NUMERICAL SIMULATIONS OF THE PULVERIZED COAL COMBUSTION IN A SWIRL COMBUSTOR

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1. Summary

A three-dimensional numerical simulation has been carried out to investigate the effects of swirl intensity on the pulverized coal combustion. The mathematical models, based on Eulerian-Largrangian descriptions, are used to describe the interaction between the gas and particle flows. The turbulent flow of the gas phase is modelled through the RNG k-ε model while the EBU (eddy break-up)-Arrhenius model is used to calculate the chemical reaction of the turbulent combustion. The six-heat-flux model is used to account for the radiation caused by the turbulent combustion. The single kinetic-rate model is used for coal devolatilization while the heterogeneous char reaction rate is calculated by the diffusion-kinetic model. The NOx formation also is predicted using the current combustion model. When the swirl number increases, the reverse-flow zone is shortened and is shifted toward the combustor inlet. Though this shift causes the maximum temperature zone to shift toward the inlet region, it has virtually no effect on the overall change in the gas temperature. The NO formation is characterized by the local gas temperature, and the intensity of the coal particle dispersion. For the case with the relatively high swirl number, no discernable increase of the gas temperature is observed; however, the overall NO emission decreases substantially. In addition, the particle trajectory is generally shortened, of which phenomenon is caused by the shift of the reverse-flow zone where the trapped particles are not readily escaped from the recirculating flow. In result, the combustion of most pulverized coal particles takes place within a shorter distance from the combustor inlet.

2. Introduction

Coal is an important energy source for the power plant which generates electricity used in our daily lives. Despite the rapid advance in the energy conversion technologies, the demand for the use of coal has never been greater because of its practicality and apt economics. Coal-fired power plants generally use the pulverized coal powder to burn the coal. Because these countless fine particles are mixed with the injecting air, this mixed flow is considered as the particle-laden two-phase flow. As soon as these coal particles enter the furnace, the particles are heated, devolatilized, and burned. The combustion stability is dependent on the particle size and the operating conditions such as the supplied air temperature and pressure. To achieve a rapid mixing and stable flame, the swirl combustion chamber is often used in the modern combustion utilities. The enhancement of the combustion efficiency and pollutant control can be achieved by th high temperature and pressure of the combustor.

The flow physics of the interaction between the particles and the radiative furnace environment is extremely complex and, thus, poses a great computational challenge. Because of its high academic challenge, the two-phase flow of the pulverized coal combustion has suscitated a strong interest in the combustion community. Abbas *et al.* (1) investigated the aerodynamics effect on the NOx formation. Their study shows the burnout performance, due to directing the initial particle flights into a fuel rich region, can be prevented if the residence time of the particles in the internal recirculation zone is sufficiently prolonged (1). Zhou *et al.* (2-3) used the USM turbulence-chemistry model and the Eulerian-Eulerian two-fluid model for simulating the coal combustion. Their numerical predictions of the NOx formation using the unified second-order moment turbulence-chemistry model were compared well with the experimental data. Li *et al.* (4) found that the modified k-ε model gave the better prediction than that obtained using the standard k-ε model. Additional numerical work can be found in Refs. (5-8), including the thorough review article by Williams *et al.* (8).

In the current work, it is our primary interest to investigate the effects of the swirl number and the inlet air temperature on the overall performance of the pulverized coal combustion.

3. Mathematical Models

The governing equations are based on the Eulerian and Lagrangian descriptions for the gas phase and coal particles, respectively.

3.1 Governing equations

The steady-state transport equation for a variable φ follows the form below:

$$\frac{\partial}{\partial x}(\rho u\phi)+\frac{1}{r}\frac{\partial}{\partial r}(\rho rv\phi)+\frac{1}{r}\frac{\partial}{\partial \theta}(\rho w\phi) = \frac{\partial}{\partial x}\left(\Gamma_\phi \frac{\partial \phi}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\Gamma_\phi \frac{\partial \phi}{\partial r}\right)+\frac{1}{r}\frac{\partial}{\partial \theta}\left(\Gamma_\phi \frac{\partial \phi}{r\partial \theta}\right)+S_\phi+S_{p,\phi} \tag{1}$$

where, S_φ represents the source terms of the gas phase. $S_{d,\varphi}$ is of the source term for the dispersed phase. Γ_φ, represents the exchange coefficient. The turbulence is modelled using the RNG k-ε model (9). The momentum equation for a particle of the Stokes flow obeys the following Lagrangian form:

$$\frac{d\vec{u}_{p,i}}{dt}=\frac{3C_D\mu \mathrm{Re}}{4\rho_p d_p^{\,2}}\left(\vec{u}_i-\vec{u}_{p,i}\right) \tag{2}$$

$$\frac{dx_{p,i}}{dt}=\vec{u}_{p,i} \tag{3}$$

where $\vec{u}_{di}$ and $\vec{x}_{di}$ represent the particle's velocity and position. $\vec{u}_i$ is the instantaneous gas phase velocity. C_D is the drag coefficient for a sphere given by Faeth (10) below:

$$C_D=\begin{cases}24/\mathrm{Re}\left(1+0.15\,\mathrm{Re}^{0.687}\right) & \mathrm{Re}\le 1000\\ 0.44 & \mathrm{Re}>1000\end{cases} \tag{4}$$

The particle temperature is obtained using the energy equation below:

$$m_p C_{P,p} \frac{dT_p}{dt} = hA_p(T - T_p) + Q_{\text{devolatilization}} + Q_{\text{char reaction}} + Q_{\text{radiation}} \quad (5)$$

where the convection coefficient, h, is obtained from the Nusselt number represented by the correlation below:

$$Nu = \frac{hd_p}{\lambda} = 2 + \frac{0.555\,\mathrm{Re}^{1/2}(\mathrm{Pr})^{1/3}}{[1 + 1.232\,\mathrm{Re}^{-1}(\mathrm{Pr})^{-4/3}]^{1/2}} \quad (6)$$

The coal devolatilization is modelled by the first-order single kinetic rate model given as follows:

$$\frac{dv}{dt} = -k_v(v - v^*) \quad (7)$$

where k_v is the rate constant given by the Arrehnius expression as $A_v \exp(-E_v/RT)$. v is the volatile-yield at a specific time, t, and v^* is the maximum value of v. The volatile gas reaction is assumed to be a global one-step reaction (11) as follows:

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O \quad (R1)$$

$$R_{ARR} = 7.2 \times 10^{11} \times [C_3H_8]^{0.25}[O_2]^{1.5} \exp(-30/RT) \quad (8)$$

The EBU model is adopted as a part of submodels. The mixing-controlled rate of the reaction is expressed in terms of the turbulence time scale k/ε. The model accounts for the dissipation rates of the fuel, oxygen and products, which are expressed as below:

$$R_{EBU} = Min\left[4\bar{\rho}\tilde{Y}_{fu}\frac{\varepsilon}{k}, 4\bar{\rho}\frac{\tilde{Y}_{ox}}{s}\frac{\varepsilon}{k}, 2\bar{\rho}\frac{\tilde{Y}_{PR}}{1+s}\frac{\varepsilon}{k}\right] \quad (9)$$

where, s is the mass-bassed stoichiometric oxygen/fuel ratio. The equation (9) can be reduced by combining with the Arrhenius fuel consumption rate, whose result is provided below:

$$R_{FU} = Min[R_{EBU}, R_{ARR}] \quad (10)$$

The char reaction rate of Baum and Street [12] is used as follows:

$$\frac{dm_{char}}{dt} = \pi d_p^2 R T_g \frac{R_k R_D}{R_k + R_D} \quad (11)$$

where

$$R_k = A_c \exp(-\frac{E_c}{RT_p}) \quad (12)$$

$$R_D = C\frac{\left[\left(T_P + T_g\right)/2\right]^{0.75}}{d_p} \quad (13)$$

The thermal NO formation model, known as "Zeldovich NO mechanism," is used as follows(13):

$$O + N_2 \xleftrightarrow{K_1} NO + N \quad \text{(R2)}$$

$$N + O_2 \xleftrightarrow{K_2} NO + O \quad \text{(R3)}$$

$$N + OH \xleftrightarrow{K_3} NO + H \quad \text{(R4)}$$

where,

$K_1 = 1.8\times10^8 \exp(-38370/T)$ $\qquad$ $K_{-1} = 3.8\times10^7 \exp(-425/T)$

$K_2 = 1.8\times10^4 \exp(-4680/T)$ $\qquad$ $K_{-2} = 3.8\times10^3 \exp(-20820/T)$

$K_3 = 7.1\times10^7 \exp(-450/T)$ $\qquad$ $K_{-3} = 1.7\times10^8 \exp(-24560/T)$ $(m^3/mol\square s)$

