EXPERIMENTAL AND NUMERICAL ANALYSIS OF SYNGAS MILD COMBUSTION

S.R. Shabanian*, M. Derudi, M. Rahimi*, A. Frassoldati**, A. Cuoci**, T. Faravelli****

masoudrahimi@yahoo.com; alessio.frassoldati@polimi.it

* CFD research center, Chemical Engineering Department, Razi University, Kermanshah, Iran

** Politecnico di Milano, Dipartimento di Chimica, Materiali e Ingegneria Chimica "G. Natta", Milano, Italy

Abstract

In this study, a CFD model was developed to predict NOx emissions, temperatures and species mole fractions in a Mild combustion experimental burner which was fed with hydrogen and hydrogen/CO_2/H_2O mixtures. Numerical simulations are performed with three turbulence models, three combustion models and two kinetic mechanisms. The temperature and flow fields data are exported to KPP numerical tool for prediction of NOx. It was found that the KPP and CFD results are in good agreement with experimental observations only when the RSM-transition turbulence model together with modified EDC and POLIMI 1101 syngas mechanism are employed in the model.

1. Introduction

Mild combustion [1], also known as flameless [2] or HiTAC [3] is a technology which offers efficient combustion with low emissions of pollutants. This technology is based on the use of high dilution of fuel, flue gases and preheated air to form a more uniform combustion region with lower temperature peaks. Derudi et al. [4] showed that Mild combustion can be applied for the coke oven gas (CH_4/H_2 mixture) using sufficiently high dilution ratios. Galletti et al. [5] investigated flame and Mild combustion regimes in a lab-scale burner for COG and showed that the NNH and N_2O routes are the dominant pathways. Parente et al. [6] performed an experimental and numerical analysis of a Mild combustion burner fed with CH_4 and CH_4/H_2 mixtures. Mild combustion of hydrogen-containing fuels was investigated also by Yu et al. [7]. In this work, experimental runs have been carried out in a lab-scale burner fed with H_2 and H_2/CO_2/H_2O mixtures in order to assess the Mild combustion regime and measure NOx and CO emissions. Then, a comparison between experimental results and CFD predictions has been performed in order to gain insight into the conditions at which the burner is operated.

2. Experimental apparatus

The experimental setup consists of a laboratory-scale atmospheric burner, an air/fuel flow-rate control system and a sampling and measurement system for measuring the temperature and exhaust compositions. The characteristics of this burner are discussed in detail elsewhere [4]. It is a quartz tube that consists of two

main sections: combustion chamber and air preheating region. Both sections of the burner are embedded in refractory insulated electrical ovens. The air preheater provides temperature up to 1300°C, while the combustion chamber oven is used only to monitor and minimize heat losses to the surrounds. Air and gaseous fuel are fed through a high velocity nozzle that is located in the bottom of the chamber. The length and radius of the chamber are 0.33 m and 0.025 m, respectively. The radius of nozzle is 0.0015 m and the nozzle enters in the chamber for 0.03 m. The burner also has a secondary air inlet only used during the start-up [4]. The exhausts go out from one central and three eccentric outlets located on the top of the combustion chamber; they are sampled, dried and analyzed by means of an on-line GC (Horiba PG-250), which measures NOx, O_2, CO and CO_2 while temperatures at two different positions inside the burner are continuously monitored.

3. Numerical model

The abovementioned experimental conditions have been modelled. Three runs of experiments were investigated in this work. In the first run the burner was fed with pure hydrogen, whereas with a $H_2/CO_2/H_2O$ (40/10/50 % by vol.) in the other runs (Table 1). The numerical model was developed using FLUENT™ version 6.3.26 using a 2D steady-state simulation. The computational domain (0.33 × 0.025 m) was described using a structured grid with ~65,500 cells. The grid-independency of the results was verified using a finer grid with ~171,000 cells. Three different turbulence models were used: standard k-ε (SKE), Reynolds stress model, and k-ω. When k-ω or RSM models were used, the Transitional flows available in the CFD code was enabled in order to model the flow with low Reynolds number inside the burner. The discrete ordinate (DO) method together with the Weighted-Sum-of-Gray-Gases (WSGG) model was used to solve the radiative transfer equation. The governing equations were discretized in the whole domain using the second-order schemes. The SIMPLE algorithm was applied to handle velocity-pressure coupling. The numerical computation was considered to be converged when the residuals for all equations were lower than 1×10^{-6}. The contour plot of temperature was also monitored and the temperature values in some selected positions of the chamber were used as additional convergence criterion.

