



## An insight into chemical kinetics and turbulence-chemistry interaction modeling in flameless combustion

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### Abstract

Computational Fluid Dynamics (CFD) study of flameless combustion condition is carried out by solving the Reynolds-Averaged Navier-Stokes (RANS) equations in the open-source CFD package of OpenFOAM 2.1.0. Particular attention is devoted to the comparison of three global and detailed chemical mechanisms using the Partially Stirred Reactor (PaSR) combustion model for the turbulence-chemistry interaction treatment. The OpenFOAM simulations are assessed against previously published CFD results using the Eddy Dissipation Concept (EDC) combustion model as well as the experimental data available in the literature. Results show that global chemical mechanisms provide acceptable predictions of temperature and major species fields in flameless mode with much lower computational costs comparing with the detailed chemical mechanisms. However, incorporation of detailed chemical mechanisms with proper combustion models is crucial to account for finite-rate chemistry effects and accurately predict net production of minor species.

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**Keywords:** Flameless combustion; Chemical mechanism; Combustion model; Jet-in-hot coflow flame; OpenFOAM; Major and minor species.

### 1. Introduction

MILD combustion is a modern combustion technology that has many advantages; such as creation of uniform combustion throughout the furnace, increasing combustion efficiency and significantly reduction of pollutant emissions [1, 2]. To establish this combustion regime, two conditions are simultaneously required; preheating the reactants above auto-ignition temperature of the fuel and oxidizer, and diluting the reaction zone from fuel or oxidizer. Dally et al. [3] reported valuable experimental information on a hybrid methane/hydrogen jet issuing into a hot and diluted coflow (JHC) in the non-premixed turbulent combustion regime. Due to comprehensiveness and accuracy of the results reported by Dally et al. [3], lots of studies have been focused on the modeling of the mentioned JHC burner. Christo and Dally [4] investigated the effect of various turbulence and combustion models and chemical kinetic schemes. They reported that the EDC combustion model is good enough to predict the behavior of MILD combustion, and for simulating this combustion regime, the detailed mechanisms like GRI 3.0 should be used. Kim et al. [5] compared four global reaction mechanisms for natural gas combustion to predict the temperature and mixture fraction of species in MILD combustion regime. Aminian et al. [6] demonstrated the development of shear layers between fuel and coflow, and also coflow and tunnel air streams by means of adjusting the turbulence intensity in the inlet of the JHC flames. They also modified the EDC combustion model for MILD regime with increasing the mixing time scale constant ( $\tau_{mix}$ ) above the

default value in the EDC approach [7]. In addition, they comprised various RANS turbulence models, and two detailed kinetics schemes namely the KEE and DRM-22 mechanisms to predict behavior of the JHC flames. It was declared that the modified  $k - \varepsilon$  turbulence model and the KEE mechanism provide the best results for MILD combustion simulation. Main purposes of the present study are to compare two combustion models namely the EDC and PaSR, and also examine capability of the Jones-Lindstedt kinetic scheme which is a global mechanism versus two detailed mechanisms, DRM-22 and KEE, for predicting the MILD combustion behavior.

## 2. Case study

According to Figure 1 the jet in hot coflow burner experimentally studied by Dally et al. [1] consists of a central fuel jet (i.d. = 4.25mm) which is surrounded coaxially by an annulus (i.d. = 82mm) equipped with a secondary burner providing hot combustion products. The hot flue gases are premixed with air and nitrogen via two side-inlets at the bottom of the annulus to vitiate the oxidizer and produce coflow streams with 3%, 6% and 9% oxygen mass fraction denoted as HM1, HM2, and HM3 flames, respectively. The whole burner has been placed inside a wind tunnel, with room-temperature air at the same velocity as the hot coflow, to help the stabilization of the flames.

