Proceedings of the
International Conference on Mechanical Engineering 2005
(ICME2005) 28- 30 December 2005, Dhaka, Bangladesh

ICME05-FL-18

MODELING AND SIMULATION OF A GAS COMBUSTOR

H. N. Mondal* and S.K. Bhattacharia

Department of Chemical Engineering
Bangladesh University of Engineering and Technology, Dhaka-1000
* hmondal@che.buet.ac.bd

ABSTRACT

A combustor is a feature of gas turbine engine. Prediction of the performance of combustor becomes an integral part for the development of efficient combustor. Primary design objectives are to burn the fuel efficiently, keep the wall temperature as low as possible and minimize emissions such as NOx and CO. Efficient burning depends on how well the fuel and air are mixed before ignition which in turn depends on the degree of turbulence. But to keep the wall temperature as low as possible, excess air with higher volume plays an important role, which affects the burning and the process becomes further complicated. To enhance the turbulence, different fuel and air injection patterns are studied and the effect of secondary air injection is investigated. For turbulence computation, *k-ε* model and for reaction dynamics eddy-dissipation model is used. FLUENT is used for numerical simulation.

Keywords: Combustion, Computational fluid dynamics (CFD), Turbulence modeling.

1. INTRODUCTION

Combustion is a mass energy conversion process during which chemical bond energy is converted into thermal energy. Combustion is the dominant technology in energy sector. Combustion and its control are very essential and it has been said that approximately 80 percent of the energy in the world come from combustion sources [1, 2]. The downside issue associated with combustion is directly associated with environmental pollution. It is well known that combustion, not only generates heat, but also produces pollutants like NO_x, SO_2, CO_2, CO, soot and unburnt Hydrocarbons [3]. Performance of the industrial and the utility combustion systems is often constrained by limitation of pollutant emissions.

Great energy savings could be made by improving combusting devices. But advanced combustor modifications require more detailed modeling of turbulent combustion when the formation and the destruction process of pollutants are to be predicted in order to reduce the harmful concentration near the furnace wall. Chemical kinetics has a major influence on pollutant formation, specifically in systems equipped with air or fuel staging. Some of the parameters that control the performance of a combustor are air/fuel ratio, degree of turbulence, wall temperature and geometry of the air and fuel inlet. These parameters should be optimized to get maximum performance from combustor. Efficient burning depends on how well the fuel and air are mixed before combustion which in turn depends on degree of turbulence. Control over the production of pollutants like NOx, SO_2, CO_2, CO, soot and unburnt hydrocarbons is another concern for better design of a combustor [4].

Homogenizing the temperature field in turbulent mixing is very important and dominates the combustion process. In the post film region, mixing with secondary air reduces the temperature. Secondary air is another factor, which also controls the emission from the combustor. Secondary air is mixed into the product stream of the flame to oxidize remaining hydrocarbons, CO, Soot and to reduce the temperature of exhaust film. The reduction in temperature also reduces the NOx formation. As lower temperature and delayed mixing are beneficial for NOx control, NOx emission is often controlled by reducing furnace temperature or by delaying mixing of fuel-rich and fuel-lean combustion reactants. Kidoguchi *et al.* studied NOx reduction for varying swirling condition. They found that on rich and high swirl condition, NO concentration decreases during the diffusion [4]. Magel *et al.* showed a combustion model that was able to handle finite rate chemistry in turbulent combustion [5]. Ravary and Johnsen developed a 2D model of the combustion in a furnace. They carried out a preliminary numerical study of the combustion of CO/SiO gas and NOx formation in a Silicon furnace [6]. A theoretical study was carried out on NOx emission in in-line NOx calciner. It was shown on the study that the mixing rate of oxygen into the main flow determined different local oxygen concentrations and different oxidation rates in the zone, which in turn affect the level of NO emission [7]. Adams *et al.* described the development of a non-equilibrium CO model and it was shown that low temperature CO oxidation can be accurately predicted with the use of CO model [8].

In this study, different air injection patterns were studied to enhance the turbulence. To maintain the wall temperature and minimize emission, different fuel/air ratios were investigated, and different geometric arrangement for primary air was also studied. Influence of the absence of secondary air in the combustor and steps of reaction were also studied. For turbulence computation, standard *k*-*ε* model and for combustion modeling, eddy dissipation model were used.

