Three-Dimensional Spray Combustion Simulation in a Practical Boiler*

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A three-dimensional computer model of a swirling fired-type furnace in which pulverized petroleum coke and ASTM No. 6 heavy oil are fed from two opposite side walls is presented. The predicted results are compared with measurements of exhaust NO concentration in an operating 125 MW(e) boiler with and without air introduced tangentially from the bottom of the furnace (below the lower burners) to convert H₂S to SO₂ effectively. Agreement between predicted and experimental data is quite satisfactory. Both show that the unburned ratio decreases with an increase in the fraction of the flow of tangential air to that of secondary air and with an increase of NO concentration. Our prediction also shows that when the tangential air is introduced from the bottom, a reduction in the H₂S formation rate is successfully effected in low-grade high-sulfur-content fuels such as heavy oil and petroleum coke.

Key Words: Pollutant, Chemical Equilibrium, Swirl, Furnace, Three-Dimensional Model, NO Formation Model, Soot Formation Model, H₂S Formation Model, Petroleum Coke Combustion, ASTM No. 6 Combustion

1. Introduction

Global warming caused by an increase in CO₂ and environmental destruction such as that caused by acid rain derived from NO_x and SO_x, are now the gravest problems on Earth. One partial solution of urgent necessity to these problems involves the enhancement of combustion efficiency. A power station boiler or an industrial furnace has mainly three-dimensional geometry and is generally operated with pulverized coal, coke and heavy oils. Combustion of low-grade, high-nitrogen and high-sulfur-content fuels such as residual oil, and pulverized coal, or coke, that are also difficult to handle is necessary from the viewpoint of effective use of energy resources.

Recently, numerical analysis of combustion characteristics in a two-dimensional axisymmetrical coordinate system, where ASTM No. 6 heavy oil⁽¹⁾, pitch-

water mixture (PWM) and coal-water mixture (CWM)⁽²⁾ are fired, has been applied to combustion systems in laboratory-scale furnaces. In a series of these studies, a more detailed examination has been described for droplet dispersion behavior and slurry (PWM, CWM) droplet combustion in spray combustion systems.

Thus the purpose of this study is to predict the efficiency of combustion, the concentration of unburned char and soot in the gas phase, and the NO concentration in the exhaust gas during the combustion of the petroleum coke together with ASTM No. 6 heavy oil in a three-dimensional furnace. The effect of secondary air on the formation of pollutants, such as concentrations of NO, unburned char and soot in the gas phase, is also estimated.

2. Theory

2.1 Governing equation

All transport equations in this study can be written for Cartesian geometry as:

$$\frac{\partial}{\partial x_j}(\rho U_j \phi) = \frac{\partial}{\partial x_j} \left(\Gamma_\phi \frac{\partial \phi}{\partial x_j} \right) + S_\phi + S_{d\phi}, \quad (1)$$

where ϕ represents the dependent variables which

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denote the momentum (U, V, W), mass (1), turbulence energy (k), eddy dissipation rate (ϵ), enthalpy (h), radiative heat flux (R_j) and mass fraction (m_i ; i = soot, volatile matter, $N_2, O_2, CO_2, H_2O, CO, NO, HCN$). Γ_ϕ is the exchange coefficient, S_ϕ is the source term in the gas phase and $S_{d\phi}$ is the source term between the particle phase and the gas phase whose coupling is calculated using the PSI cell method⁽³⁾. The inlet conditions such as velocity components, temperatures and concentrations of gases are given directly by the experimental condition. The turbulence parameters of k and ϵ are determined in the same manner as in Khalil et al⁽⁴⁾. The wall boundary condition for the flow field is estimated by the standard wall function method⁽⁵⁾.