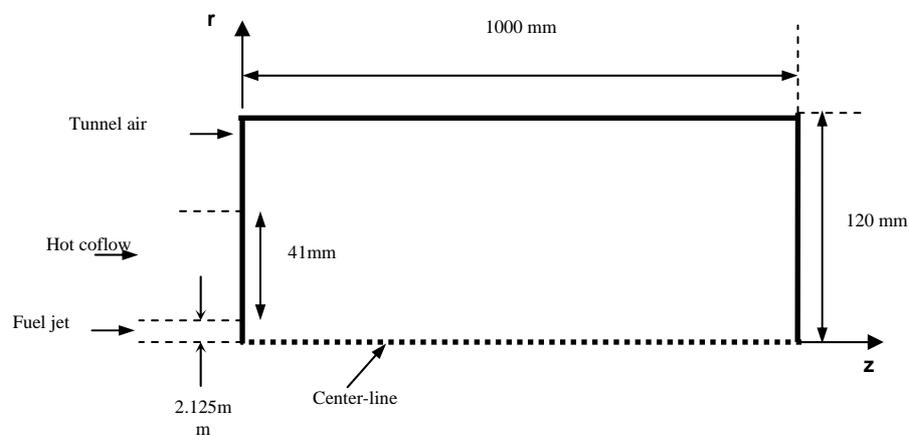


Figure 1. Two dimensional, axisymmetric computational domain

## 3. Physical model

The steady-state Favre-Averaged Navier-Stokes (FANS) equations were solved in a finite volume scheme using the open-source package OpenFOAM 2.1.0. The Reynolds stress tensor was resolved applying a modified version of the  $k-\varepsilon$  model with the constant  $C_{1\varepsilon}$  set to 1.6 (instead of 1.44) to compensate for the round jet/plane jet anomaly [8, 9]. The discrete ordinate (DO) method together with the Weighted-Sum-of-Gray-Gases (WSGG) model with coefficients from Smith et al. [10] was employed to solve the radiative transfer equation (RTE). The DO method solved the RTE in 16 different directions across the computational domain. Second-order upwind scheme was applied for the space derivatives of the advection terms in all transport equations. The PIMPLE algorithm was also employed to handle velocity-pressure coupling in flow field equations. Preliminary cold-flow simulations were conducted to check for grid independency and finally a computational domain with 31k cells was chosen to continue the hot-flow realistic simulations.

### 3.1 Boundary conditions

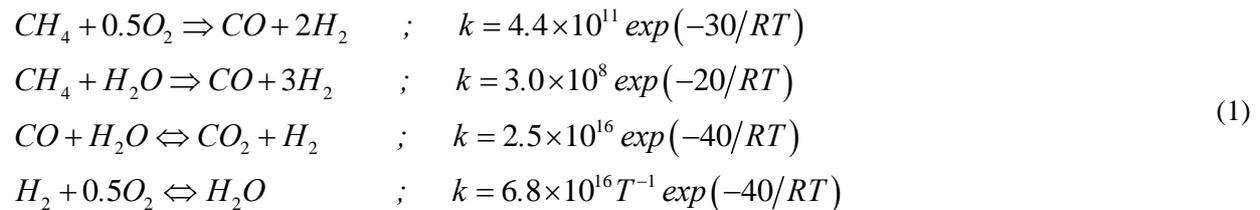
The HM1 and HM3 flames which represent the MILD and flame-like conventional regimes, respectively, were investigated numerically in this study. Uniform velocity and composition profiles, presented in Table 1, are given to the unmixed fuel jet, coflow oxidizer and tunnel air inlet streams. Combustion products and part of non-reacted tunnel air exhaust through the exit which was treated as a pressure outlet. A zero-shear stress wall was adopted to the side boundary, instead of a more realistic pressure inlet/outlet conditions. However, as the tunnel air was considered wide enough this boundary condition was not affected the flame structure, while largely improved the convergence and simulation time.

Table 1. Boundary conditions for simulation setup [3]

Flame	Fuel jet				Oxidant coflow					Tunnel air		
	$Q$ (kg/s)	$T$ (K)	CH <sub>4</sub> (wt. %)	H <sub>2</sub> (wt. %)	$u$ (m/s)	$T$ (K)	O <sub>2</sub> (wt. %)	H <sub>2</sub> O (wt. %)	CO <sub>2</sub> (wt. %)	$u$ (m/s)	$T$ (K)	O <sub>2</sub> (wt. %)
HM1	3.12e-4	305	88	11	3.2	1300	3	6.5	5.5	3.2	294	23.2
HM3	3.12e-4	305	88	11	3.2	1300	9	6.5	5.5	3.2	294	23.2

### 3.2 Chemical kinetics mechanisms

The global mechanism of Jones-Lindstedt (JL) is a four-step reaction mechanism including 4 elements and 7 species with Arrhenius reaction rates as follows:



The first two irreversible global reactions are representing the breakdown of the hydrocarbon fuel. The first reaction is important at fuel-lean, and the second one is dominant at fuel-rich conditions. The third reaction is the water-gas-shift reaction and the fourth one describes the oxidation of hydrogen [11].