2. MODEL EQUATIONS

2.1 The Standard k-ε Model

The Standard k-ε model of turbulence is a two-equation model in which solution of two separate transport equations allows the turbulence velocity and length scales to be independently determined. It is semi-empirical model, and the derivation of the model equations relies on phenomenological considerations and empiricism. It is based on model transport equation for the turbulence kinetic energy (*k*) and its dissipation rate (*ε*). The model transport equation for *k* is derived from the exact equation and that of *ε* obtained using physical reasoning and bears little resemblance to its mathematically exact counterpart. In the derivation of k-ε model, flow is assumed as fully turbulent, and the effect of molecular viscosity is fully negligible. The following two equations represent the transport of turbulent kinetic energy, *k*, and its rate of dissipation, *ε*, respectively

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_j}(\rho k u_i)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] \qquad (1)$$
$$+G_k+G_b-\rho\varepsilon-Y_M+S_k$$

and

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\frac{\partial}{\partial x_i}(\rho\varepsilon u_i)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial \varepsilon}{\partial x_j}\right] \qquad (2)$$
$$+C_{1\varepsilon}\frac{\varepsilon}{k}(G_k+C_{3\varepsilon}G_b)-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}+S_\varepsilon$$

Where G_k represents the generation of turbulence kinetic energy due to the mean velocity gradients, G_b is the generation of turbulence kinetic energy due to buoyancy. Y_M represents the contribution of fluctuating dilation in compressible turbulence to the overall dissipation rate, $C_{1\varepsilon}$, $C_{2\varepsilon}$ and $C_{3\varepsilon}$ are constants. σ_k and σ_ε are the turbulent Prandtle numbers for *k* and ε and S_k and S_ε are user defined source terms.

The turbulent viscosity, μ_t, is computed by combining *k* and *ε* as follows:

$$\mu_t=\rho C_\mu\frac{k^2}{\varepsilon} \qquad (3)$$

The model constants have the following default values:

$$C_{1\varepsilon}=1.44,\ C_{2\varepsilon}=1.92,\ C_\mu=0.09,$$
$$\sigma_k=1.0,\ \text{and}\ \sigma_\varepsilon=1.3$$

2.2 Eddy Dissipation model for Combustion

The intrinsic idea behind the eddy dissipation model is that the rate of combustion is determined by the rate at which parcent of unburned gas are broken down into smaller ones, such that there is sufficient interfacial area between the unburned mixer and hot gases to permit reaction [9]. The implication of this is that chemical reaction rates play no role in determining the burning rates, but, rather, turbulent mixing rates completely control combustion. The model assumes that the reaction rate may be related directly to the time required to mix reactants at the molecular level. Since in turbulent flows, the mixing rate is dominated by the eddy properties, the rate is proportional to a mixing time defined by k/ε. Multiple simultaneous reactions are modeled with reactions occurring in the bulk phase or on wall or particle surfaces. It is modeled with the mixing and transport of chemical species by solving conservation equation describing convection, diffusion and reaction sources for each component species. Conservation equation takes the following general form for *i*-th species:

$$\frac{\partial}{\partial t}(\rho Y_i)+\nabla\cdot(\rho u_i Y_i)=-\nabla\cdot J_i+R_i+S_i \qquad (4)$$

Where R_i is the net rate of production of specie '*i*' by chemical reaction and S_i is the rate of creation by addition from the dispersed phase. An equation of this form will be solved for N-1 species where N is the total number of fluid phase chemical species present in the system. In addition to the transport equation of all the species, a transport equation for mixer fraction is also solved to deduce the product and oxidizer mass fractions

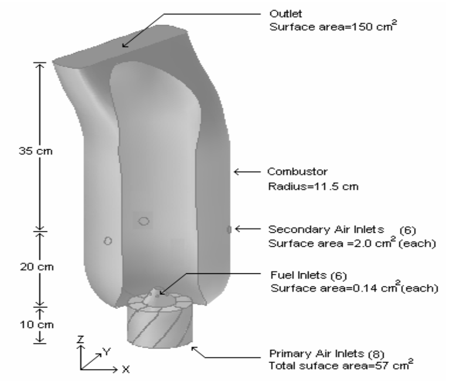

Fig 1. Geometry of the model considered

3. DESCRIPTION OF THE UNIT

The basic geometry is shown in Fig 1 with a section of the outer wall cut away. There are six secondary air inlets, each with a surface area of 2 cm^2. The outlet has a surface area of 150 cm^2. There are six small fuel inlets, each with a surface area of 0.14 cm^2. Primary air inlet is guided by vanes to give the air a swirling velocity. Its total surface area is 57 cm^2. Input parameters are velocity of fuel, primary air and secondary air.

