

Computer Simulation of NO_x Formation in Boilers

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Abstract

Understanding of how and where NO_x formation occurs in industrial boiler is very important for efficient and clean operation of utility boilers. This study aims to numerically simulate the NO_x formation using a 3D model furnace of an industrial boiler. The studied boiler is a 160 MW and is gas fired with natural gas. The boiler combustion model is a 3D problem that involves turbulence, combustion, radiation in addition to NO_x modeling. The 3D model is developed by dividing the volume of the furnace into 371000 control volumes with more concentration of grids near solid walls and regions of high property gradients. The simulation study provided the 3D temperature distribution as well as the rate of formation of the NO_x in the combustion chamber and in the exhaust gas at various operating conditions.

Keywords: NO_x Emission, Boilers, CFD Simulation, Combustion, Boiler Management.

1. Introduction

The management and protection of the environment have captured the interest of the international community in view of the problems of increasing pollution and environmental degradation. The ratification of the Kyoto agreement in 2005 enforces new environment protection measures. A number of countries have already introduced new laws to limit the emission from a large spectrum of commercial and industrial facilities. Because of the wide use of utility boilers in commercial and industrial facilities, there is a need for studies for better understanding of how and where NO_x formation occurs in such boilers. These studies are important for efficient and clean operation of utility boilers (Baubilis 1992), for improving boiler/burner design (Kokkinos 2000), and for development of

inferential methods for emission monitoring, (Elshafei et. al., 2006).

This paper presents the results of 3D computer simulation of the combustion chamber of a 160 MW boiler to study NO_x formation under various operating conditions of the boiler. The formation of NO_x in industrial boilers is a very complicated problem due to many parameters that influence its formation process. The numerical calculation of the combustion process in industrial boilers is a 3D problem that involves turbulence, combustion, radiation in addition to NO modeling. In the combustion chamber of a boiler, the heat transfer is dominated by radiation. Hence accurate prediction of the radiative heat transfer is necessary to obtain a correct estimate of the thermal boiler performance. In addition, correct computation of the thermal radiation is needed to accurately predict the temperature field as well as the heat fluxes at the walls of the boiler. The mechanisms of NO_x formation and combustion properties, and their dependence on furnace operating conditions, can be captured by mathematical models based on Computational Fluid Dynamics (CFD), (Li and Thompson (1996), Dong (2000), Habib et al (2004).

A fully three-dimensional flow, heat transfer and combustion computer model was developed by Boyd et al (1985) for tangentially fired pulverized fuel furnaces. The complete model solves equations for gas momentum and mixing, particle trajectories and combustion and energy conservation with radiation transfer. Zheng et al. (2000) presented numerical and experimental study on reduction of NO_x emissions in the furnace of a tangentially fired boiler under different operating conditions using a simplified NO_x formation mechanism model.

Other recent studies (Coelho and Carvalho, 1996, Chung et al 2002 and Habib et al, 2004) have involved the total flow and energy modeling of industrial gas furnaces. The focus in these studies was on improving the efficiency of furnaces and reducing NO_x pollution among other considerations.

Measurements of the stability limits and temperature contour maps of flame inside a water-cooled tangentially-fired model furnace were performed by Habib et al (1992). The limits of ignition were found to depend on the inclination angle of the burners and on the temperature levels. A one-component model to represent oil- and gas-fired boilers was developed and implemented in a system simulation program by Handby and Li (1997). The objective of their study was to calculate the emissions of NO_x, CO and SO_x, in addition to prediction of the performance of the boiler. The model was developed for boilers with outputs in the range 100 kW to 3 MW. The application of a full three-dimensional mathematical model to a fuel-oil fired power station boiler was conducted by Coelho and Carvalho (1995). Several variants of thermal and fuel-NO formation models were applied to the prediction of NO concentration in a utility boiler.

Based on the above literature search, it is clear that the problem of NO_x formation in industrial boilers although received much attention in regard of coal fired boilers, a limited portion of research work was focused on gas fired boilers. The present work is aimed at conducting a numerical investigation of the problem of the influence of the air to fuel ratio, the inlet combustion air temperature and the swirl angle on NO formation.