The detailed chemical mechanism KEE [12] includes 17 species and 58 reversible chemical reactions related to the oxidation of methane. The DRM-22 [13] also is a detailed chemical mechanism consists of 22 species and 104 reversible reactions for methane and ethane oxidation, unlike two previous mechanisms that were only for oxidation of methane [7].

### 3.3 Turbulence-Chemistry Interaction (TCI) model

#### 3.3.1 Eddy Dissipation Concept (EDC) model

The Eddy Dissipation Concept (EDC) combustion model provides an empirical expression for the mean reaction rate based on the assumption that the chemical reactions occur in the region of the flow where the dissipation of turbulent kinetic energy takes place. According to EDC model dissipation of energy to heat is performed in regions, for which the entire volume is only a fraction of the fluid volume. These regions are denoted as fine structures and they are believed to be vortex tubes, sheets or slabs, whose characteristic dimensions are in the same order of the Kolmogorov length scale [14]. From the concept of step-wise turbulence energy cascade [15], characteristic scales of the fine structure have been introduced in the EDC model as follows:

$$\gamma^* = \left( \frac{3C_{D_2}}{4C_{D_1}} \right)^{3/4} \left( \frac{\nu \mathcal{E}}{k^2} \right)^{3/4} = C_\gamma \left( \frac{\nu \mathcal{E}}{k^2} \right)^{3/4} \tag{2}$$

$$\tau^* = \left( \frac{C_{D_2}}{3} \right)^{1/2} \left( \frac{\nu}{\mathcal{E}} \right)^{1/2} = C_t \left( \frac{\nu}{\mathcal{E}} \right)^{1/2} \tag{3}$$

Here  $\gamma^*$  is the fine structure volume and  $\tau^*$  is the time scale for mass transfer between fine structure and surrounding fluid.  $C_{D_1}$  and  $C_{D_2}$  are the model constants set equal to 0.134 and 0.5 leading to fine structure volume and residence time constants equal to  $C_\gamma = 2.1637$  and  $C_t = 0.4083$ .

It has been demonstrated that a modification on the EDC model is necessary for treating turbulence-chemistry interaction under the MILD combustion conditions [7, 16]. This modification is mainly focused on the increasing mixing rate time scale between fine structures and surrounding fluids comparing with its default value.

### 3.3.2 Partially stirred reactor (PaSR) model

The Partially Stirred Reactor (PaSR) combustion model is an extension of the EDC approach. In this model, the computational cell is divided into two distinct areas; in one area all reactions occur, and in the other area no reaction occurs. The relationship between the concentrations in the computational cell is as follows:

$$c_1 = k^* c + (1 - k^*) c_0 \quad (4)$$

In which,  $c_0$  is the concentration in the feed stream of the cell or the initial concentration of the cell,  $c$  is the unknown concentration in the reaction zone,  $c_1$  is the reactor exit concentration or concentration of the cell, and  $k^*$  is the mass fraction of the mixture which reacts. The whole process can be described in two steps; in the first step, the initial concentration in reaction zone changes from  $c_0$  to  $c$ , in second step the reactive mixture  $c$  mixes with non-reactive mixture  $c_0$  by available turbulence in the cell to produce the output concentration  $c_1$ . The duration between  $c_0$  converting to  $c_1$  is called the integration time,  $\tau$ , and since the turbulence mixes  $c_0$  with  $c$ , the time between  $c$  and  $c_1$  is denoted as the characteristic time for turbulence,  $\tau_{mix}$ . Based on these time scales,  $k^*$  can be introduced as follows:

$$k^* = \frac{\tau}{\tau + \tau_{mix}} \quad (5)$$

There are several methods to calculate the mixing time scale  $\tau_{mix}$ . The method that gives the best results and OpenFOAM uses it, is the Taylor time scale which uses turbulence parameters as Eq. (6):

$$\tau_{mix} = C_{mix} \frac{k}{\varepsilon} \quad (6)$$

The model constant  $C_{mix}$  is equal to 1 for laminar flows, and varies between 0.001 to 0.3 for turbulent flows depending on the flow turbulency. Reduction of flow turbulency, increases the value of  $C_{mix}$ .

