Numerical Study of Oxygen Enrichment on NO Pollution Spread in a Combustion Chamber

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Abstract-In this study, a 3D combustion chamber was simulated using FLUENT 6.32. Aim to obtain detailed information on combustion characteristics and nitrogen oxides in the furnace and the effect of oxygen enrichment in a combustion process. Oxygenenriched combustion is an effective way to reduce emissions. This paper analyzes NO emission, including thermal NO and prompt NO. Flow rate ratio of air to fuel is varied as 1.3, 3.2 and 5.1 and the oxygen enriched flow rates are 28, 54 and 68 lit/min. The 3D Reynolds Averaged Navier Stokes (RANS) equations with standard k-ɛ turbulence model are solved together by Fluent 6.32 software. First order upwind scheme is used to model governing equations and the SIMPLE algorithm is used as pressure velocity coupling. Results show that for AF=1.3, increase the oxygen flow rate of oxygen reduction in NO emissions is Lance. Moreover, in a fixed oxygen enrichment condition, increasing the air to fuel ratio will increase the temperature peak, but not the NO emission rate. As a result, oxygen enrichment can reduce the NO emission at this kind of furnace in low air to fuel rates.

Keywords—Combustion chamber, Oxygen enrichment, Reynolds Averaged Navier- Stokes, NO emission

I. INTRODUCTION

DUE to increased demand for energy, clean cut fossil fuel resources, and growing concern over environmental pollution and global warming, mainly caused by the greenhouse effect is a urgent need for advanced energy systems to provide efficient power, with harmful consequences there is less environmental.

Currently, the main pollution from nitrogen oxides destroys ozone in the upper atmosphere. Nitrogen oxides and nitrogen oxide containing complex reaction mechanisms, resulting in accelerated depletion of ozone in the oxygen cycle are on the ground. Hence, the combustion engineers to develop various strategies used to reduce NO_x emissions and improve combustion process have focused. Oxy-fuel firing is more energy efficient and environmental friendly than conventional air-fuel firing and its application to reheating furnaces has begun since 1990s.

During air-fuel combustion, the chemically inert nitrogen in the air dilutes the reactive oxygen and carries away some of the energy in the hot combustion exhaust gas. Increased oxygen in the combustion air can cause loss of energy in the exhaust gases and reduce and increase the efficiency of the heating system. No_x are very hazards [1], because the produced pollution by nitrogen oxides have remained harmful effects on human health and the environment, play an important role the formation of ozone hole and react at atmosphere pressure and form ozone what one of the main sources of photochemical smog according to (1).

$NO_2 + Solar \quad Energy \longrightarrow NO + O + PhotochemicalSmog$ (1)

So, Combustion engineers have focused their attention to develop many strategies to reduce NO_x emission.

Two general methods for reducing pollutants are unusable: improvement combustion cycle, treatment exhaust gases.

Today, oxygen enrichment combines with oxidizer in the chemical reaction to reduce NO to improve the combustion cycle. The main objective of this study was to compare the amount of air to fuel ratio of NO_x emissions, including and without oxygen enrichment.

Using oxygen enrichment, different percentages of air has been removed and will replace with O_2 , so N_2 is reduced in combustion chamber and also NO_x pollutant.

Oxygen enrichment reduces or eliminates the need for combustion air, resulting in less nitrogen oxide production. Oxy-fuel combustion also increases the flame temperature without increasing fuel cost [2].

Benefits of oxygen enrichment are [3]: lower emissions, increase efficiency, increase productivity, improve temperature stability and heat transfer, and reduce costs of fuel consumption and pollutants.

Frassoldati et al. performed an integrated CFD based procedure in order to determine NO_x emissions by a swirling confined flame [4]. A very detailed and comprehensive reaction schemes was used by the model based upon the results obtained from CFD computations.

The procedure was validated with high swirled confined natural gas diffusion flames. Hamzeh Jafar Karimi, Mohammad Hassan Saidi [5] had done computational method on a type reheating furnace in which combustion air was enhanced by oxygen.

The results showed that the best range of oxygen enrichments was between 21% and 45% by volume, as the higher slope of flame temperature and production increase occurs in this range.

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S.S. Daood, W. Nimmo, P. Edge, B.M. Gibbs [6] had worked on Deep-staged, oxygen enriched combustion of coal.

Resulting in comparison to air staged combustion, oxygen enriched air staged combustion at the 31% level of staging resulted in approximately 7%, 20% and 35% NO reduction for 28%, 30% and 35% overall oxygen concentration, respectively. Experimental evidence has also indicated that oxygen enrichment does appear to reduce NO levels along with improvement of carbon burnouts.

A numerical investigation of NO emission from an entrained flow reactor are done with L. Álvarez, M. Gharebaghi, J.M. Jones, M. Pourkashanian, A. Williams, J. Riaza, C. Pevida, J.J. Pis, F. Rubiera[7]. A decrease in NO emissions was observed when N_2 was replaced by CO_2 for the same oxygen concentration for both the experimental and computed results.

II. GOVERNING EQUATION

Combustion simulation of turbulent flow with heat transfer, species transport and chemical reactions is typically solved. FLUENT [8] to solve the physical equations (energy, continuity, momentum equations) using finite volume deals.