4. RESULTS AND DISCUSSION

4.1 Variation in Geometry

Different parameters were varied to study the performances of the combustor. Effects of swirl velocity on combustion process were investigated varying the pattern of rotation of the primary air inlet. Angles of rotation used for the investigation were 30°, 45°, 60° and 90°. Investigation revealed significant changes of the distribution of static temperature. Contour of static temperature on the plane y=0 in Fig 2(a) and 2(b) showed that wall temperature was higher while the angle of rotation of the primary air inlet was 60°, compare to that of 90°. Temperature at the central part of the combustor was produced to be higher when the angle of the rotation was 90° and thus produced gradual decrease of temperature to the direction of wall. So increasing the turbulence by increasing the angle of rotation decreases the wall temperature and increases the temperature at the center. Swirl velocity and degree of turbulence made considerable effect for the production of NOx in combustor. Investigation showed that NOx production is low when the angle of rotation for the primary air inlet is 30° and highest when the angle of rotation is 90° [Fig 3(a) and 3(b)]. So the result revealed that NOx production was increased with the increase of the degree of turbulence. This is happened because higher turbulence produces higher temperature at the center, which causes more Nitrogen to convert to its oxides.

Production of CO_2 [Fig 4(a) and 4(b)] in reactor showed almost identical pattern. In case of 30° rotation, produced CO_2 concentrated at the center while for other cases, it gradually dispersed towards the wall.

4.2 Variation in Percent of Excess Air

Excess air in the combustor affects the wall temperature and the performance of the combustor considerably. To study the influence of excess air, 50%, 100% and 125% of excess air were used to monitor the performance. Contour of the static temperature of the planes y=0 showed that increase of excess air increased the burning efficiency [Fig 5(a), 5(b) and 5(c)]. Increase of excess air also decreased the wall temperature because excess air facilitates the burning and increases the temperature at the central region of the combustor. Production of NOx in the combustor is also influenced by the amount of excess air. Investigation [Fig 6(a, b and c)] revealed that NOx production is less at higher percentage of excess air [Fig 5(a), 5(b) and 5(c)]. At lower percentage of excess air, NOx production dispersed in the combustor, while at higher percentage, NOx production concentrated near the outlet.

4.3 Variation in Reaction Steps

FLUENT offers two models for burning of CH_4. One is a single step model where CH_4 converts to CO_2 and H_2O in a single step and another is a two step model where CH_4 converts to CO_2 and H_2O in two steps. It was found that variation of reaction steps influenced the production of NOx and CO_2. Fig 7(a) and 7(b) showed that two step reactions produced more NOx than single step, while Fig 8(a) and Fig 8(b) showed that more CO_2 produced in single step reaction.

4.4 Secondary Air off

Reduction of the wall temp is one of the important targets while designing a combustor. It appeared that secondary air inlet is the most important factor to control the wall temperature in the upper part of the combustor. Investigation of the absence of secondary air revealed this effect. Fig 9(a) and Fig 9(b) showed how secondary air influenced wall temperature. It was found from Fig 9(a) that the absence of secondary air increased the wall temperature drastically. Average temperature of the combustor increased to a great extent compare to the presence of secondary air. This is happened because secondary air facilitates burning and impedes heat to spread near the wall. Fig 10(a) and 10(b) showed the comparative performance of production of NOx in the combustor. Fig 10(a) also showed that absence of secondary air also enhances the production of NOx, and spread the NOx around the combustor. Absence of secondary air also influenced the pattern of production CO_2 as shown in Fig 11(a) and 11(b).

5. CONCLUSIONS

This study revealed some important features, which can be considered for better design of a can combustor. It showed that higher swirl velocity of the primary air reduced the wall temperature, but produced more NOx. Both the wall temperature and NOx are reduced by higher percentage of excess air. It also clearly revealed that the injection of secondary air helped to maintain wall temperature lower and the absence of secondary air increased the wall temperature drastically, and reduced overall efficiency of the combustor.

6. REFERENCES

1. Turns, S. R. 2000, *An Introduction to Combustion*, Second edition, McGraw Hill International Edition .
2. Toong, T. Y., 2000, *Combustion Dynamics*, Second edition, McGraw Hill International Edition.
3. Glarborg, P., Miller, J. A., & Kee, R. J, 1986, “Kinetic Modeling and Sensitivity Analysis of Nitrogen Oxide Formation in Well Stirred Reactor”, Combustion and flame 65, 177-202.
4. Kiduguchi, Y., Miwas, K & Mohammadi, A., 2001 “Reduction mechanism of NOx in rich and high turbulence diesel engine”, *Proc. Fifth international symposium on diagnostic and modeling of combustion in internal combustion engine*, July 14, Nagoya, Japan.
5. Magel, H., C., Schneider, R., Risio, B., Schnell, U., & Hein, K., R., G., 1995 “Numerical Simulation of Utility Boilers with advanced combustion. Technologies”, *Proc. Eighth International Symposium on Transport Phenomena in Combustion,* San Fransisco, USA.
6. Ravary, B., & Johansen, S.,T., 1999 “2D Modeling of the Combustion and NOx Formation in Furnaces Producing Fesi”, *Second International Conference on CFD in the Minerals and Process Industries, CSIRO,* Melbourne, Australia.

