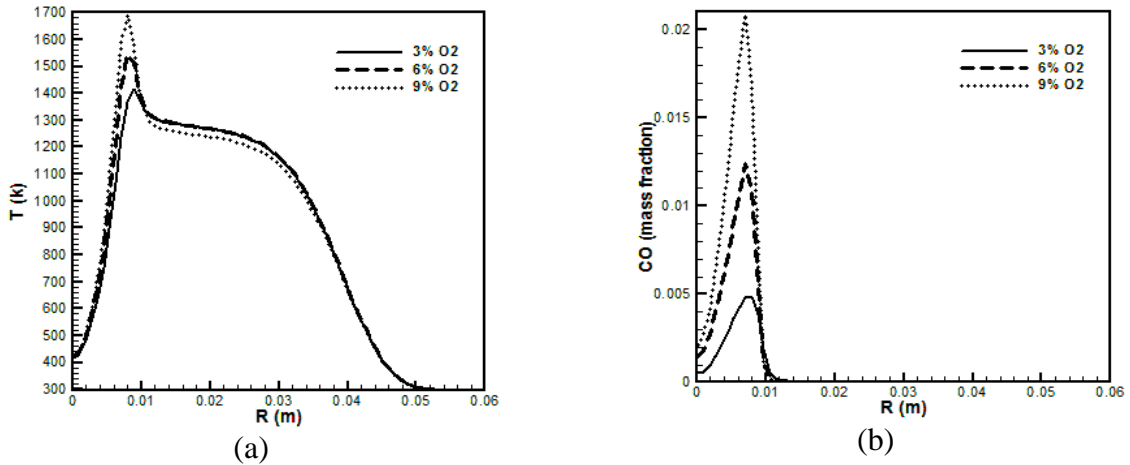


Figure 7. The effect of Change of O₂ concentration in the hot oxidant stream on the radial distribution of temperature (a) and CO (b) at $z=30\text{mm}$.

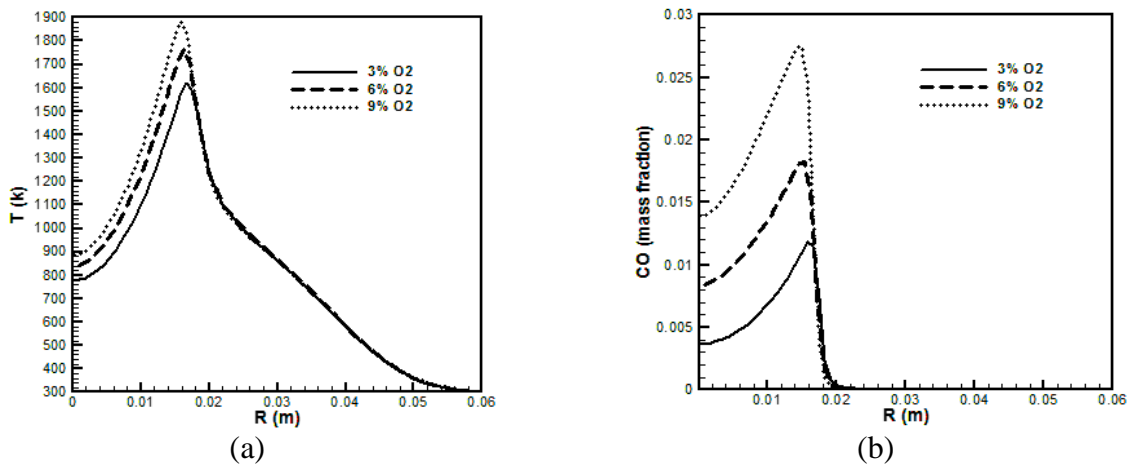


Figure 8. the effect of O₂ concentration in the hot oxidant stream on the radial distribution of temperature (a) and CO (b) at $z=120\text{mm}$.

The effect of oxygen concentration, in the hot oxidant stream, on the mean flame temperature is considerable. It drops from 1700 K for 9%O₂ to 1400 K for 3% O₂ at $z=30\text{mm}$. The temperature of the centreline is 400 K and it is the same for all cases. Therefore, increasing the oxygen mass fraction in the hot oxidant stream, increases the maximum temperature. Higher temperature is a main cause of higher pollution (such as CO, that is shown in Figs. 8b and 9b) and depriving the main advantage of the MILD combustion.

Conclusions

Detailed comparison with experimental data is presented to evaluate the performance of the PaSR model in predicting temperature and species concentration in the MILD combustion mode. The modeling results demonstrated that the PaSR model with a detailed kinetic scheme is suitable for modeling JHC flames. The numerical modelling shows that the flame characteristics, such as temperature and species concentration, predicted by PaSR model are closer to the experimental measurements than the results predicted by PDF and EDC models. The numerical results, in agreement with experimental observations, show that increasing the oxygen mass fraction in the hot oxidant stream causes the flame temperature increases that is a disadvantage in the MILD combustion mode.

Nomenclature

ρ	density
u_i	velocity in i-direction
g	gravity
p	pressure
Y_k	mass fraction of species k
h	enthalpy
T	temperature
c_k	Concentration for species k
τ_{ij}	viscous tensor
μ	dynamic viscosity
Sc_k	Schmidt number for species k
$\dot{\omega}_k$	mass reaction rate of species k per unit volume
Pr	Prandtl number
μ_t	turbulent viscosity
Pr_t	turbulent Prandtl number
Sc_{tk}	turbulent Schmidt number for species k
k	turbulent kinetic energy
ε	kinetic energy dissipation rate
κ_k	reactive fraction of species k

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