Continuity Equation

$$\frac{\partial}{\partial t}(\rho) + \nabla .(\rho V) = S_m$$
Momentum Equation
$$\frac{\partial}{\partial t}(\rho V) + \nabla .(\rho V V) = \nabla .((\mu + \mu_t)\nabla V) + F$$
(3)

Energy Equation

$$\frac{\partial}{\partial t}(\rho E) + \nabla .(\rho V E) = \nabla .((k + k_t)\nabla T) + \nabla .(\tau .V) - \nabla (pV)$$

$$+ S_r + S_h$$
(4)

It is common to use the Reynolds-averaged form of the governing equation in conjunction with a suitable turbulence model.

The 3D Reynolds Averaged Navier Stokes (RANS) equations together with standard k turbulence model [9] are solved by Fluent 6.32. Physical integration of the equations used in the finite volume method.

$$\frac{\partial}{\partial t}(\rho k) + \nabla (\rho V k) = \nabla \left(\frac{(\mu + \mu_t)}{\sigma_k}\nabla k\right) + G_k - \rho \varepsilon$$
(5)

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla (\rho V\varepsilon) = \nabla \left[\frac{(\mu + \mu_t)}{\sigma_{\varepsilon}} \nabla \varepsilon \right] + C_{1\varepsilon} \frac{\varepsilon}{k} G_k - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k}$$
(6)

Where $C_{1\varepsilon} = 1.44$ $C_{2\varepsilon} = 1.92$ $\sigma_k = 1$ $\sigma_{\varepsilon} = 1.31$

III. NITROGEN OXIDE MODELING

In this study, two different mechanisms have been identified for the formation and destruction of NO, i.e., thermal NO and prompt-NO mechanism:

The formation of thermal NO is determined by the following three extended Zeldovich mechanism:

$$O + N_2 \xleftarrow{k_1, k_2} NO + N \tag{7}$$

$$N + O_2 \xleftarrow{k_3, k_4} NO + O \tag{8}$$

$$N + OH \xleftarrow{k_5, k_6} NO + H \tag{9}$$

Based on the quasi-stead state assumption for N radical concentration, the net rate of NO formation via the foregoing reaction can be determined by:

$$\frac{d[NO]}{dt} = \frac{1}{1 + \frac{k_2[NO]}{k_3[O_2] + k_5[OH]}} * \\
\left[2k_1[O][N_2] - \frac{2k_2}{k_3[O_2] + k_5[OH]} * (k_4[O][NO]) + \\
k_6[H][NO] \right]$$
(10)

Where

$$k_i = A_i T^{B_i} \exp\left(\frac{-C_i}{T}\right) \tag{11}$$

Where T is temperature, K. The reaction constants, Ai, Bi and Ci, were taken from Baulch et al. [10].

IV. COMBUSTION MODELING

In the present study, a 3D combustion chamber was simulated by FLUENT 6.32. First, the geometry is modeled in GAMBIT. The computational domain is a rectangular cube which is 60 cm wide, 90 cm high and 190 cm long.

Fluent software uses two resolutions, namely pressure based and density based resolutions. In this study modeling is based on pressure. In order to resolve the chemical reaction and its modeling, species are selected from species transport in models menu. In reaction, volumetric option is selected. Then, inlet diffusion, diffusion energy source, full multi component diffusion, thermal diffusion options are all checked and eddydissipation is selected in turbulence-chemistry interaction menu. From Material menu, density option, incompressible gas is selected. Then, by clicking species, all components of reaction can be observed.

V.NUMERICAL CALCULATION

A standard k- ϵ turbulence model as a simplest complete model of turbulence is widely used in turbulent combustion simulation. The pressure velocity coupling is resolved using SIMPLE algorithm. The descritization model is first order upwind scheme. The grid independence was checked and finally a grid with 83320 cells was selected as the computational grid. Cells near the entrance of air and fuel in order to illustrate the rapid changes in the parameters refined (fig. 1).



Fig. 1 Computational Mesh in solution domain at plan Z=0.

After writing chemical reaction of methane combustion in stoichiometric and use from thermodynamic tables, adiabatic flame temperature calculates 2320°K. When the residual comes down to near zero and reach convergence, solution will be finish.

VI. BOUNDARY CONDITION

Flow conditions are steady, turbulent flow, heat transfer and chemical reactions, also under flow condition; Mach number is very low; hence, the flow in assumed incompressible.

Inlet temperature of 300 $^{\circ}$ K for all the input. Since the fuel and air are quite distinct, this model can be used effectively. In mixture material menu, methane-air is selected since methaneair reactions are involved. In reaction, volumetric option is selected.

VII. RESULT AND DISCUSSION

After numerical calculation, it is easy to see results. By plotting the NO mole fraction vs. X, according to the fig. 2, with the increase of air to fuel ratio, as expected, NO increases substantially due to an increase in N_2 inflow, while such NO changes are less with the increase of air to fuel ratio from 3.2 to 5.1.