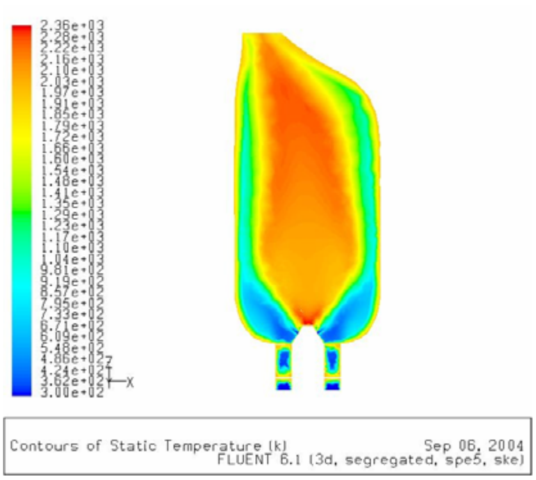

Fig 2(a). Contours of Static Temperature at the plane y=0, when angle of rotation is 60°.

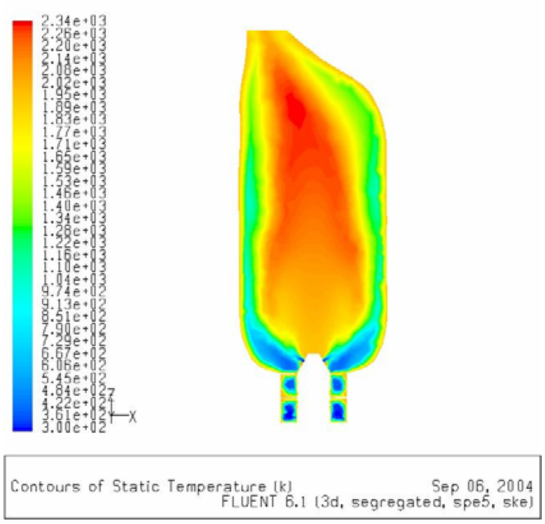

Fig 2(b). Contours of Static Temperature at the plane y=0, when Angle of Rotation is 90°

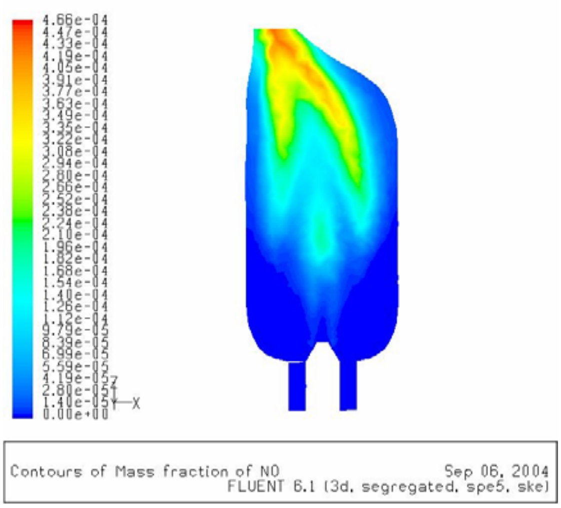

Fig 3(a). Contours of Mass fraction of NOat the plane y=0 when Angle of Rotation is 30°.

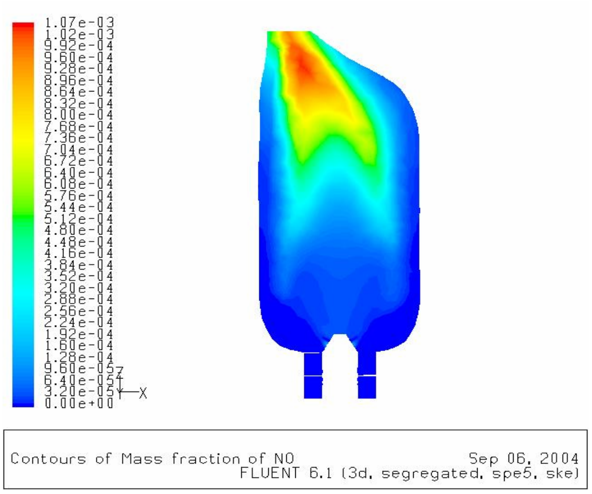

Fig 3(b). Contours of Mass fraction of NO at the plane y=0 when Angle of Rotation is 90°