Under the quasi-steady assumption for [N] atom, the overall rate for thermal NO reaction is reduced as follows:

$$\frac{d[NO]_T}{dt} = 2K_1[O][N_2]\left(1-\frac{K_{-1}K_{-2}[NO]^2}{K_1K_2[O_2][N_2]}\right)\Big/\left(1+\frac{K_{-1}[NO]}{K_2[O_2]+K_3[OH]}\right) \quad (14)$$

[OH] and [O] radicals are determined by the partial equilibrium assumption below:

$$[OH] = 2.129\times10^2 T^{-0.57} \exp(-4595/T)[O]^{0.5}[H_2O]^{0.5} \quad (15)$$

$$[O] = 36.64T^{1/2}[O_2]\exp(-27123/T) \quad (16)$$

The fuel NOx formation is calculated by the De Soete's mechanism (13) as follows:

$$HCN + O_2 \rightarrow NO \quad \text{(R5)}$$

$$HCN + NO \rightarrow N_2 \quad \text{(R6)}$$

$$C + NO \rightarrow N_2 \quad \text{(R7)}$$

3.2 Analysed swirl combustor

Figure 1 depicts the geometries and dimensions of the pulverized coal combustion chamber scenariorized in the current study. The chamber is cylindrical in shape and 3.0 m long and 0.6 m in diameter. The primary air mixed with coal is injected into the chamber through the annulus "A" (see Fig. 1) while the secondary swirling air is injected into the annulus "B", whose dimensions and operating conditions are listed in Table 1 and in Fig. 1. The pulverized coal particles are categorized into 10 size group with an average size of approximately ~45 μm.

A 65×60×27 non-uniform grid (in the axial, radial, and azimuthal directions, respectively) is employed with grid stretching employed to enhance the resolution near

the combustor inlet region. The operating conditions and the coal properties are listed in Tables 1 and 2.

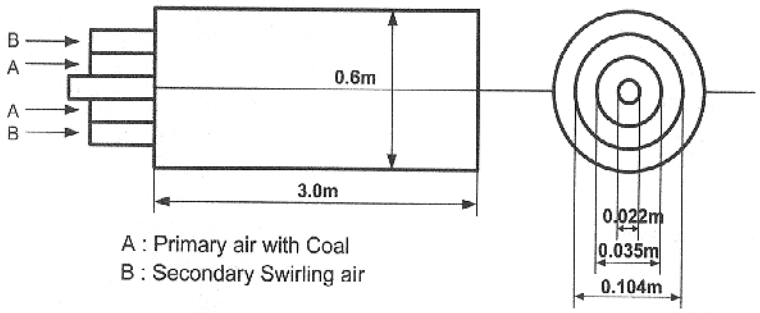

Fig. 1 Configuration of Combustion Chamber

Table 1 Operating conditions

Coal feed rate(kg/h)	14.0
Primary air flow rate(kg/h)	31.3
Secondary air flow rate(kg/h)	120
Secondary air swirl number	0.5, 0.8, 1.0
Primary air temperature(°C)	80
Secondary air temperature(°C)	300

Table 2 Proximate analysis of the coal

Volatile(%)	Char(%)	Water(%)	Ash(%)	N(%)
35.8	53.7	6.3	4.2	1.29

4. Results

Simulation of pulverized coal combustion and NO formation has been performed. The velocity vectors and isothermal lines are shown in Fig. 2 for SN = 0.5 and in Fig. 3 for SN = 1.0. No recirculation zone is observed for the case of SN=0.5. When the swirl number increases, the reverse-flow zone is shortened and is shifted toward the combustor inlet. The high temperature zone is also shifted toward the combustor inlet wall. However, the overall gas temperature is not greatly influenced by this shift. Figures 4 and 5 show the trajectories of the pulverized coal particles with an average diameter of 45 μm. It should be noted that the results shown in Figs. 4 and 5 shows the unburned coal particles trajectories only and those of the remaining ash is not

included in the figures. For the case of SN = 0.5, the coal particles move along the reverse flow zone caused by the sudden expansion of the step-flow. When increasing the swirl number, the particle trajectory is shortened. Because of the shorter particle trajectory at higher swirling number, the internal reverse flow is shifted toward the inlet zone. In this case, most injected coal particles do not travel further downstream and, rather, be trapped within the recirculating flow of the reverse zone. This phenomenon works favourably for an efficient turbulent mixing between the particles and the hot gas, whose interaction results in more stable and efficient coal combustion within the furnace.

In Fig. 6, the predictions for the NO formation level (in ppm) from the computation are well compared to the experimental data of Abbs *et al.* [1]. The pattern indicates that the NO emission can be reduced when the combustion takes place under the higher swirling number. It is noted that the predicted NO level is the mean value obtained at the combustor exit. The minor difference between the experimental data and the computational prediction is attributed to the shortcoming of the k-ε turbulence model which tends to underpredict the turbulent kinetic energy, resulting in the some error in the turbulent dispersion of the particles.