Fig. 2 NO mole fraction along the torch centerline with different airfuel inlets and oxygen enrichment

Obviously, Minimum NO mole fraction happens when the AF ratio is 1.3. With air to fuel ratio of 3.2, as the intake oxygen discharge increases, more NO are produced.

The comparison of contours of NO mole fraction, also confirms this truth. For example, the contours in enriched oxygen flow rate =54 are shown in fig. 3.



Fig. 3 No mole fraction enriched combustion 54 lit/min, (a) AF = 1.3 (b) AF = 3.2, (c) AF = 5.1

There is a comparison between all of temperatures in fig. 4.



Fig. 4 compares temperature along the torch centerline with different air-fuel inlets and oxygen enrichment.

With the increase of air-fuel ratio, the maximum torch flame increases too. According to figure 4, this increase is very strict from air-fuel ratio of 1.3 to 3.2. The temperature becomes uniform along the torch centerline.

With oxygen enrichment, variations are observed in maximum temperature of AF ratio of 1.3. As the oxygen inlet increases, the temperature decreases dramatically. However, changes in oxygen enrichment are negligible in AF ratio of 3.2 and 5.1.

In fig. 5-7, NO mole fractions are plotted in each air to fuel ratio, separately. According to fig. 5, amount of NO decreases from normal combustion to 28 lit/min enriched oxygen, also from 28 flow rate to 54, but NO mole fraction increases from 54 lit min flow rate to 68 lit/min, so minimum pollutant related to NO mole fraction occurs at 54 lit/min enriched oxygen.



Fig. 5 NO mole fraction distribution at AF = 1.3



Fig. 6 NO mole fraction distribution at AF = 3.2



In 2005, M. Darbandi, A. Banaeizadeh and G. E. Schneider had been done numerical simulation on reacting flow [11] and compared their results with results of experimental data and other numerical results which is gotten by Elkaim, D., Reggio, M., and Camarero, R and Smoot, J.L, and Lewis, H.M. Fig. 8 plotted those results and results of this study and shows comparison between them. According to this figure, there is good agreement between all of results.



Fig. 8 Mixture fraction distribution of species and a comparison between present study, Elkaim et al. [12] and experimental data [13]

In summary, optimum way in NO production belongs to enriched oxygen with 54 lit/min flow rate and AF flow rate ratio=1.3. Some parameters of chemical reaction were checked and compared at state AF=1.3 for normal combustion and enriched oxygen flow rate= 54 lit/ min in below figures. For example, fig. 9 compares temperatures.



Fig. 9 Comparison of temperature along the axis of the combustion chamber (normal combustion and enriched combustion)

The temperature at 54 lit/min enriched combustion from 1m along combustion chamber is greater than normal combustion, considerably.



Fig. 10 Comparison of CH_4 mole fraction along the axis of the combustion chamber (normal combustion and enriched combustion)

Fig. 10 shows CH_4 mole fraction is approximately the same. According to figure 11, difference in O_2 mole fraction begins from 1m along chamber for two considered states, while before location 1m they are approximately the same.



Fig. 11 Comparison of O_2 mole fraction along the axis of the combustion chamber (normal combustion and enriched combustion)

Fig. 12 shows amount of CO_2 mole fraction vs. length of chamber. It is obvious that in each location amount of CO_2 mole fraction for 54 lit/min enriched combustion is greater than that for normal state.



Fig. 12 Comparison of CO_2 mole fraction along the axis of the combustion chamber (normal combustion and enriched combustion)

Fig. 13 is approximately the same fig. 12, by difference in vertical axis. It shows H_2O mole fraction vs. position.



Fig. 13 Comparison of H_2O mole fraction along the axis of the combustion chamber (normal combustion and enriched combustion)



Fig. 14 Comparison of N_2 mole fraction along the axis of the combustion chamber (normal combustion and enriched combustion)

At fig. 14 it can be seen comparison of N_2 mole fraction for two selected states.



Fig. 15 Comparison of NO mole fraction along the axis of the combustion chamber (normal combustion and enriched combustion)

Fig. 15 is most important graph. In that, NO mole fraction is shown for normal and 54 lit/min enriched combustion.

At finally, we will see comparison of all species mole fraction along the axis of the normal combustion and 54 lit/min enriched combustion.

VIII.CONCLUSION

Computational results for the pollutant emissions resulting from combustion of fuel are evaluated. A 3D combustion chamber was simulated using FLUENT6.32 software. Air/fuel ratio is varied as 1.3, 3.2 and 5.1 and the oxygen enriched flow rates are 28, 54, 68 lit/min. The results show that for AF=1.3, increasing oxygen flow rate at the oxygen lance decreases the NO emission. Minimum NO pollutant is related to 54 lit/min oxygen enrichment flow rate. Additionally, in a fixed oxygen enrichment condition, increasing the air/fuel ration will increase the temperature peak, but not the NO emission rate. As a result, oxygen-enrichment can reduce the NO emission at this kind of furnace in low air/fuel rates.

ACKNOWLEDGMENT

Author thanks from hydropower and dam research office at Khuzestan water and power authority.

International Journal of Mechanical, Industrial and Aerospace Sciences ISSN: 2517-9950 Vol:6, No:9, 2012

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