2. Description of the Boiler Model

The boiler considered in the present study is 160 MW, natural gas, water-tube boiler, having two vertically aligned burners. The boiler is composed of a furnace (radiation section) and return tube bank (convection section). The boiler is used for production of superheated steam for process industry. The steam flow rate is 240 t/h. Steam pressure and steam temperature are 51 bar and 330°C. The combustion chamber has 12.541 m length in the direction of flame, 4.579 m width of front wall and 7.925 m (distance between drums). A schematic of the boiler is shown in Fig.1. The primary air has a swirl angle of 45° and the secondary air has no swirl.

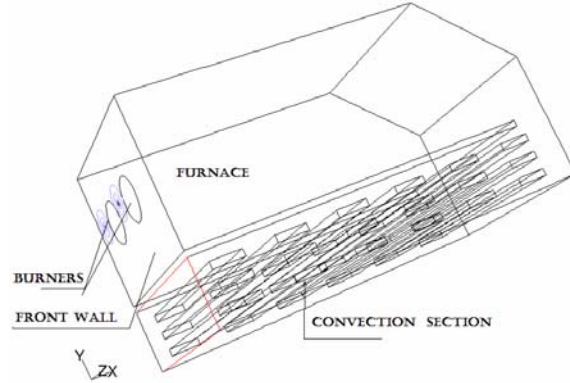


Fig. 1. 3D illustration of the boiler furnace.

3. Mathematical Formulation

The mathematical model is based on the numerical solution of the conservation equations for mass, momentum, and energy, and transport equations for scalar variables. The equations, which are elliptic and three-dimensional were solved to provide predictions of the flow pattern, thermal and pollution characteristics of reacting flows inside a model of an industrial boiler. Operating parameters include the air to fuel ratio, combustion air temperature and swirl angle. The governing equations, turbulence model, the boundary conditions and the solution procedure are presented in the following sections. The equations which govern the conservation of mass, momentum and energy as well as the equations for species transport may be expressed in the following general form (Reynolds, 1987 and Shih et al, 1995):

$$\frac{\partial}{\partial x_j} \left(\bar{\rho} \bar{U}_j \Phi + \bar{\rho} u_j \phi \right) = \frac{\partial}{\partial x_j} \left[\Gamma_\phi \frac{\partial \Phi}{\partial x_j} \right] + \bar{\rho} S_\phi \quad (1)$$

Where Φ is the dependent variable and u_j is the velocity component along the coordinate

direction x_j , $\bar{\rho}$ is the fluid density; Γ_ϕ is the diffusion coefficient and S_ϕ is the source term,

U_j : is the velocity component in the x_j directions,

\bar{U}_j : is the average velocity component,

x_j : is the a space coordinate, and

ρ : is the density.

Equation (1) stands for the mass conservation equation when $\Phi = 1$; the momentum conservation equation when Φ is a velocity component; the energy equation when Φ is the stagnation enthalpy.

Renormalized group turbulence model, Wilcox (2000), was used to provide better results for vortex flows. In order to correctly predict the temperature distribution in the furnace a radiative transfer equation (RTE) for an absorbing, emitting and scattering medium was solved. Once the radiative intensity is obtained, the gradient of the radiative heat flux vector was found and substituted into the enthalpy equation to account for heat sources (or sinks) due to radiation. The solution of the RTE for this application was obtained using the discrete ordinates. The blackbody spectral emissive power is calculated through using variables by Liu et al. (1998) and Zheng et al (2000) based on expressions of Modak (1979) and Smith et al (1982). The set of governing differential equations together with the boundary conditions are solved numerically by an iterative, line-by-line procedure (Patankar 1980). The details of the calculation procedure can be found in previous work such as Habib and Whietelaw (1982), Attya and Habib (1990) and Shuja and Habib (1996). The investigators used CFD packages Fluent 6.1.22.

4. NOx Generation

The combustion process considered in the present study has two mechanisms for NOx formation. The first is the thermal NOx which is controlled by the nitrogen and oxygen molar concentrations and the temperature of combustion in excess of 1,300 °C. The second is the prompt NOx which is formed from molecular nitrogen in the air combining with fuel in fuel-rich conditions. This nitrogen then oxidizes along with the fuel and becomes NOx during combustion. The mass transport equation for the NO species, including convection, diffusion, production and consumption of NO was solved. To consider the effect of residence time in NO mechanisms, a Lagrangian reference frame concept is included through the convection terms in the governing equations written in the Eulerian reference frame. The mechanisms of NOx formation and correlations can be captured by mathematical models (Li, 1997, Dong, 2000, Habib et al, 2004), and their dependence on furnace operating conditions and fuel composition. The Fluent simulation package provides state-of-the-art models for prediction of combustion and pollutant formation, including built-in NOx prediction. Fluent provides both finite rate and PDF combustion models, along with state-of-the-art NOx prediction capability.