For the case of SN = 0.5, the NO level is slightly higher than that predicted using SN = 1.0. This difference is probably because of the ignition delay of the particles of which reasons are discussed as follows: In general, the devolatilization and its subsequent char combustion take place when the particle temperature reaches approximately 500 K [5]. For the case of SN = 0.5, the coal particles are not well preheated with sufficient amount of time and, thus, results in poor devolatilization. This difference in preheating condition causes the ignition delay, which results in less efficient combustion and more NO emission. On the other hand, for the of SN = 1.0, the injected particles into the recirculation zone are relatively well preheated, which causes relatively rapid volatilization and, therefore, the more efficient combustion takes place. In this case, the NO level is also favourably reduced.

Figures 7 through 12 show the velocity vectors and temperature contour of the swirling gas flow for various inlet temperatures, T = 773, 1073, and 1273 K. As shown, the turbulent mixing is greatly intensified as the air's inlet temperature increases. For the given inlet air flowrate, the increase in the secondary swirl air temperature causes the increase in the gas velocity because of the air density reduction at higher temperature. The gas velocity increase and the gas density reduction provide a suitable environment for less drag and, in result, the deeper penetration is achieved.

The recirculation zone with relatively high temperature has expanded toward the combustor centre because of the increase in the secondary swirl air temperature. As mentioned above, the devolatilization and char combustion are initiated when the particle temperature reaches approximately ~500 K. In general, it requires a sufficient amount of time for the devolatilization through the preheating process. When the inlet air temperature increases, the drag force exerted on the coal particles is decreased, of which process reduces the preheating time by increasing the temperature difference between the particles and the surrounding gas. This increase in the temperature difference leads to the larger heat flux provided to the particles. The drag reduction yields the formation of the fuel-lean zone and, eventually, leads to the sufficient mixing with oxygen-rich air prior to the ignition. For these reasons, the high temperature zone is expanded toward the combustor centre when the inlet air temperature is increased.