2.2 Overall paths of the combustion reaction

The paths of the combustion reactions of the droplet, particle and combustible gas are shown in Table 1 where the indices (i) and (ii) denote heterogeneous and homogeneous reactions, respectively. For the homogeneous reaction step, both the volatile matter and CO are assumed to have infinite chemical reaction rates and thus be limited by the turbulent diffusivity where the eddy-dissipation model⁽⁶⁾ is utilized.

2.3 Modelling of swirl burner

Figure 1 is an illustration of the burner cross section in a theoretical model designed for calculation purposes. Although the outlet shapes of the actual

Table 1 Particle, droplet and gas-phase reaction mechanism

(i)	
Pet. coke	$\rightarrow N_2 + O_2 + SO_2 + H_2O + Ash + CO$
	$\downarrow$ (ii)
	CO_2
	$\uparrow$ (ii)
	CO
	$\uparrow$ (i)
ASTM No. 6 (i), (ii)	
heavy oil	$\rightarrow N_2 + O_2 + CO_2 + SO_2 + H_2O + C(\text{residual}) + Ash$
(i): Heterogeneous reaction, (ii): Homogeneous reaction.

Fig. 1 Illustration of swirl burner model

burners and combustion air flow-off pipe are circular, the shapes are modified to be rectangular for the convenience of computation. These areas are equivalent to those of the practical system. The hatched region in the center of Fig. 1 corresponds to the petroleum coke particle ejection part, and the center point (symbol of $\bullet$) of this region corresponds to the heavy oil droplet-ejection point. Combustion air is supplied to the furnace in 8 sections (for ease of calculation) outside the circumference of the hatched region. Swirling air is generated by V and W (symbol of $\rightarrow$) which are computed from the vane angle whose velocities are given on the staggered mesh.

2.4 Radiative heat transfer model

Radiative heat transfer is handled by the ordinary 6-flux method⁽⁷⁾. With a gray gas assumption, the emissivity of the combustion gas is calculated from the partial pressure of the emissive gas species (CO_2, SO_2, H_2O) and the gas-phase soot-mass fraction⁽⁸⁾. The overall emissivity, which also contains the particle, is as follows:

$$\epsilon = 1 - (1 - \epsilon_g) \exp(-\pi D_p^2 \rho_N \Delta x_j / 4), \quad (2)$$

where D_p is particle diameter, ρ_N is particle number density and Δx_j is the length of the cell in direction j . The absorption coefficient of the gas is given as

$$a_R = 0.025 a_R' = 0.025 \epsilon / \Delta x_j. \quad (3)$$

Although the scattering coefficient s_R varies greatly with particle number density and gas composition, it is assumed to be 0.13⁽⁹⁾ in the spray combustion system.

2.5 NO formation model

Thermal NO formation is calculated using the extended Zeldovich mechanism, as shown in Eqs. (4) - (6), where the local chemical equilibrium is assumed.

The reaction sequence of fuel NO is estimated using the model of Scott et al⁽¹⁰⁾.

2.6 H₂S formation model

All of the sulfur in the fuel is assumed to be converted to SO_2 , which is reduced to H_2S due to the lack of oxygen. SO_2 and H_2S concentrations are calculated in every control volume under the assumption of the following local equilibrium:

The gas composition at the state of equilibrium is calculated in the same way as the thermal NO calculation.

2.7 Gas-phase soot-formation model

The concentration of soot in the gas phase is calculated by the model⁽¹¹⁾ which takes both rates of formation and burnout into consideration.

2.8 Analysis of particle and droplet dynamics and reaction

2.8.1 Momentum equation The particle and droplet momentum equation is

$$m_p \frac{du_j}{dt} = \frac{1}{2} C_D \rho (U_j - u_j)^2 + m_p g_j, \quad (8)$$

where the drag coefficient C_D is a function of Reynolds number⁽¹²⁾. The dispersion model of the particle and droplet is illustrated in Fig. 2. For petroleum coke, the axial component of the initial ejection velocity, u_{in} , is assumed to be equal to the inlet velocity of the carrier air, and the other ejection velocity components are zero. The ejection point of the particle is assumed to be dispersed randomly in the outlet of the burner. For ASTM No. 6 heavy oil, the axial component of the initial ejection velocity is the same as the ejection velocity. On the other hand, the perpendicular velocity components, v_{in} and w_{in} are given randomly with the spray angle of 2θ and the standard deviation of 0.5θ . As a result, droplets are dispersed inside the cone of spray. The influence of gas-phase velocity fluctuation upon the particle and droplet trajectory is considered using the method of Boyd and Kent⁽⁹⁾.

