

## CHEMICAL EQUILIBRIUM ANALYSIS AND CFD SIMULATION OF COAL COMBUSTION AND NO<sub>x</sub> FORMATION

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### ABSTRACT

A full two-fluid model of reacting gas-particle flows with an algebraic unified second-order moment (AUSM) turbulence-chemistry model is used to simulate Beijing coal combustion and NO<sub>x</sub> formation. The sub-models are the k-ε-k<sub>p</sub> two-phase turbulence model, the EBU-Arrhenius volatile and CO combustion model, the six-flux radiation model, coal devolatilization model and char combustion model. The blocking effect on NO<sub>x</sub> formation is discussed. In addition, the chemical equilibrium analysis is used to predict NO<sub>x</sub> concentration at different temperature. Results of CFD simulation and chemical equilibrium analysis show that, optimizing air dynamic parameters can delay the NO<sub>x</sub> formation and decrease NO<sub>x</sub> emission, but it is effective only in a restricted range. In order to decrease NO<sub>x</sub> emission near to zero, the re-burning or other chemical methods must be used.

**Keywords:** NO reduction, reburning, inlet air parameter.

### INTRODUCTION

Swirl coal burners are widely used in the utility boilers of power stations in China. Nowadays it is important to develop low-pollutant swirl burners. Presently, most of studies on reducing pollutant formation are focused on chemical reactions and using the aerodynamics to form fuel rich combustion. As to the aerodynamics, it was found recently by both experiments and numerical simulation that as the swirl increases, the NO formation at first decreases and then increases. There is a swirl number of the lowest NO formation [1]. It was still found that, a blocking body, which located between the primary and secondary air can reduce NO emission remarkably [2]. Furthermore, the effect of many coal concentrators on NO reduction has been reported in these years [3]. But, Up to now no systematic studies on the effective range of using aerodynamics to reduce NO are reported. As to the chemical method, re-burning is one of the effective ways to reduce NO formation. It was found that, swirl coal combustion with natural gas re-burning can reduce NO emission to less 30% of what

without re-burning[4,5]. But, except NO reduction re-burning may still decrease burnout rate and increase CO emission. In this paper, both CFD analysis and chemical equilibrium analysis are used to simulate coal combustion and NO formation. The effective range of using aerodynamics to reduce NO and re-burning's effect to NO and CO emission had been studied.

### THE FULL TWO-FLUID MODEL FOR REACTING GAS-PARTICLE FLOWS AND COAL COMBUSTION

For the comprehensive modeling of reacting gas-particle flows and coal combustion, a full two-fluid model is used, that is, the continuity, momentum, energy and turbulent kinetic energy equations for both gas and particle phases are derived and solved in Eulerian coordinates. The sub-models are: the k-ε-k<sub>p</sub> two-phase turbulence model, the EBU-Arrhenius combustion model, a six-flux radiation model, a two-equation model of coal devolatilization, a diffusion-kinetic model of char combustion. The detailed description of this comprehensive model can be found in [6].

The AUSM turbulence-chemistry model for NO formation is incorporated into the comprehensive model [7].

For the full two-fluid model the basic equations of 3-D turbulent reacting gas-particle flows and coal combustion can be expressed in the following generalized form:

Gas-phase equations

$$\begin{aligned} & \frac{\partial}{\partial x}(\rho u \varphi) + \frac{\partial}{r \partial r}(r \rho v \varphi) + \frac{\partial}{r \partial \theta}(\rho w \varphi) \\ &= \frac{\partial}{\partial x} \left( \Gamma_{\varphi} \frac{\partial \varphi}{\partial x} \right) + \frac{\partial}{r \partial r} \left( r \Gamma_{\varphi} \frac{\partial \varphi}{\partial r} \right) + \\ & \frac{\partial}{r^2 \partial \theta} \left( \Gamma_{\varphi} \frac{\partial \varphi}{\partial \theta} \right) + S_{\varphi} + S_{\varphi}^p \end{aligned} \quad (1)$$

Particle-phase equations

$$\begin{aligned}
& \frac{\partial}{\partial x}(\rho_p u_p \varphi_p) + \frac{\partial}{r \partial r}(r \rho_p v_p \varphi_p) \\
& + \frac{\partial}{r \partial \theta}(\rho_p w_p \varphi_p) \\
& = \frac{\partial}{\partial x} \left( \Gamma_{\varphi p} \frac{\partial \varphi_p}{\partial x} \right) + \frac{\partial}{r \partial r} \left( r \Gamma_{\varphi p} \frac{\partial \varphi_p}{\partial r} \right) \quad (2) \\
& + \frac{\partial}{r^2 \partial \theta} \left( \Gamma_{\varphi p} \frac{\partial \varphi_p}{\partial \theta} \right) \\
& + S_{\varphi p} + S_{\varphi pg}
\end{aligned}$$

Where  $\varphi$  and  $\varphi_p$  are the generalized dependent variables,  $S_{\varphi p}$  and  $S_{\varphi pg}$  are the source items. The meanings of these variables and terms are given in [6].

The boundary conditions for the gas phase and particle phase are specified as in usual treatment: fully developed-flow conditions at the exit; symmetrical conditions at the axis; no-slip condition for the gas velocity at the wall. the wall function approximation is used for near-wall grid nodes. The particle-phase conditions at the wall are: zero normal mean velocity and zero gradients of other variables.