Table 1. Experimental and modelling runs investigated.

Run number	H_2 (Nml/min)	Air1 (Nml/min) (preheated)	N_2 (Nml/min) (preheated)	CO_2 (Nml/min)	H_2O (Nml/min)	Preheater temperature (K)
1	407.6	999.5	1293.1	0	0	1173
2	596.6	1463.1	2705.6	149	745	1373
3	596.6	1463.1	543.3	149	745	1373

3.1. Turbulence/chemistry interaction models

In this work, Turbulence/chemistry interactions have been modelled with two main approaches: the Eddy dissipation/Finite Rate (ED/FR) and the Eddy Dissipation Concept (EDC). The EDC model has been largely used for conventional combustion systems, for which provides precise results and allows incorporating detailed kinetics in a computationally reasonable method. Recently, some researches have been done to discuss about the use of EDC model for non conventional systems. De et al. [8] and Aminian et al. [9] proposed a modified EDC model to improve model predictions for Mild combusion conditions. In this study, the effect of the modified EDC, obtained by changing of residence time constant of the EDC model (3 instead of 0.4083) was also adopted.

3.2. Kinetic mechanisms and NOx formation models

Two different kinetic mechanisms were employed to explain the oxidation of the $H_2/CO_2/H_2O$ mixture: global kinetic rates [10] with the ED/FR and EDC models, and a detailed mechanism POLIMI-H_2CO1101 [11] with the EDC.
A numerical tool called Kinetic Post Processor (KPP) is employed for calculating NOx emissions. Details on the KPP can be found elsewhere [12, 13]. The KPP uses the input data of temperature and flow fields calculated by the CFD code and each computational cell is modelled using a chemical reactor. The kinetic mechanism used in the KPP calculations is the same used in the CFD modelling but also includes the NOx chemistry: POLIMI-H_2CO1101NOx [11].

4. Results and discussion

4.1. Effect of turbulence model

Precise prediction of turbulent mixing is important in modelling turbulent combustion because it has a large effect on the flow field and turbulence–chemistry interaction. In this section, predicted temperatures and CO concentrations obtained with different turbulence models, in combination with the modified EDC model and POLIMI-H_2CO1101 mechanism, are compared with the results of the experiments of Table 1.

Table 2. Experimental and predicted values using various turbulence models

CO (ppm, dry basis)		EXP	SKE	k-ω-Transition	RSM-Transition
Run 1	CO (ppm)	0.5	0	0	0
	Temperature (K)	1060	1090	1090	1080
Run 2	CO (ppm)	130	2	42	129
	Temperature (K)	1284	1335	1330	1290
Run 3	CO (ppm)	18	0.7	6	23.2
	Temperature (K)	1285	1300	1294	1280

Table 2 shows middle temperature and outlet CO concentration for the investigated runs. It can be observed that all three turbulence models predict temperature well, although the RSM-Transition gives a slightly better prediction. For the CO concentration, there are large differences between SKE and k-ω-Transition predictions and the measurements; the performance of neither SKE nor k-ω-Transition is satisfactory. On the contrary, CO concentration predictions of RSM-Transition model are in good agreement with measurements.

4.2. Effect of turbulence/chemistry interaction models

The effect of the combustion models and kinetic mechanisms on the temperature was also studied. The ED/FR and modified EDC with two-step chemistry as well as the EDC and modified EDC with POLIMI syngas mechanism were used to model the combustion of $H_2/CO_2/H_2O$ mixture (Run 2, Table 1).