2.8.2 Reaction model The particle and droplet energy equation is

$$\frac{d(m_p h_p)}{dt} = h_p \frac{dm_p}{dt} + Q_{pc} + Q_{pr} + Q_{pb} + Q_{pl}, \quad (9)$$

where Q_{pc} , Q_{pr} , Q_{pb} and Q_{pl} are rates of convective and radiative heat transfers, the rate of combustion heat release of the particle and the latent heat of droplet evaporation, respectively. The heat transfer rate is modified by the transfer number.

The reaction rate coefficient of petroleum coke

Table 2 Underrelaxation factor for dependent variables

P	U_j	k	ϵ	μ_t	ρ	h	$\dot{m}_i$	R_j
1.0	0.3	0.7	0.7	0.7	0.7	0.5	0.7	1.0

Fig. 2 Illustration of particle and droplet dispersion model

combustion, k_c , is given by Young and Smith's equation⁽¹³⁾. ASTM No. 6 heavy oil is assumed to be composed of volatile matter and residual carbon. The evaporation rate of volatile matter is estimated by the Ranz-Marshall equation and includes the blowing effect of volatile matter:

$$\frac{dm_p}{dt} = -\frac{\pi D_p^2}{C_p} \ln(1+B) h_c, \quad (10)$$

$$B = C_p (T_p - T_s) / L_H, \quad (11)$$

where B is the transfer number, and C_p , T_s and L_H are the constant pressure specific heat, the saturated temperature and the latent heat of the heavy oil, respectively. The combustion rate of the residual carbon after the evaporation of volatile matter is considered to have the same reaction rate as petroleum coke combustion. The reaction rate of the coke and residual carbon is estimated using the general overall reaction rate coefficient, k_t , as follows:

$$\frac{dm_p}{dt} = -\pi D_p^2 k_t, \quad (12)$$

$$k_t = \frac{1}{(1/k_c) + (1/k_d)}, \quad (13)$$

where k_d is the oxygen diffusion rate coefficient⁽¹⁴⁾.

3. Numerical Solution

3.1 Solution of partial differential equations

The solution of a system of partial differential equations such as Eq. (1) must be performed in an iterative manner because of the high degree of non-linearity and interconnection of equations. Finite-differential equations for ϕ can be expressed using the general form⁽¹⁵⁾:

$$A_P \phi_P = A_E \phi_E + A_W \phi_W + A_N \phi_N + A_S \phi_S + A_T \phi_T + A_B \phi_B + S_U, \quad (14)$$

$$A_P = A_E + A_W + A_N + A_S + A_T + A_B - S_P, \quad (15)$$

where A_i ($i = E, W, N, S, T, B$) are the coefficients around the point P . The convection-diffusion flux is evaluated using the power-law scheme. The source term is linearized as follows:

$$S_U + S_P \phi = \iiint S_\phi(x, y, z) dx dy dz. \quad (16)$$

The underrelaxation method is further employed for successive iteration, and the underrelaxation factor for each variable is shown in Table 2. The coupling of pressure and velocity fields is followed by the SIMPLE algorithm⁽¹⁵⁾. The convergence criterion is assumed to correspond to normalized residuals in all conservation equations which are less than 0.01 of the values at the inlet condition for mass and momentum equations and at the adiabatic temperature for enthalpy and radiative flux equations.