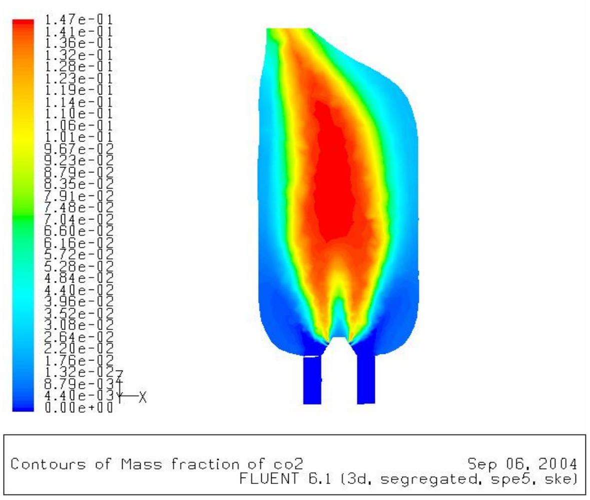

Fig 4(a). Contours of Mass fraction of CO_2 at the plane

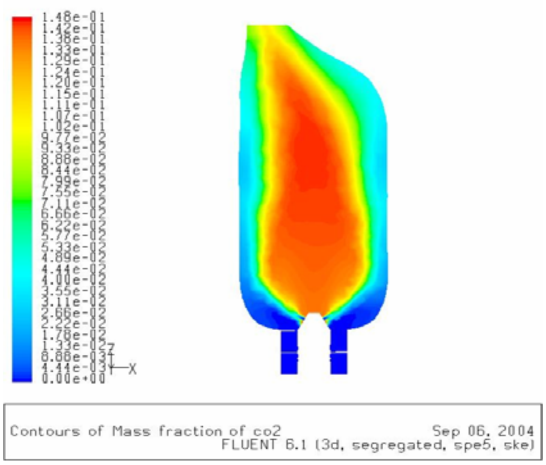

Fig 4(b). Contours of Mass fraction of CO_2 at the plane y=0 when Angle of Rotation is 30°

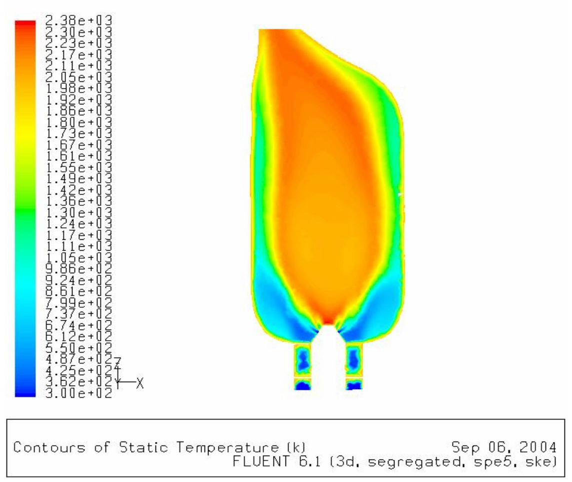

Fig 5(a). Contours of Static Temperature at the plane y=0 when 50% Excess air is used in the primary air inlet.

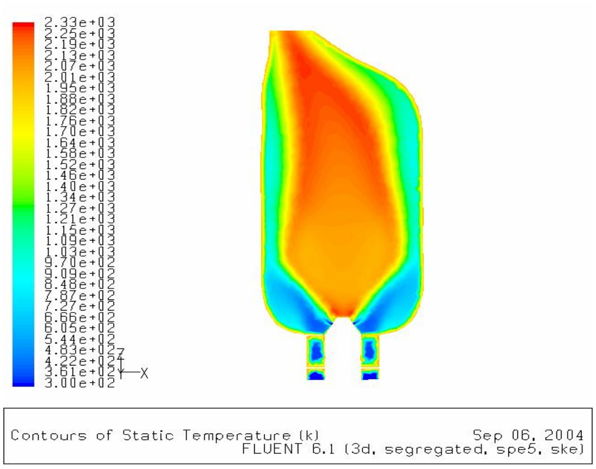

Fig 5(b). Contours of Static Temperature at the plane y=0 when 100% Excess air is used in the primary air inlet.

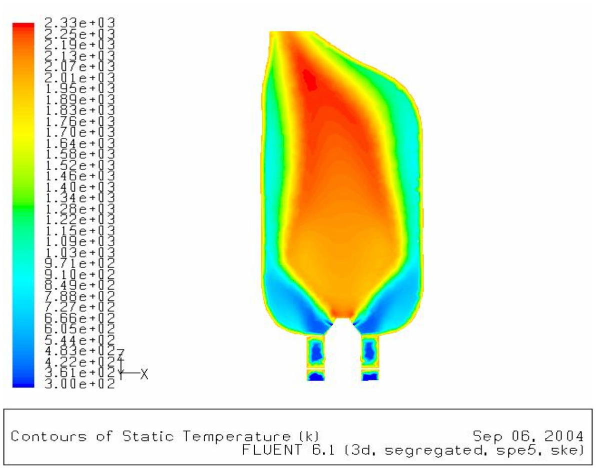

Fig 5(c). Contours of Static Temperature at the plane y=0 when 125% Excess air is used in the primary air inlet.