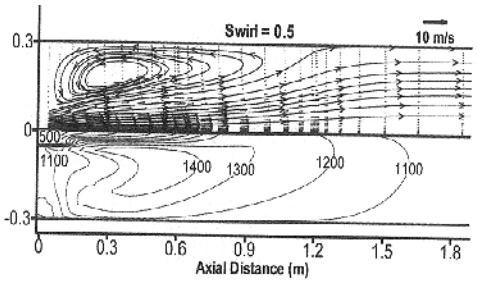

Fig. 2 Velocity vector and isotherms for SN=0.5

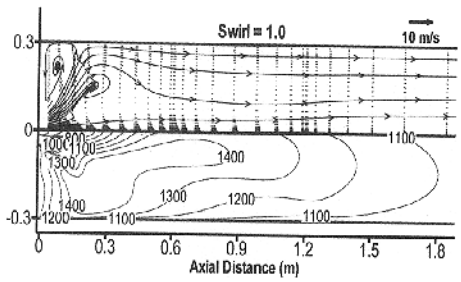

Fig. 3 Velocity vector and isotherms for SN=1.0

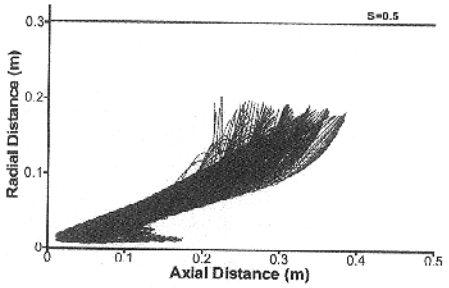

Fig. 4 Particle trajectory for SN=0.5

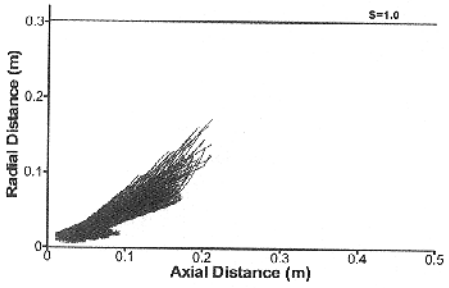

Fig. 5 Particle trajectory for SN=1.0

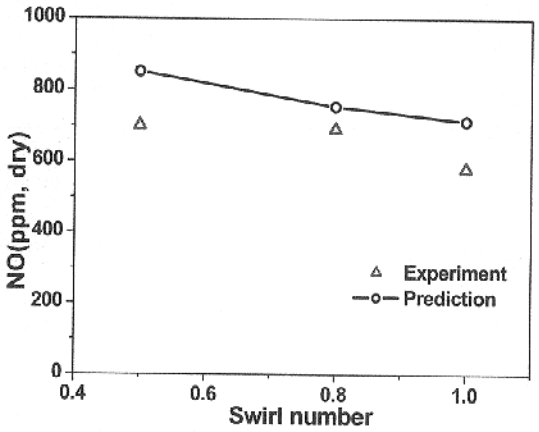

Fig. 6 Effect of Swirl on NO emission

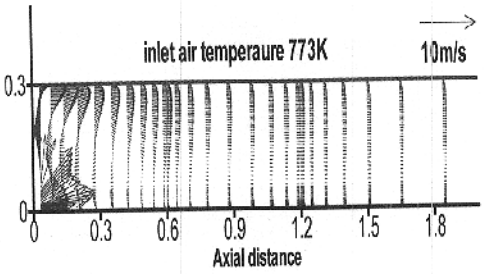

Fig. 7 Velocity vectors for 773K

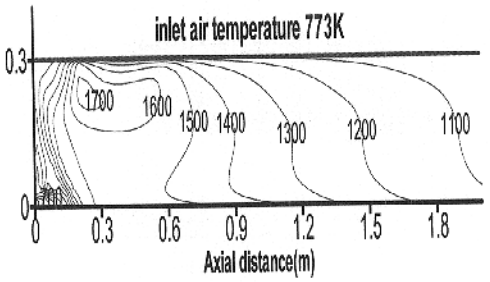

Fig. 8 Gas temperature contour for 773 K

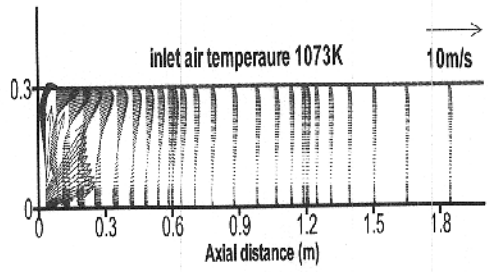

Fig. 9 Velocity vectors for 1073K

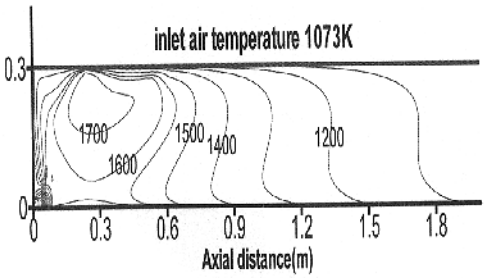

Fig. 10 Gas temperature contour for1073K

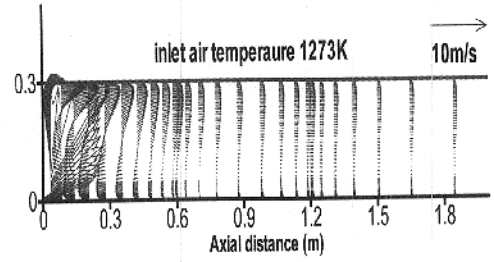

Fig. 11 Velocity vectors for 1273K

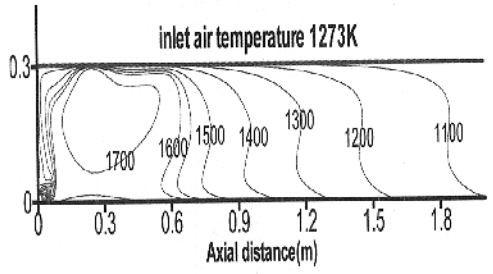

Fig. 12 Gas temperature contour for 1273K

5. Conclusion

The simulations of the pulverized coal combustion and NO formation have been performed. When the swirl number is increased, the high temperature zone is shifted toward the combustor inlet; however, little influence on the overall gas temperature is observed. The NO emission level predicted using the current modelling approach is well compared with the experimental data. The increase in the secondary swirl air temperature causes the gas velocity to rise because of the air density reduction. The density reduction and the gas velocity increase provide a suitable condition for less drag and, therefore, a deep penetration length. The drag reduction yields the formation of the fuel-lean zone and, eventually, leads to the sufficient mixing with oxygen-rich air

prior to the ignition. It is concluded that the high temperature air enhances the pulverized coal combustion with greater swirling strength.

Acknowledgements

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