3.2 Solution of ordinary differential equations

The ordinary differential equations are simultaneously integrated using the Runge-Kutta-Gill method

Table 3 Fuel properties and initial conditions of numerical analysis

Fuel	Petroleum coke	ASTM No.6 heavy oil
Proximate		
volatile matter (%)	-	87.95
fixed carbon (%)	98.8	12.0
fly ash (%)	1.2	0.05
Ultimate		
C (%)	88.6	84.65
H (%)	4.0	10.0
O (%)	0.2	0.0
N (%)	2.2	0.35
S (%)	5.0	5.0
Lower calorific value (MJ/kg)	34.7	40.0
Initial velocity (m/s)	50.0	150.0
Initial diameter (μm)	10.0~130.0	25.0~325.0
class division number	7	7
Ejection point	20(Gaussian dist.)	Fixed in nozzle tip
Ejection angle (deg.)	0	10(at random)
Number of nozzles	6	12
Total calculated number of trajectories	840	840

Table 4 Operating conditions

Fuel flow rate		
Petroleum coke(provided with lower burner)	3.47 (kg/s)	
ASTM No.6 heavy oil (upper burner)	0.96 (kg/s)	
(lower burner)	3.21 (kg/s)	
Air flow rate and temperature		
Lower burner(with EGR=0.147, S=1.3)	39.0 (Nm^3/s), 563 (K)	
Upper burner(with EGR=0.147, S=1.3)	39.0 (Nm^3/s), 563 (K)	
Upper air port	16.6(1- α) (Nm^3/s), 556 (K)	
Lower air port	16.6 α (Nm^3/s), 556 (K)	
Air ratio		1.1 [-]

for each particle or droplet. The integration time step is taken to be the lesser of the eddy lifetime and characteristic time for a particle to traverse an eddy⁽⁹⁾.

4. Experimental Apparatus

Combustion of petroleum coke together with ASTM No. 6 heavy oil is investigated in a 125 MW(e) universal pressure utility boiler. The configuration and grid arrangement of the furnace are shown in Fig. 3. The furnace is operated using a total of 12 swirl burners on two opposite walls, on which each has three burners located at the lower part of the furnace (lower burner for coke and heavy oil combustion) and three other burners located above those. The upper burners are only used in heavy oil combustion. Nonswirling overfiring air is introduced from 5 air ports (UAP: upper air port) which are located above the upper burners that face each other. Air is also introduced from 4 air ports (LAP: lower air port) which are located below the lower burners to allow tangential air flow. The fuel properties and initial conditions of trajectory calculations of fuels are shown in Table 3. Fuel droplet diameter distribution is shown in Fig. 4. The operating conditions are shown in Table 4 where EGR is exhaust gas recirculation, S is the swirl number and α is the fraction of the total secondary air flow rate that is attributable to the LAP air flow rate.

Fig. 3 Configuration and grid arrangement of the furnace

Fig. 4 Initial coke particle and oil droplet diameter distribution

5. Result and Discussion

5.1 Trajectories of fuels

Particle and droplet trajectories in the furnace are shown in Fig. 5 with variations of α , where the upper figure represents the particle flow behavior and

the lower one represents the droplet flow behavior. In both, the trajectories illustrate that particle or droplet dispersion occurs with a change of starting locations or initial velocities. Since the reverse flow near the burner caused by the swirling flow influences the dynamics of the particle and droplet, the residence time near the burner is relatively long, especially for a particle or droplet whose initial velocity is very small. Most small particles or droplets burn out in this region. As α increases, both the particle and droplet fly below the lower burner and burn well. Most particles or droplets near the wall of the furnace have a long lifetime since the gas temperature near the wall region is relatively low.

5.2 Distribution of gas temperature

Figure 6 shows the temperature distribution at the center plane of the furnace with variations of α . When $\alpha=60\%$, the higher-temperature zone which is caused by the mixing and combustion of LAP air with combustible gas, is observed below the lower burners.