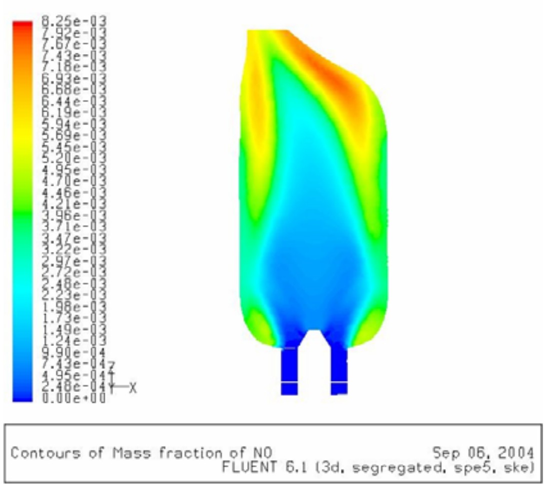

Fig 6(a). Contours of Mass fraction of NO at the plane y=0 when 50% Excess air is used in the primary air inlet.

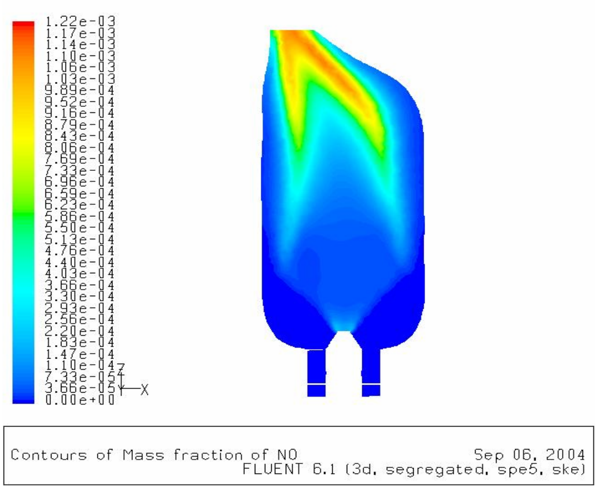

Fig 6(b). Contours of Mass fraction of NO at the plane y=0 when 100% Excess air is used in the primary air inlet.

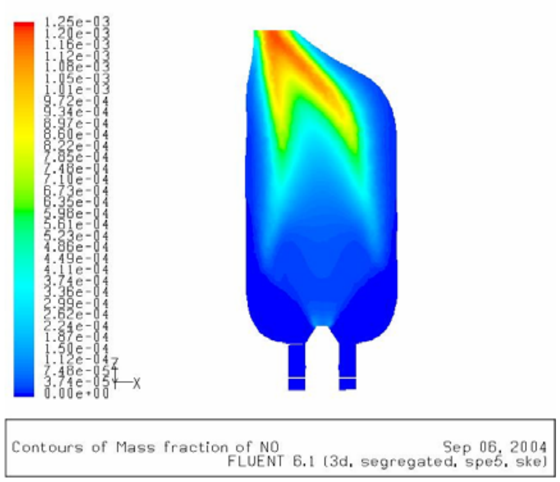

Fig 6(c). Contours of Mass fraction of NO at the plane y=0 when 50% Excess air is used in the primary air inlet.

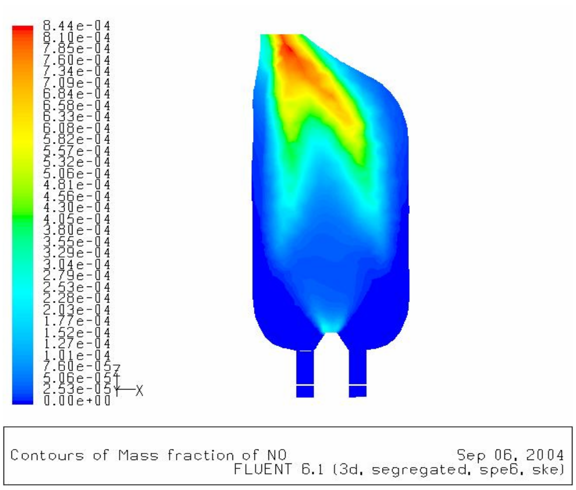

Fig 7(a). Contours of Mass fraction of NO at the plane y=0, when Methane Air reaction is completed in 2 steps.

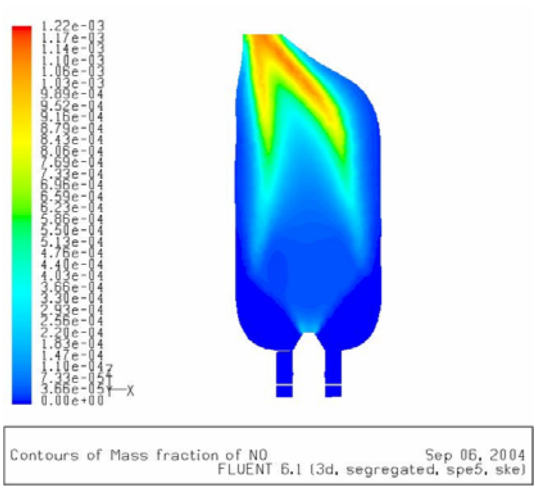

Fig 7(b). Contours of Mass fraction of NO at the plane y=0, when Methane Air reaction is completed in single step.

