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Chemical and Physical Effects of Carbon Dioxide Injection with Different Preheating Temperature in Flameless Combustion

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ABSTRACT: The purpose of the present study is the numerical simulation of the flameless burner with carbon dioxide injection into the oxidizer stream using OpenFOAM software. Also, the effect of different amounts of oxidizer preheating temperature has been studied. In order to perform simulations from the partially stirred reactor combustion model, the standard k-ε turbulence model with modified coefficients and discrete phase radiation model with the calculation of adsorption and emission coefficients using weighted sum of gray gases mode model with non-gray gas coefficients have been used. The results of the present study indicate that the physical effects of carbon dioxide degradation will reduce the amount of heat release and the amount of carbon monoxide produced, while the chemical effects of this injection result in a significant increase in these amounts. Increasing the mass fraction of injection from 0.25 to 0.75 leads to a change in the maximum mass fraction of carbon monoxide produced from 0.05 to 0.072. Also, the chemical effect of the injection changes the flame structure and increased carbon monoxide emissions by increasing the preheating temperature. The chemical effect of carbon dioxide injection on the production of NOx pollutants is such that, with increasing temperature, the amount of NOx emission is increased.

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1. INTRODUCTION

Flameless combustion is one of the combustion regimes based on the strong recirculation of the combustion products into the oxidizer to dilute and pre-heat the reacting mixture. Therefore, the structure of the oxidizer plays a major role in the heat transfer and flame structure in this combustion process. Extensive studies have been done on the effect of oxidizer structures on the flameless combustion. Tu and et al. [1] examined the physical and chemical effects of Carbon dioxide (CO_2) injections into the hot co-flow in the flameless combustion burner. The results show that the replacement of CO_2 with N_2 causes delayed ignition of oxy-fuel combustion.

In the present study, the physical (specific heat capacity, radiation properties, molecular mass, density and molecular diffusion coefficients of carbon dioxide in comparison with nitrogen) and chemical (active carbon dioxide in chemical reactions compared with nitrogen) effects of replacement of CO_2 by N_2 has been investigated. In addition, the oxidizer pre-heating temperature effects have been discussed on the physical and chemical effects of carbon dioxide injections.

2. COMPUTATIONAL DETAILS

In order to perform the numerical simulations, flameless combustion burner made by Dally et al. [2] has been used.

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In accordance with Fig. 1, the axisymmetric computational domain is used for the simulations. The governing boundary conditions are shown in Fig. 1 and these applied in accordance with Table 1.

OpenFOAM software has been used to perform numerical simulations. The standard k-ε model was used with the modified coefficient $C_{\varepsilon 1}$ from 1.44 to 1.6. In addition, for the modeling interactions of turbulence and chemistry of reactions, the Partially Stirred Reactor (PaSR) combustion model has been used.

Discrete Ordinate (DO) model is used to calculation of radiative heat transfer. Also, the GRI2.11 chemical mechanisms have been used due to better prediction of the temperature and combustion species distribution (especially NOx) [3].

The PIMPLE algorithm is used for the elimination of coupling between velocity and pressure. The convergences criteria of the solution also take into account the residuals of all equations equal to 10^{-7}.