Fig. 5 Predicted particle and droplet trajectories with variations of α (upper figure: particle, lower figure: droplet)

The high-temperature region in the center plane of the furnace also enlarges toward the outlet of the furnace with an increase in α .

5.3 Distribution of oxygen concentration

The oxygen concentration distribution at the center plane of the furnace is shown in Fig. 7 with variations of α . As α is increased, the combustion region is extended throughout the furnace.

5.4 Distribution of NO concentration

The NO concentration distribution at the center

Fig. 6 Predicted contours of temperature (K) at the center plane of the furnace with variations of α (contour lines in intervals of 100 K)

Fig. 7 Predicted contours of oxygen concentration at the center plane of the furnace with variations of α (contour lines in intervals of 2%)

plane of the furnace is shown in Fig. 8 with variations of α . The low-NO region at the center of the furnace appears to be a NO reduction region since it is a region of high temperature and low oxygen concentration. As the NO reduction region becomes small with an increase in α , the NO concentration at the outlet plane gradually increases.

5.5 The effect of α on NO and soot in exhaust gas

Figure 9 shows the effect of α on NO and soot (a summation of unburned char and soot in gas phase) concentrations in the exhaust gas. The calculated result is in good agreement with the experimental result for NO concentration in the exhaust gas. With an increase in α , NO concentrations in both the experimental and calculated results gradually increase, and this tendency is clearly illustrated in Figs. 6-8. On the

Fig. 8 Predicted contours of NO concentration at the center plane of the furnace with variations of α (contour lines in intervals of 50 ppm)

Fig. 9 Effect of α on NO and soot concentrations in exhaust gas

other hand, the soot concentration in the exhaust gas decreases with an increase in α . Consequently, the soot-formation rate in the region of high equivalent ratio is high and burnout is not completed under the condition of a small α .

5.6 Effect of α on the maximum H_2S concentration at the bottom of the furnace

Figure 10 shows the effect of α on the maximum H_2S concentration at the bottom plane of the furnace and Fig. 11 shows the contours of oxygen concentration at this same plane. As α increases from 0% to 60%, the H_2S concentration sharply decreases from 3500 to 150 ppm. Consequently, the oxygen concentration below the lower burners increases with an increase in α , as shown in Fig. 11, and H_2S in Eq. (7) is converted to SO_2 . The introduction of LAP air below the lower burners is effective in the reduction of H_2S formation which causes sulfur corrosion.

6. Conclusions

A three-dimensional theoretical model for spray combustion in flames of ASTM No. 6 heavy oil with petroleum coke, which includes the effects of swirling flow near the burner and combustion air introduction from the lower air port, has been described. The reduction of NO and soot emissions in exhaust gas and of the formation of H_2S at the bottom of the furnace were studied.

Fig. 10 Effect of α on maximum H_2S concentration at a bottom plane of the furnace

Fig. 11 Predicted contours of oxygen concentration at the bottom plane of the furnace with variations of α (contour lines in intervals of 1%)

(1) The predicted NO concentration in the exhaust gas is in good agreement with experimental results, and both show that the NO concentration in the exhaust gas increases with an increase in α (the fraction of the total secondary air flow rate that is attributable to LAP air flow rate). However, the soot concentration in the exhaust gas decreases.

(2) The prediction shows that the H₂S concentration at the bottom of the furnace sharply decreases from 3 500 to 150 ppm, when α increases from 0 to 60%. The introduction of LAP air at the bottom of the furnace will thus be effective in the oxidation of H₂S which causes sulfur corrosion.

Our predicted results demonstrate that it is difficult to reduce emissions of both NO and soot by only controlling α . Finally, in order to determine the optimum combustion condition using this simulation method, further research involving the change of the flow rate ratio of exhaust gas recirculation, temperature of combustion air, location and number of burners, secondary air ports and swirl intensity of the burner must be conducted.

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