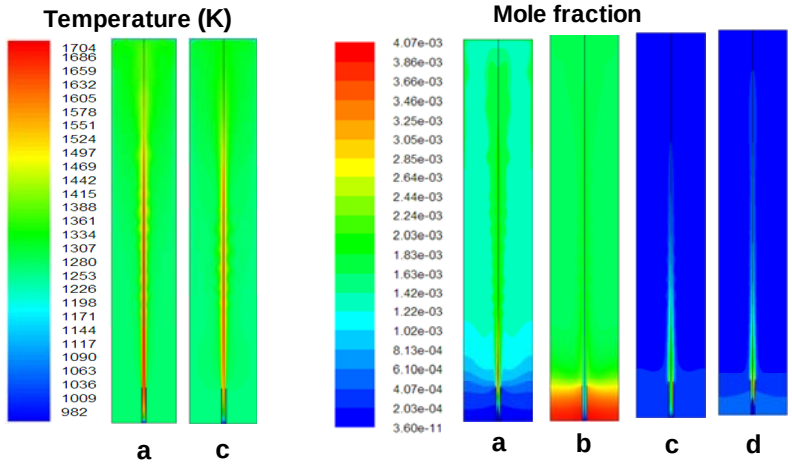

Figure 1. Temperature and CO distribution in the burner fed with $H_2/CO_2/H_2O$ mixture (Run 2, Table 1), predicted using: (a) ED/FR with 2-step mechanism, (b) modified EDC with 2-step mechanism, (c) modified EDC with POLIMI 1101, (d) EDC with POLIMI1101

Fig. 1 shows the temperature distribution inside the burner obtained with ED/FR with two step mechanism and modified EDC with POLIMI syngas mechanism (the models which have largest difference in temperature predictions). The modelling results show that there is a high temperature reaction zone near the central axis of the burner with different peak value of temperature for different models and mechanisms. The ED/FR model with 2 step mechanism predicts a maximum temperature of 1704 K, while the modified EDC with POLIMI mechanism gives a peak of 1615 K. Although the temperatures are almost similar for all the mechanisms, the CO mole fraction distributions are quite different. As shown in Fig. 1, when the 2 step mechanism is used, the value of CO emission is higher than that of the detailed mechanism. This might be due to incorrect prediction of equilibrium constant of the CO oxidation reversible reaction.

4.3. Prediction of CO and NO emissions

Fig. 2 shows the predicted profile of carbon monoxide (CO) along the central axis of burner for two experimental runs (runs 2, 3 of Table 1). The figure reveals that the CO concentration increases at the beginning of combustion chamber and then decreases for higher axial distances.

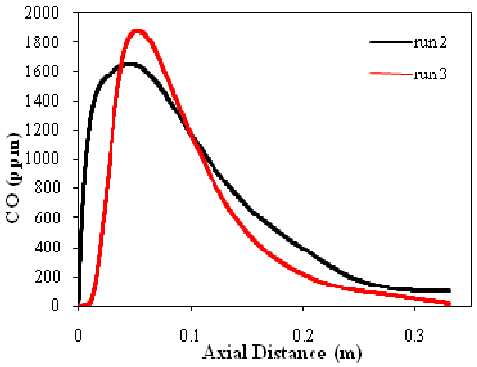

Figure 2. Predicted profile of CO along the burner axis for runs 2 and 3 of Table 1: RSM-Transition model, modified EDC-POLIMI 1101 mechanism.

This trend can be explained by CO formation in high temperature region at the beginning of chamber and then CO consumption along the burner length. It is useful to mention that CO formation occurs from CO_2 decomposition because CO_2 is not stable in high temperature region. In addition, it can be observed when the flow rate of N_2 in inlet mixture is increased, the peak value of CO profile at the beginning of chamber decreases. This can be due to a decrease of the peak temperature induced by N_2 increase in the inlet.

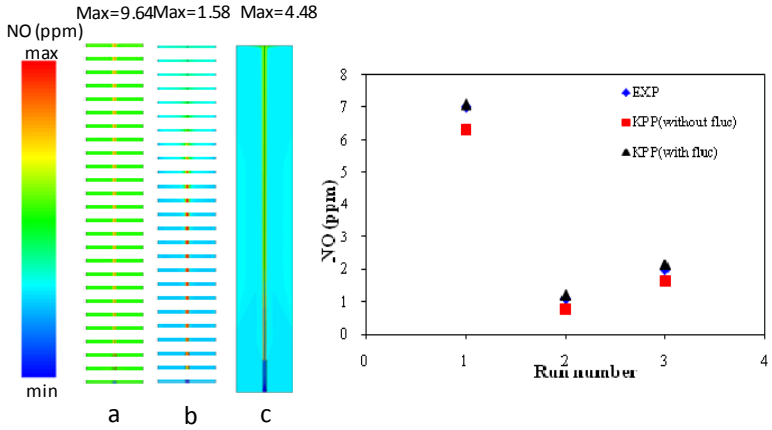

Figure 3. NO field (left) as well as prediction and experimental values of NO (right, dry basis) at the burner outlet for different runs: a=run1, b=run2 and c=run3.