The NOx calculations are based on a model of NO emissions for a power plant boiler by Li and Thompson (1996). The model is derived from the extended Zeldovich mechanism and requires only a few physical parameters obtained from experiments. The expressions for the reactions rate coefficients used in the NO model are given in Hanson and Salimian (1984). The rate of formation of thermal NO is significant only at high temperatures (greater than 1800 K) because fixation of nitrogen requires the breaking of the strong N₂ triple bond. It is known that during combustion of hydrocarbon fuels, the NO formation rate can exceed that produced from direct oxidation of nitrogen molecules (i.e., thermal NO). Many investigations have shown that the prompt NO contribution to total NO from stationary combustors is small. This is investigated in the present work. The turbulent mixing process results in temporal fluctuations in temperature and species concentration which will influence the characteristics of the flame in a nonlinear form. Thus, employing time-averaged composition and temperature in any model to predict the mean NOx formation rate can result in significant errors. In the present work, temperature fluctuations were taken into account by considering the probability density functions which describe the time variation. The model was validated through comparison with available experimental data of Yaga et al (2000).

5. Simulation Results

The general features of the flow and combustion characteristics are presented in Figures 2-6 for the velocity vectors, temperature contours, NOx and O₂ contours. These results are provided at the typical in-operation boiler as shown in Table 1.

Table 1. Typical data for Excess air factor $\lambda = 1.15$

Parameter	Value
Fuel flow rate	4.14 kg/s
Air flow rate	80.46 kg/s
Steam Pressure	51 bar
Steam temperature	538 K
Fuel	Methane
Steam flow rate	240 t/h
Swirl angle, primary air	45°
Radial angle for fuel	45°
Air Temperature	300 K

The results are presented at two different planes. The first is a vertical plane ($y=-2.24\text{m}$) passing through the two burners and the second is a horizontal plane ($z=4.662\text{m}$) passing through the

upper burner. The velocity vectors of are shown in Fig. 2. The velocity of fuel decreases as the fuel is mixed by turbulent diffusion with air due to air entrainment. The velocity along the burner axis decreases slightly towards the exit of the furnace. The flow velocity increases again in the passage to the convection section and maintains the same level throughout the convection chamber.

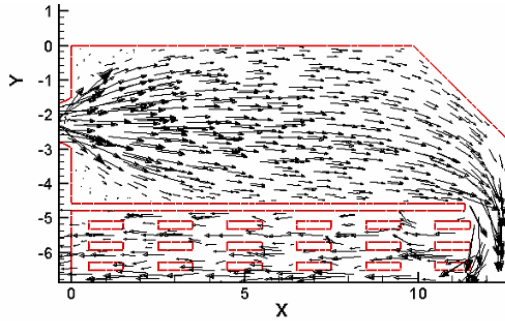


Fig 2. Velocity vectors of the flow field in a horizontal plane passing through the upper burner.

The temperature distributions in a horizontal section passing through the two burners are shown in Fig. 3. The temperature distribution in a vertical section passing through the upper burner is shown in Fig. 4. The temperature reaches its maximum of about 2000 K at the flame front where stoichiometric mixture occurs. Temperature then decreases to around 1500 K at exit of the furnace before entering the convection section. The interaction of the two flames is shown in Figure 3 where a complete mixing occurs, providing quasi-homogeneous temperature in the last one third of the furnace. Figure 5a presents the distribution of NO in the burners' plane. The NO concentration reaches its maximum value at the flame front. This is attributed to the elevated value of temperature at these locations which result in elevated value of the thermal NO. The NO value decreases towards the exit of the furnace. The NO distribution in a horizontal plane is shown in Fig. 5b and shows that NO stays unchanged in the convection part (tube bank passage). This is attributed to the low temperature values. The distributions of the mole fraction of oxygen in a horizontal section passing through the upper burner are shown in Fig. 6. The oxygen concentration is reaching its minimum values at the locations of maximum temperature.