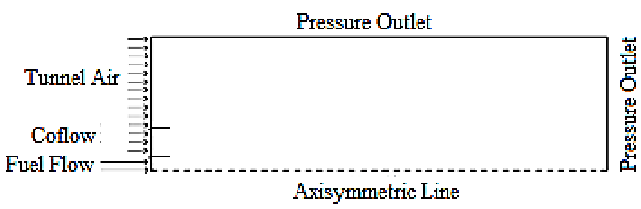

Fig. 1: Computational domain and boundary conditions

Table 1. The governing boundary conditions

No.	$T_{product}$ (K)	Co-flow Mass Fraction (%)	Tunnel Air Mass Fraction (%)
1	1300	O_2=3 , CO_2=5.5 , H_2O=6.5 , N_2=85 , XCO_2=0	O_2=23 , CO_2=0 , H_2O=0 , N_2=77 ,XCO_2=0
2	1300	O_2=6 , CO_2=5.5 , H_2O=6.5 , N_2=82 , XCO_2=0	O_2=23 , CO_2=0 , H_2O=0 , N_2=77 ,XCO_2=0
3	1300	O_2=9 , CO_2=5.5 , H_2O=6.5 , N_2=79 , XCO_2=0	O_2=23 , CO_2=0 , H_2O=0 , N_2=77 ,XCO_2=0
4	1300	O_2=3 , CO_2=0 , H_2O=0 , N_2=97 , XCO_2=0	O_2=23 , CO_2=0 , H_2O=0 , N_2=77 ,XCO_2=0
5	1300	O_2=3 , CO_2=25 , H_2O=0 , N_2=72 , XCO_2=0	O_2=23 , CO_2=25 , H_2O=0 , N_2=52 ,XCO_2=0
5X	1300	O_2=3 , CO_2=0 , H_2O=0 , N_2=72 , XCO_2=25	O_2=23 , CO_2=0 , H_2O=0 , N_2=52 ,XCO_2=25
6	1300	O_2=3 , CO_2=50 , H_2O=0 , N_2=47 ,XCO_2=0	O_2=23 , CO_2=50 , H_2O=0 , N_2=27 ,XCO_2=0
6X	1300	O_2=3 , CO_2=0 , H_2O=0 , N_2=47 ,XCO_2=50	O_2=23 , CO_2=0 , H_2O=0 , N_2=27 ,XCO_2=50
7	1300	O_2=3 , CO_2=75 , H_2O=0 , N_2=22 ,XCO_2=0	O_2=23 , CO_2=75 , H_2O=0 , N_2=2 ,XCO_2=0
7X	1300	O_2=3 , CO_2=0 , H_2O=0 , N_2=22 ,XCO_2=75	O_2=23 , CO_2=0 , H_2O=0 , N_2=2 ,XCO_2=75
8	1100	O_2=3 , CO_2=0 , H_2O=0 , N_2=97 ,XCO_2=0	O_2=23 , CO_2=50 , H_2O=0 , N_2=27 ,XCO_2=0
9	1100	O_2=3 , CO_2=50 , H_2O=0 , N_2=47 ,XCO_2=0	O_2=23 , CO_2=50 , H_2O=0 , N_2=27 ,XCO_2=0
9XT	1100	O_2=3 , CO_2=0 , H_2O=0 , N_2=47 ,XCO_2=50	O_2=23 , CO_2=0 , H_2O=0 , N_2=2 ,XCO_2=50

3. RESULTS AND DISCUSSION

The grid independency results show that the network with 42550 cells has independent results for the simulations.

The results of the solver validation are presented. An average error of 10% indicates a good agreement between the results with experimental data (Fig. 2).

As shown in Fig. 3, the physical effect of CO_2 injection leads to a significant reduction in the maximum Hydroxyl (OH) mass fraction, which increases with an increase in CO_2 injection. decreasing of OH produced is due to higher heat absorption by CO_2 injection due to its higher heat capacity than nitrogen. The chemical effect of CO_2 injection is such that it leads to an increase in the OH mass fraction through the reaction $H + O_2 \leftrightarrow O + OH$.

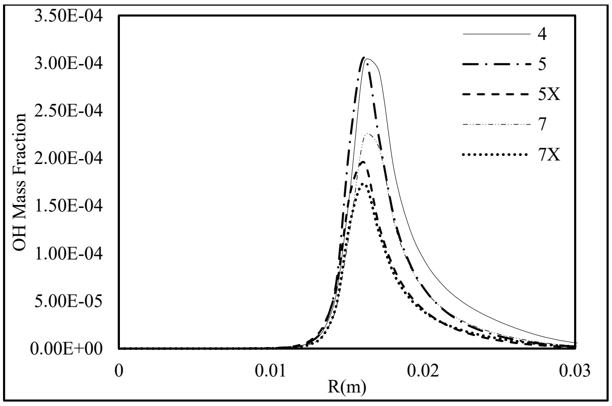

Fig. 3. OH distribution in 90 cm from inlets in different CO_2 mass fraction injection