Fig. 3 shows the predicted NO mole fraction for the investigated runs. The temperature fields for the prediction of NO were provided by the modified EDC and POLIMI syngas mechanism. The maximum value of NO belongs to run 1. This can be due to higher peak value of temperature in the burner in these conditions, i.e. lower dilution with inert gases. In addition, a high concentration region of NO

can be observed near the central axis of burner in all three runs. The temperature, which controls the thermal NOx formation, is high in the regions near the central axis. This could be the reason of high concentration of NO in the central regions of burner. Moreover, H and O radicals involved in the NNH and N_2O mechanisms have higher concentrations in this flame region. Fig. 3 shows also the predicted and measured values of NO emissions. It can be observed that KPP is a powerful tool for the prediction of NO in a low turbulence regime as the one found for the syngas Mild combustion in this study. The predictions are improved by employing temperature fluctuations in KPP. A decrease of 6%-33% on the predicted values is observed when T fluctuations are not taken into account.

Conclusion

A numerical and experimental study of a Mild combustion burner fed with H_2 and $H_2/CO_2/H_2O$ mixtures has been presented. Results showed that the turbulence model and kinetic mechanisms are important factors in the simulation of the Mild combustion regime. SKE and k-ω-Transition models were found to be unable to reproduce the experimental values of CO within the exhausts. The temperature distributions inside the combustion chamber are almost similar for the all used combustion models and kinetic mechanisms, but the CO mole fraction distributions are quite different. NOx and CO results predicted with a Modified EDC combustion model, POLIMI 1101 mechanism and the RSM-Transition turbulence model are in good agreement with the experimental results. The results also revealed that as the nitrogen flow rate in the gas mixture increased (runs 2 and 3), the CO mole fraction at the burner outlet increased.

References

[1] Hasegawa, T., Mochida, S., Gupta, A., *AIAA J. Propul. Power* 2: 233–239 (2002).

[2] Wünning, J.A., Wünning, J.G., *Progr. Energy Combust. Sci.* 23: 81–94 (1997).

[3] Cavaliere, A., de Joannon, M., *Progr. Energy Combust. Sci.* 30:329–366 (2004).

[4] Derudi, M., Villani, A., Rota, R., *Proc. Combust. Inst.* 31: 3393-3400 (2007).

[5] Galletti, C., Parente, A., Derudi, M., Rota, R., Tognotti L., *Int. J. Hydrogen Energy* 34: 8339-8351 (2009).

[6] Parente, A., Galletti, C., Tognotti , L., *Int. J. Hydrogen Energy* 33: 7553-7564 (2008).

[7] Yu, Y., Gaofeng, W., Qizhao, L., Chengbiao, M., Xianjun, X., *Int. J. Hydrogen Energy* 35: 2694-2697 (2010).

[8] A., De, E., Oldenhof, P., Sathiah, D., Roekaerts, Flow Turbulence Combust. DOI 10.1007/s10494-011-9337-0.

[9] Aminian, J., Galletti, C., Shahhosseini, S., Tognotti, L., *Proc. of the 5th European Combustion Meeting*, Cardiff, UK, 2011, pp 1-6.
[10] Westbrook, C.K., Dryer, F.C., *Prog. Energy Combust. Sci.* 10:1 (1984).
[11] Frassoldati, A., Faravelli, T., Ranzi, E., *Int. J. Hydrogen Energy* 32: 3471-3485 (2007), Available at: (http://www.chem.polimi.it/CRECKModeling).
[12] Cuoci, A., Frassoldati, A., Buzzi Ferraris, G., Faravelli, T., Ranzi, E., *Int. J. Hydrogen Energy* 32: 3486–3500 (2007).
[13] Frassoldati, A., Cuoci, A., Faravelli, T., Ranzi, E., Astesiano, D., Valenza, M., Sharma, P., *Metall. Plant Technol. Int.* 31: 44–46 (2008).

10.4405/34proci2011.II18