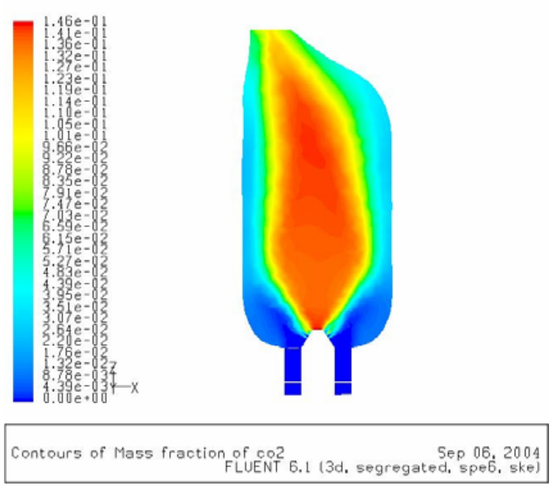

Fig 8(a). Contours of Mass fraction of CO_2 at the plane y=0, when Methane Air reaction is completed in 2 steps.

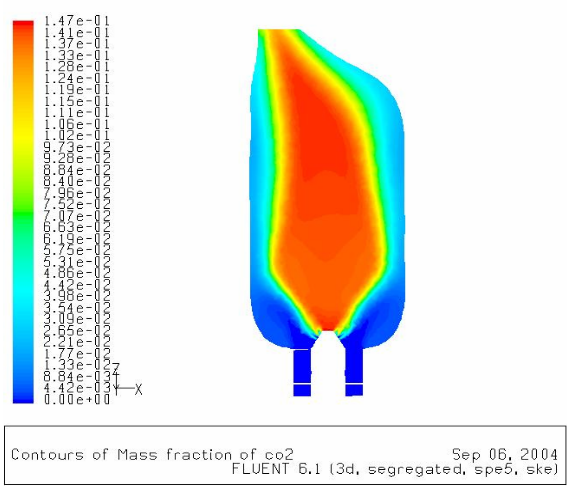

Fig 8(b). Contours of Mass fraction of CO_2 at the plane y=0, when Methane Air reaction is completed in single step.

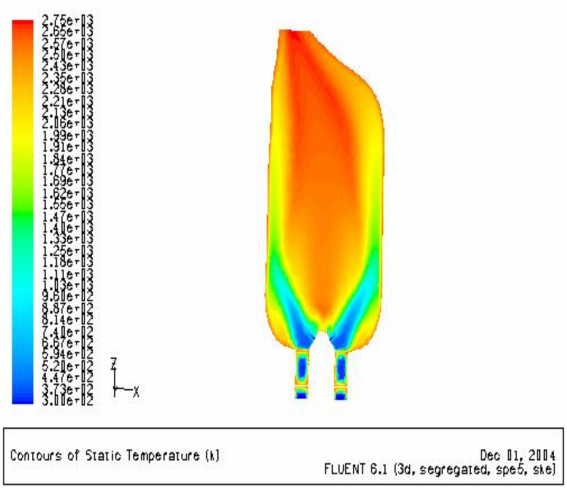

Fig 9(a). Contours of Static Temperature at the plane y=0, when secondary air is off.

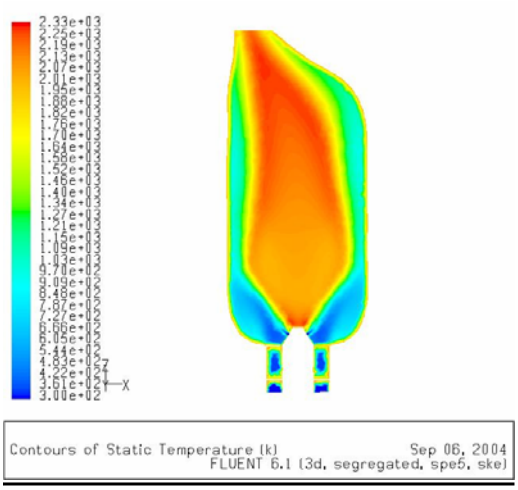

Fig 9(b). Contours of Static Temperature at the plane y=0 with secondary Air.