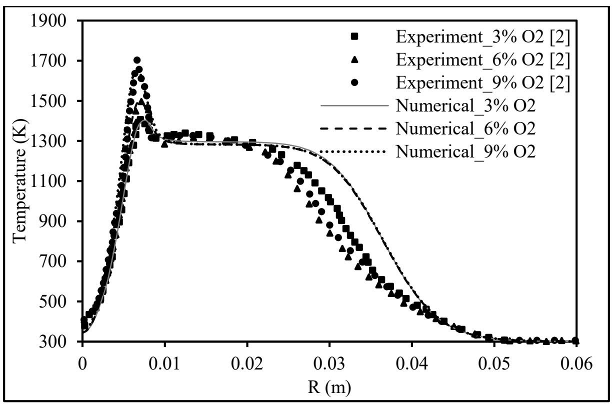

Fig. 2.Temperature variation in 90 cm from inlets

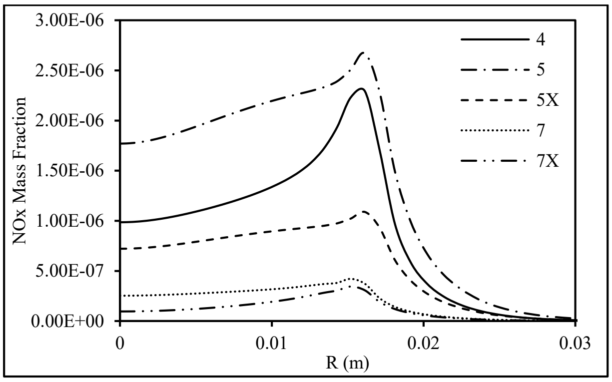

Fig. 4: NOx distribution in 90 cm from inlets in different CO_2 mass fraction injection

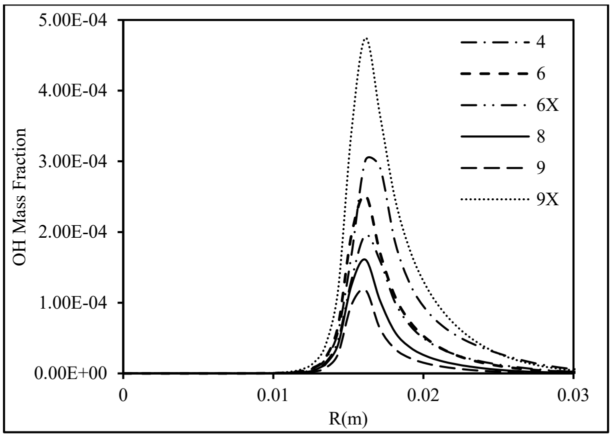

Fig. 5: Effect of co-flow pre-heating temperature on the CO_2 injection in oxidizer on OH distribution

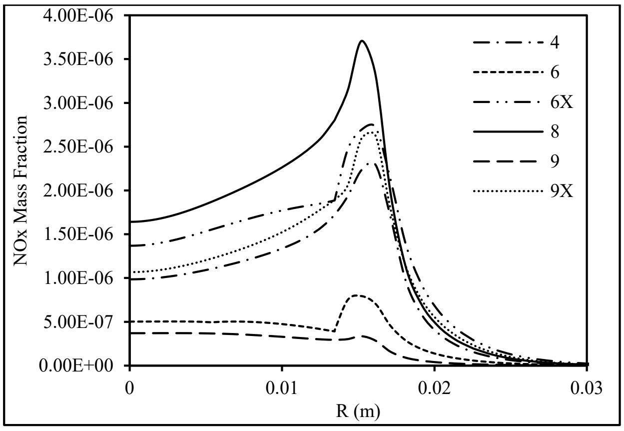

Fig. 6. Effect of coflow pre-heating temperature on the CO_2 injection in oxidizer on NOx distribution

The effects of CO_2 injection into the oxidizer is shown in Fig. 4. As can be seen, injection of high levels of carbon dioxide, physically and chemically, results in a reduction in the mass fraction of NOx. while CO_2 injection equals 25% of the oxidizer mass fraction of different physical and chemical behaviors. In this case, the physical effect of the injection results in a reduction in the NOx production due to a decrease in the maximum temperature and also a reduction in the amount of nitrogen available for the production of NOx, while the HCN behavior results in a significant increase in the production of NOx.

The OH mass fraction increases in higher preheating temperature. The increase in temperature led to a further dissociation of H_2O through the reaction of OH + H_2↔H + H_2O, which increases the hydroxyl produced.

The physical impact of the injection of CO_2 into oxidizer leads to a significant decrease in NOx emissions due to a reduction in the maximum temperature. Contrary to the physical effect, the chemical effect of carbon dioxide injections results in an increase in the amount of NOx released. This issue is due to the presence of CO_2 in the reaction N_2 + CO_2↔NO + NCO (Fig. 6).

4. CONCLUSION

The important results of the chemical and physical effects of CO_2 added to oxidizer in different preheating temperature into the Flameless burner are included: The increase in the amount of CO_2 injected leads to a decrease in the rate of reactions by reducing the concentration of radical hydroxyl. In addition, with increasing injection rates due to the decrease in maximum temperature, NOx contamination levels are significantly reduced; increasing the oxidizer pre-heating temperature increases the chemical effect of CO_2 injection into the oxidizer stream.

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