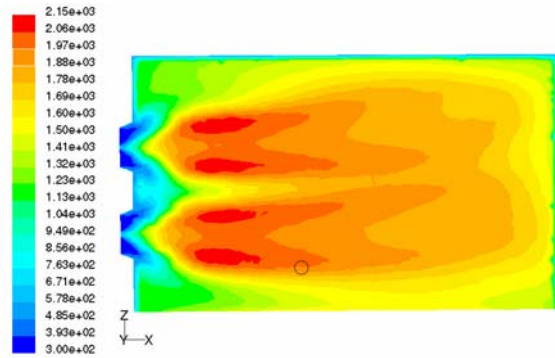


Fig 3. Temperature distributions at a vertical plane passing through the two burners.

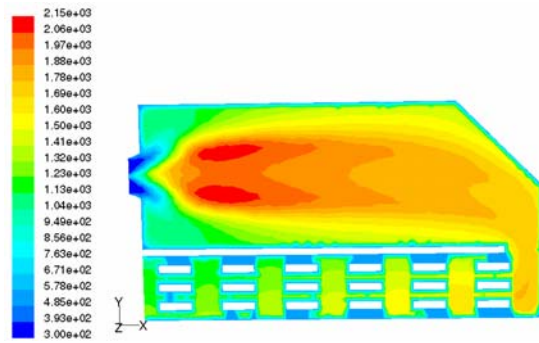


Fig 4. Temperature (K) distribution at a horizontal plane passing through the upper burner.

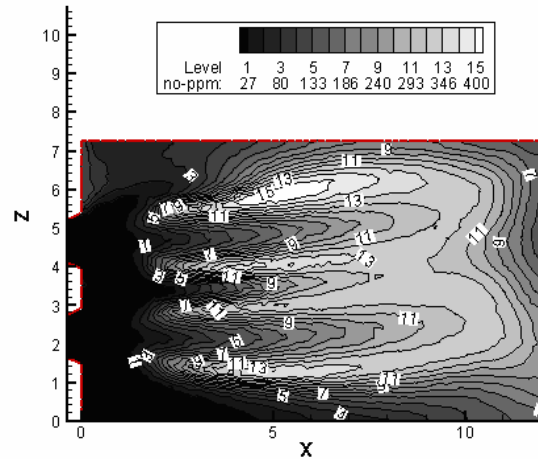


Fig 5a. Concentration distributions of NO (ppm) at a vertical plane passing through the two burners.

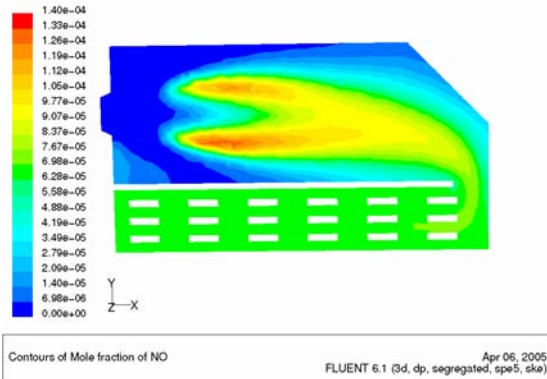


Fig 5b. Concentration distributions of NO (ppm) at a horizontal plane passing through the upper burner.

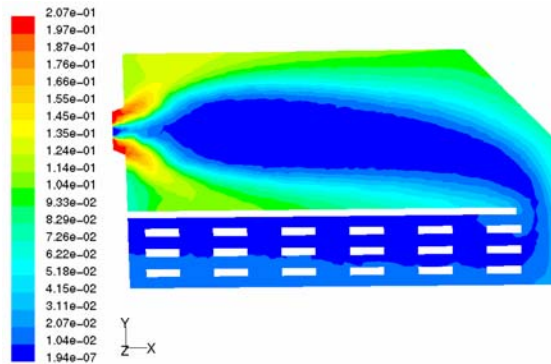


Fig. 6 O₂ (mole fraction) at a horizontal plane passing through the upper burner.

The boiler was simulated under various operating conditions to study the influence of varying air to fuel ratio by varying fuel or air mass flow rates, inlet combustion air temperature and combustion air swirl angle on the maximum and average temperature inside the furnace as well as NO concentration. The various operating conditions and the resulting NO concentrations are summarized in Table 2.

The air to fuel ratio is expressed in terms of the excess air factor, λ . The excess air factor is defined as the air to fuel ratio divided by the theoretical value for complete burning of fuel. Several conclusions could be drawn from these extensive simulations of the boiler. When the fuel flow rate increases at a fixed air mass flow rate, the maximum temperature does not change significantly, but the zones of maximum temperatures increase leading to increase in the thermal NO_x. The average chamber temperature, the exit air temperature, the prompt NO_x, and the thermal NO_x, all increase with fuel consumption.