There is another time scale in PaSR model called chemical time scale and defines as follows:

$$\frac{1}{\tau_{ch}} = - \frac{\partial f_m}{\partial c_r} \quad (7)$$

In which,  $\tau_{ch}$  is the chemical time scale,  $f_m$  is the reaction rate at the reaction zone and  $c_r$  is the concentration of reference specie. Since  $c$  is unknown sub-grid information, correlation between grid level and sub-grid level must be determined. This relation is as follows:

$$f_m(c) = \kappa f_m(c_1) \quad (8)$$

where:

$$\kappa = \frac{\tau_c}{\tau_c + \tau_{mix}} \quad (9)$$

## 4. Results and discussion

### 4.1 Comparison of combustion models

Figure 2 shows the effect of combustion models on the prediction of temperature and major species mass fraction at two axial locations for HM1 and HM3 flames. As can be seen, using the KEE mechanism, the PaSR combustion model can predict temperature and mass fraction of species better than the EDC model. This arises from the fact that in the EDC combustion model, the outlet concentration of computational cell is considered equal to reactor (fine structure) concentration, and hence, fast chemistry assumption establishes like the situation occurs in well-stirred reactors. However, in the PaSR approach, the reactor outlet mixes with non-reactive mixture and produces the cell outlet concentration. As generally known, in MILD combustion the reaction rates are slow, and fast chemistry assumption is not true. Therefore, it can be concluded that the PaSR approach is more appropriate than the EDC model for MILD combustion. However, the best results, both for temperature and combustion products mass fractions belongs to the modified EDC model for MILD combustion proposed in [7]. Note that despite more relative accuracy of the PaSR model in comparison with the EDC model, the PaSR model still has low accuracy for predicting the behavior of MILD combustion and requires more investigations for MILD combustion regime.

### 4.2 Comparison of chemical kinetics

Due to the excellence of the PaSR combustion model, the simulations with kinetic mechanisms in this section were performed using the PaSR model. As can be seen in Figure 3, the JL chemical mechanism can predict temperature and major species profiles with reasonable accuracy. In the case of temperature, the accuracy of JL mechanism is even higher than the detailed mechanism DRM-22. The reason is that the detailed mechanism DRM-22 involves reactions for methane ( $C_1$ ) and ethane ( $C_2$ ). The existence of  $C_2$  reactions in the kinetic mechanism DRM-22 violates reaction path which actually did not occur in the methane/hydrogen combustion. In other words, the negative impact of  $C_2$  existence in the makes the DRM-22 mechanism lead to overestimation of temperature at both upstream and downstream locations in both HM1 and HM3 flames.

Figure 4 reveals that despite the ability to predict the temperature and major species profile, the global kinetic mechanism JL overestimates mass fraction of carbon monoxide. The reason is that the detailed reaction paths for production and consumption of CO are not considered in the JL mechanism. As can be seen in Figure 4, among the three global and detailed chemical mechanisms investigated here, the KEE mechanism provides best prediction for minor species like CO.