## SIMULATION OF SWIRLING COAL COMBUSTION AND NO FORMATION

Simulation of coal combustion and NO formation was carried out for a swirl combustor as shown in Figure 1. The geometrical sizes and inlet-flow conditions are given in Tables 1 and 2. The coal proximate analysis is given in Table 3. The mean size of coal particle at the inlet is  $45 \mu m$ . Figure 2 shows two cases: Case 1—blocking is placed at the central tube a, the primary-air with pulverized coal is supplied from the annular space b; the secondary-air is supplied from the annular space c; Case 2—blocking is placed at the annular space b; the primary-air with pulverized coal is supplied from the central tube a, the secondary-air is supplied from the annular space c; 3-D staggered grid nodes of  $30 \times 30 \times 7$  are used. Fine grid nodes were also tested, and the same results were obtained.

Figure 4 and Figure 5 show the isolines of temperature. Case 2's temperature is higher, but in general, there is no big difference between two cases. Figure 6 and Figure 7 give the isolines of char concentration. The annular blocking hinders the mixing between the primary air and the secondary air, therefore the high value zone of case 1 is closer to the inlet compared with case 2. In general there is no big difference between two cases in the downstream, this means burnout rates of two cases are similar. Figure 8 and Figure 9 give the isolines of NO concentration. The NO concentration for case 1 is higher than what of case 2. Case 1's NO emission is 820ppm while case 2's is 460ppm. For case 2, the blocking is located between the primary-air and the secondary-air inlets, the coal is fed through the central tube. In this case, compared with case 1, annular blocking hinders the mixing between the primary air and the secondary air and forms lean oxygen combustion, so the NO

formation is lower. The effect of blockings, concentrators and swirl numbers to coal combustion and NO formation had been studied [1,8,9], among them, the most effective way to reduce NO formation is placing an annular blocking between primary and secondary air.

Figure 10-12 show the analysis results by chemical equilibrium software. Figure 10 -11 give the NO and NO<sub>2</sub> concentration with increasing temperature. As the temperature increases, both NO and NO<sub>2</sub> chemical equilibrium concentrations increase and compared with NO concentration NO<sub>2</sub> concentration can be omitted. As the combustion temperature is from 1500 K to 1700 K (from Fig 4, 5), the NO equilibrium concentration is from 500ppm to 1000ppm. For the nitrogen is very hard to be at equilibrium during combustion process, the CFD simulation result and chemical equilibrium analysis result can not be in good agreement with each other, but in general they can be compared. So, it is very hard to reduce NO emission to very low level only by optimizing air dynamic parameters, because of chemical equilibrium restrict.

Figure 12 gives the NO and CO concentration along the increase of re-burning fuel proportion at temperature 1550 K, the re-burning fuel was CH<sub>4</sub>. As the CH<sub>4</sub> proportion increases the CO concentration increases while the NO concentration decreases. When the CH<sub>4</sub> proportion is greater than 0.17 the NO concentration can be reduced to less than 100ppm. When the CH<sub>4</sub> proportion is greater than 0.11 the CO concentration increases sharply.

## CONCLUSION

1. The inlet blocking located between the primary-air inlet and the secondary-air inlet with pulverized coal fed from the central tube can reduce the NO formation near to 50%.
2. Farther NO reduction needs using re-burning technology or other chemical treatment ways.
3. Re-burning can reduce NO emission to very low level but meanwhile increase CO emission.
4. Reasonable re-burning fuel proportion, re-burning fuel inlet position, re-burning fuel type and how to combine re-burning with aerodynamics to reduce NO emission need to be farther studied.

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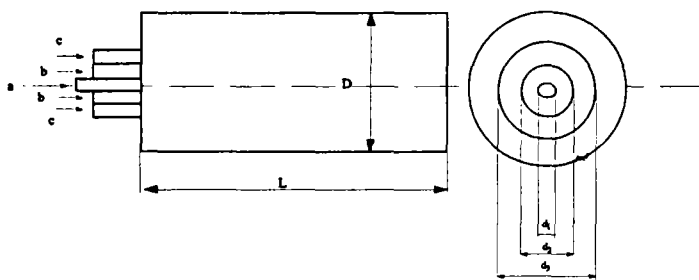


Fig 1 The Swirl Combustor

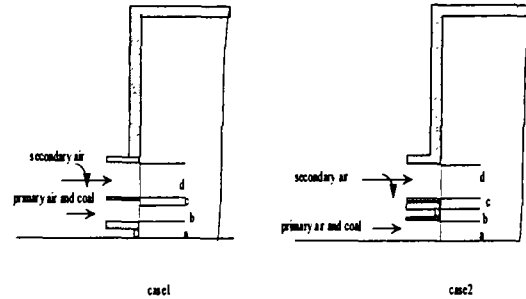


Fig 2 Two Cases

Table 1 Geometrical Sizes

D	L	$d_1$	$d_2$	$d_3$
0.6m	3.0m	0.022m	0.035m	0.104m

Table 2 Inlet Flow Parameters

	Air Flow Rate (kg/h)	Coal Feeding Rate (kg/h)	Swirl Number
Primary Air	31.8	14	0.0
Secondary Air	120.4	0	1.0

Table 3 Coal Proximate Analysis

Volatile (%)	Fixed Carbon (%)	Moisture (%)	Ash (%)	Nitrogen (%)
25.37	50.847	10.59	10.59	0.78

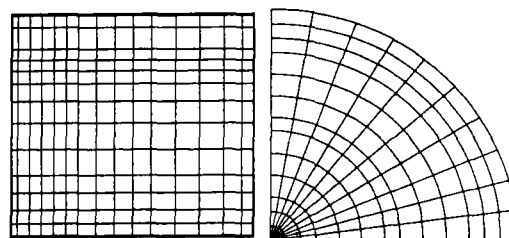


Fig 3 Grids Arrangement