Table 2 Temperature and NO Results.

Parameter (changed)	Parameter Value	Furnace Max Temp	Furnace Avg. Temp	Furnace Exh. Temp	NO Concentration	
					Thermal	Prompt
T=300						
Fuel Flow	$\lambda=1.05$	2131.6	1446.1	1171.5	230.3	73.2
Fuel Flow	$\lambda=1.15$	2132	1409	1130	210.5	46.4
Fuel Flow	$\lambda=1.25$	2133.8	1372.9	1092.1	192.6	25.4
Air Flow	$\lambda=1.1$	2128	1420	1144	210.4	59.4
Air Flow	$\lambda=1.2$	2136.6	1397.8	1122.9	210.7	34.7
Air Flow	$\lambda=1.3$	2144.7	1372	1108.4	207.9	17.1
Air Temp	T=300	2132	1409	1130	210.5	46.4
Air Temp	T=500	2221.9	1497.6	991.7	588	106.1
Swirl Angle	30	2116.8	1465.8	1137.1	212.1	51.9
Swirl Angle	45	2132	1409	1130	210.5	46.4
Swirl Angle	60	2158.8	1420	1107.7	231.6	37.5

On the other hand, when the fuel mass flow rate is kept constant and the air flow increases, the maximum temperature again does not change significantly, but the average temperature and the exit temperature decrease, which indicate that prompt NO decreases monotonically with the air to fuel ratio. It is shown that the average furnace temperature as well as the boiler exit temperature decrease as the A/F ratio increases. As the air flow rate is increased above the theoretical value, the boiler input energy per kg of flue gases is reduced and, thus, the exhaust gas temperature decreases. However, the maximum temperature starts to decrease only at excessive air/fuel ratio.

Inlet air temperature has more significant effect on the maximum temperature and the average temperature, and can cause rapid increase in thermal NO_x. Increasing the inlet air temperature from 300 K to 550 K, triples the thermal NO and almost doubled the prompt NO.

The NO distribution in a horizontal plane stays unchanged in the convection part (tube bank passage). This is attributed to the low temperature values. Thermal NO and prompt NO, increase with increased exhaust gas temperature. As the combustion air temperature increases, and furnace temperature increases, and NO concentration increases. The study indicates clearly that thermal NO formation is highly dependent on temperature. In fact, the thermal NO_x production rate doubles for every 90 K temperature increase beyond 2100 K. According, installation of proper instrumentation for monitoring the combustion and flue temperatures

would be very useful for monitoring and for estimating NO formation.

The simulation study indicates as well an increase in the maximum furnace temperature and a reduction in exhaust gas temperature as swirl angle is increased. The average temperature decreases until a value of swirl angle of 52.5° is reached and then increases. As θ increases Thermal NO, decreases showing a minimum at $\theta=45^\circ$. Higher swirl angle leads to faster mixing of the fuel and air, thus, lowering the temperature levels of the flame and reducing the NO emissions. The results also show that further increase in the swirl number results in increased furnace maximum temperature and increased values of thermal NO concentrations at exit of the boiler. This may be attributed to the very high maximum temperature values. Similar simulations were performed for the distribution of CO and O₂. Prediction of CO and O₂, together with NO_x are important for efficient operation of the boiler while maintaining the emissions within a given regulatory level.

6. Conclusions

The computer simulation of a 160 MW boiler provided insight on the correlation between the maximum furnace temperature, furnace average temperatures, inlet air temperature, and average exhaust gas temperature on the NO emission. The simulation studies showed clearly NO_x formation zones strongly correlate with the temperature zones. The results of this simulation could help in improving the predictive emission monitoring techniques, development of more effective instrumentation and monitoring of the combustion conditions, and better control of the boilers. The study recommended installation of non contact temperature measurements, as infrared imaging, or IR pyrometers for monitoring the combustion zones. The study showed that the most effective parameters for prediction of NO_x, CO, and O₂ emission are the flame temperature, the chamber combustion temperature, the exhaust temperature, the fuel flow rate, air flow rate, and A/F ratios. Predicting O₂ and CO is important to operate the boiler efficiently, while NO_x prediction enable the operator to maximize the operation while keeping the emission within the regulatory levels.

7. Acknowledgment

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