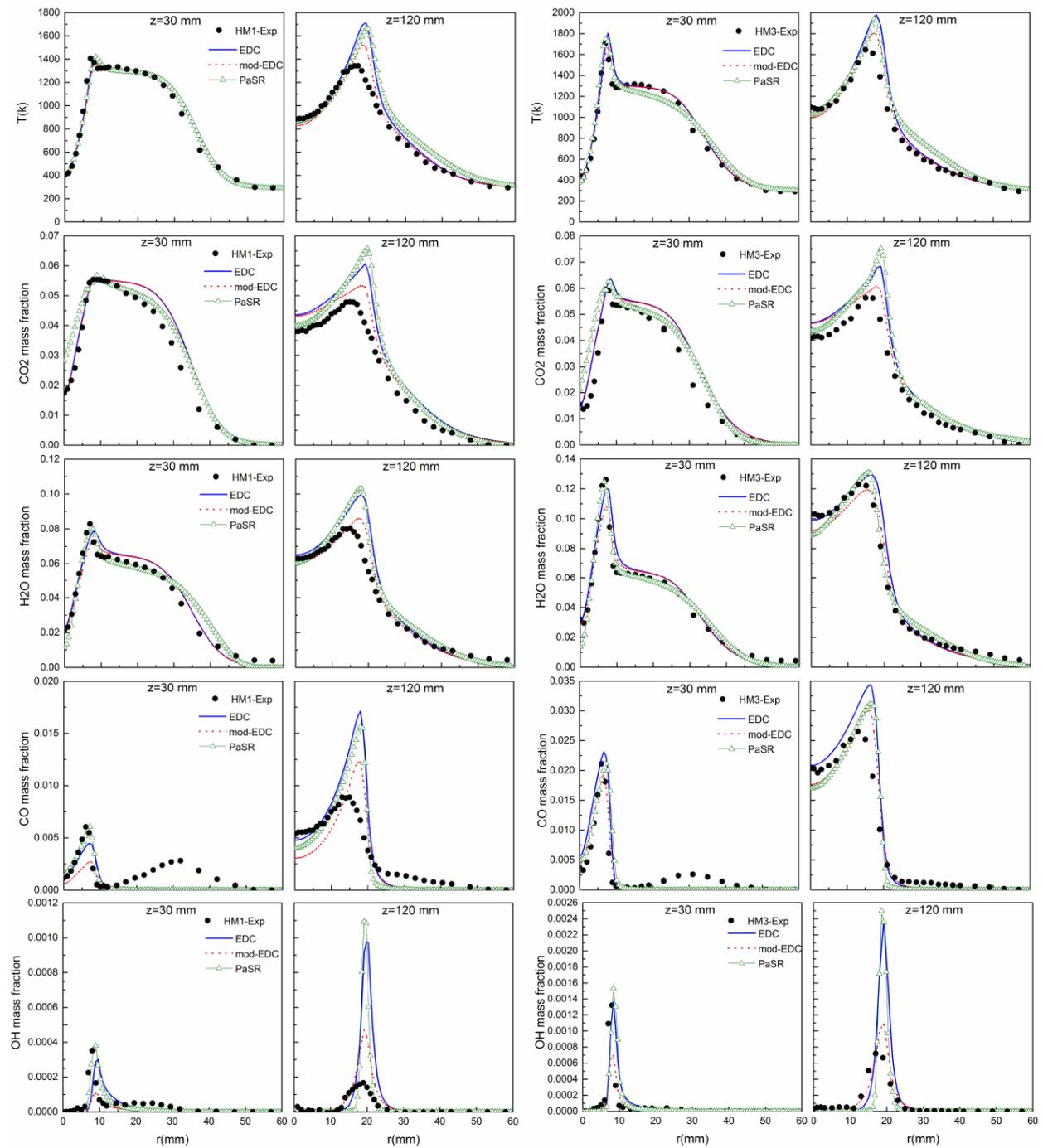


Figure 2. Comparison between profiles of experimental temperature and major and minor species, and those predicted with the EDC, modifies EDC and PaSR for HM1 and HM3 flames