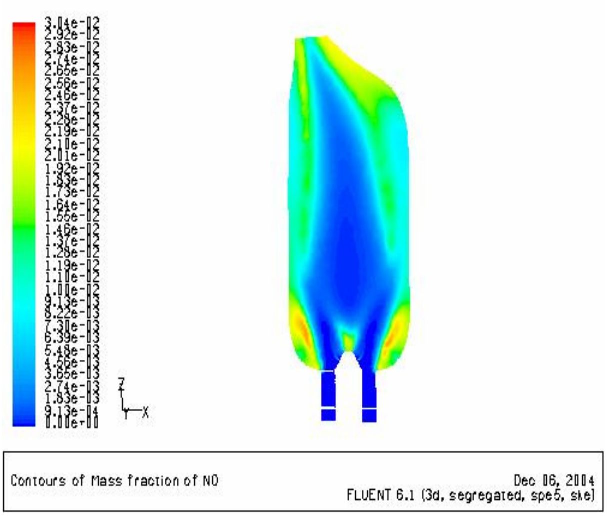

Fig 10(a). Contours of Mass fraction of NO at the plane y=0, when secondary air is off.

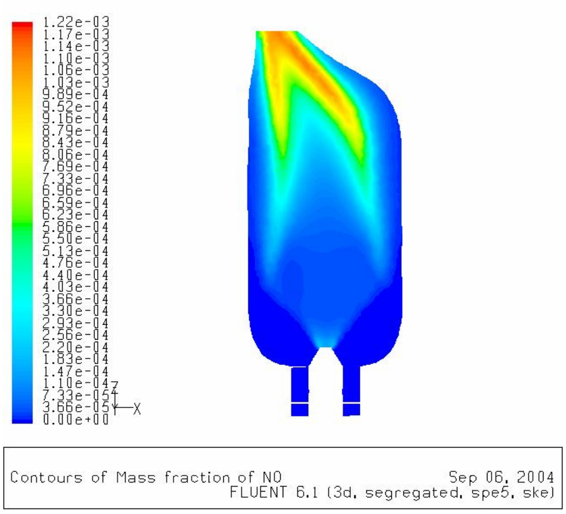

Fig 10(b). Contours of Mass fraction of NO at y=0 plane at the plane y=0 with secondary Air.

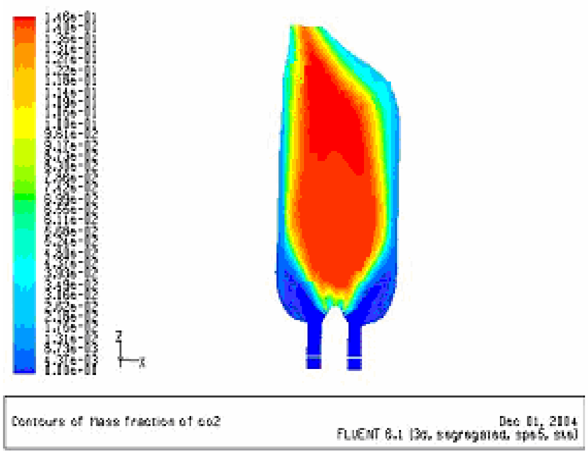

Fig 11(a). Contours of Mass fraction of CO_2 at the plane y=0, when secondary air is off.

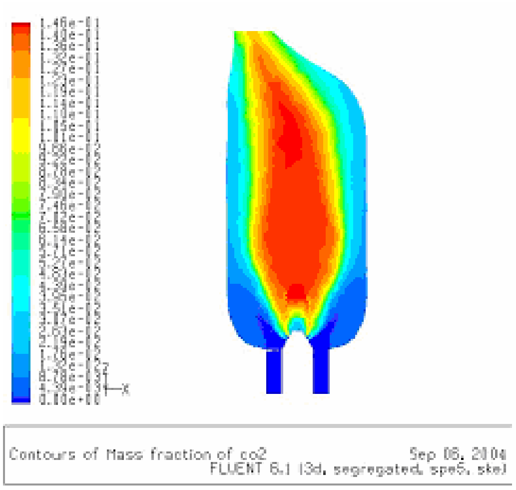

Fig 11(b). Contours of Mass fraction of CO_2 at the plane y=0 with secondary Air.

7. Iliuta, I and M. Iliuta, M., 2003., “NOx Emission in In-Line Low-NOx Calciner-A theoretical study”, International Journal of Chemical Reactor Engg. Vol. 1, Article A28.
8. Adams, B., R., Cremer, M., A., and Wang, D.,H., 2000, “Modeling Non-Equilibrium CO oxidation in Combustion systems”, *International Mechanical Engineering Congress & Exposition*, Orlando, Florida, USA.
9. Bray, K., N., C., 1980,“Turbulent flows with premixed reactants”, in Topics in Applied Physics,. 44, Turbulent Reacting Flows, Springer-Verlag, NY, 44, 115-183.