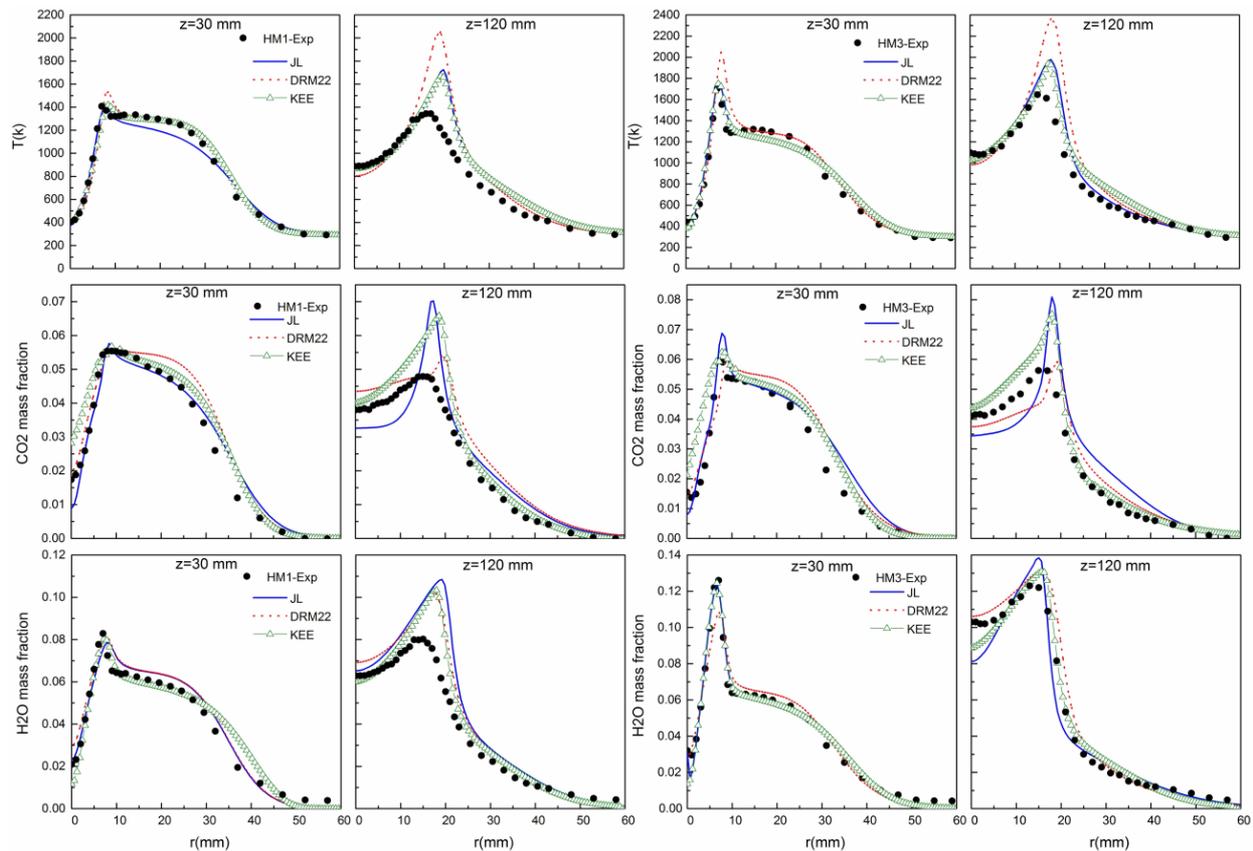


Figure 3. Comparison between profiles of experimental temperature and major species, and those of predicted with KEE, DRM-22 and JL kinetic mechanisms for HM1 and HM3 flames

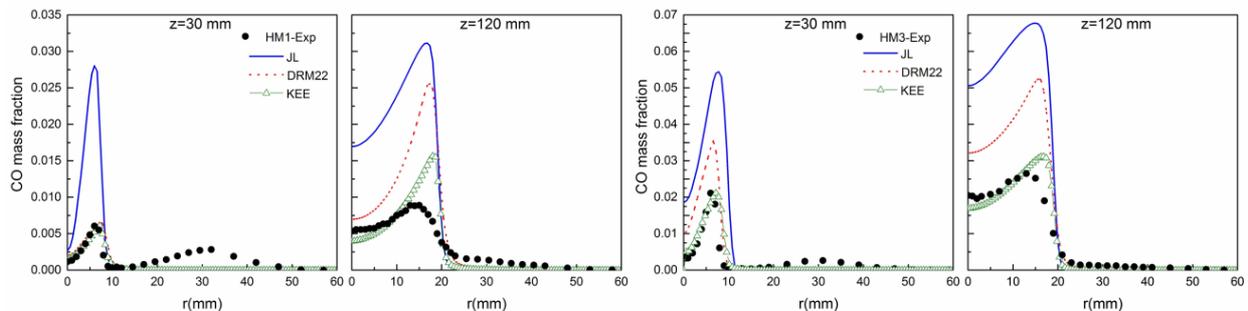


Figure 4. Comparison between profiles of experimental minor specie CO and predicted with the KEE, DRM-22 and JL mechanisms for the HM1 and HM3 flames

## 5. Conclusion

In this paper, various global and detailed chemical mechanisms together with two combustion models (EDC and PaSR) were studied in the context of turbulent jet flames issuing into a heated and diluted coaxial oxidizer stream. It was found that PaSR combustion model is more appropriate than the EDC model to simulate the behavior of MILD combustion. Also to predict the temperature and major species, the JL chemical mechanism can be used. The global chemical mechanism of JL with much less computational cost than the detailed mechanisms of KEE and DRM-22, can predict the temperature and major species profiles for MILD combustion with a reasonable accuracy. However, for accurate prediction of minor species like CO, detailed mechanisms must be employed.

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