Study on the Simulation Method for Wall Burning in Liquid-bath Combustor

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Abstract: - Considering the limitation of existing simulation method for burning characteristics in the liquid-bath combustor, this paper puts up a new wall-burning model from the true physical phenomenon of coal particle deposition. Combined with conventional coal combustion simulation program, the total computational frame also is introduced. From the comparison of simulation results from several kinds of methods, the differences of them are analyzed, which can provide a new computational idea for the simulation of liquid-bath combustor.

Key-Words: - Coal combustion, liquid-bath, combustor, wall-burning, particle deposition, simulation

1 Introduction

Almost all processes of coal combustion are comprehensive and intensive. With the development of computational fluid dynamics for twenty years, many colleges, institutes and other special research groups have developed lots of computational programs. But most simulation results from these programs cannot have the very satisfying agreement with the experimental data. The possible reason is the lack of precision of sub-models on one hand, but on the other hand, the most important reason is the half-baking of the total combustion model, that is to say, many factors that can affect the burning characteristics have not been considered. For example, coal ash or particles will deposit on the wall during the process of coal combustion. The decreasing or increasing of ash deposition will change the wall boundary condition and affect the heat transfer through the wall and burning characteristics in the combustor. But in existing CFD software, this important heat process has not been considered, so the authentic combustion condition can not be simulated well, which makes the simulation results can not provide the good guidance for the design and operation of coal furnaces or combustors. In a word, it is a critical problem need to be solved necessarily that how to simulate deposition process in order to modify the existing computational frame of coal combustion.

For making the analyzed results more precise and acceptable, many researchers have carried on many studies for ash deposition in coal combustors. Wang et al. [1] summarized several existing models and classified total process into nine issues: (1) ash formation; (2) fluid dynamics and particles transport; (3) particle impaction; (4) particle sticking; (5) deposition growth as a function of location in the combustion chamber; (6) deposition properties and strength development; (7) heat transfer through the deposition layer; (8) the effect of deposition on operating conditions (e.g. temperatures and heat fluxes) in the combustor; (9) deposition structure and its effect on flow patterns in the combustion facility. These issues are shown on Fig.1. Based on this classification and summarization, Wang et al. [1], Lee et al. [2], Fan et al. [3] studied the particle deposition respectively. For several experimental coals used in the solid-bath furnaces, the simulation results have been compared with the experimental data and acceptable agreement was achieved. But in liquid-bath combustor or furnace, the temperature is high, molten slag layer will cover the wall and capture the particles. If these particles contain combustible matters, they will continue to burn on the wall. The left coal ash will flow with the slag layer, which makes the total amount of ash deposition be much more than that in solid-bath combustor and the wall boundary condition change

sharply. So above nine issues are not enough to describe the deposition in liquid-bath combustor. In this paper, the wall-burning model is developed as



in modeling ash deposition [1]

2 Mathematical models

2.1 Coal combustion model

Under the 2D cylindrical coordinate, the Lagrangian/Eulerian mixed model is used to simulate the coal combustion, the governing equation of mass, momentum and energy for gas and particle will be solved under Eulerian and Lagrangian coordinate respectively. Some models, including k- ε /RNG model, two competing steps model, diffusion/dynamics mixed model, EBU/Arrhenius model, stochastic separate flow model and discrete transfer radiation model are used simulate gaseous turbulent flow. coal to devolatilization, char combustion, gaseous combustion, particle turbulent flow and radiation heat transfer, as shown in [4]. The governing equation under 2D cylindrical Eulerian coordinate can be described as:

$$\frac{\partial}{\partial x}(\rho u \varphi) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v \varphi) = \frac{\partial}{\partial x} \left(\Gamma_{\varphi} \frac{\partial \varphi}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \Gamma_{\varphi} \frac{\partial \varphi}{\partial r} \right) + S_{\varphi} + S_{\varphi p} (1)$$

Where φ , Γ_{φ} , S_{φ} , $S_{\varphi p}$ stand for some parameters, which are described in detail in [5].

2.2 Particle deposition model

Dominating by drag force, gravity force and other forces (such as Brownian force, thermophoresis force, electrical force, lift force, etc.), some particles will move towards wall, and only part of them can arrive. Deciding by the characteristics of arriving particles and wall, some arriving ones can stick and deposit, others maybe re-bounce and be carried by the accessory for above nine issues in order to simulate total process more reasonably.



gas again. So it is a critical problem while describing particle deposition that how to compute the arriving efficiency and sticking efficiency of particles. The different ways to affirm it are given in [1] and they will be selected to simulate coal combustion in this article.

2.2.1 Arriving efficiency of particles

The definition of arriving efficiency is:

$$\eta_{imp} = \frac{J}{J_0} \tag{2}$$

Where *J* is the arriving mass rate of particles, J_0 is the total mass rate of particles that ejected into combustor. Borrowing ideas from free-flight model developed by Friedlander & Johnstone [6]: when particles move to stop distance H_0 (deviated from wall), they will traverse the sub layer at the speed of u_d and arrive at wall, as shown on Fig. 2.

Usually the results of deposition experiments or calculations are presented as curves of non-dimensional deposition velocity u_d^+ versus non-dimensional particle relaxation time τ_p^+ . The deposition velocity, u_d , is the particles mass transfer rate, J, normalized by the mean or bulk concentration, C_0 . All of these can be described as:

$$\tau_{p}^{*} = \tau_{p} \frac{u^{*2}}{v} = C_{c} \frac{\rho_{p} d_{p}^{2}}{18\mu} \frac{u^{*2}}{v}$$
(3)

$$u_{d}^{+} = \frac{u_{d}}{u^{*}} = \left(\frac{J}{C_{0}}\right) \frac{1}{u^{*}}$$
(4)

$$C_{c} = 1 + \mathrm{Kn} \left[1.257 + 0.4 \exp\left(1 - \frac{1.1}{\mathrm{Kn}}\right) \right]$$
(5)

Where u^* is friction velocity, C_c is Cunningham correction factor.

In the computer simulation, the particle

non-dimensional deposition velocity is estimated as:

$$u_{d}^{+} = \left(\frac{N_{d}/t_{d}}{N_{0}/H_{0}}\right) \frac{1}{u^{*}}$$
(6)

Where N_d is the number of deposited particles in the time duration t_d , N_0 is the initial number of particles uniformly distributed in the region within a distance of H_0 . In this paper, the distance H_0 is predefined as the position that is just at the edge of the viscous sub-layer with $y^+=5$, which has been described in the standard wall function.

Wood [7] summarized deposition mechanism of different particles. It is observed that the particle non-dimensional deposition velocity u_d^+ has a V-shape variation along with the particle non-dimensional relaxation time τ_p^+ . This can be described by Wood's empirical equations:

$$u_d^+ = 0.1$$
 $\tau_p^+ \ge 10$ (7)

$$u_d^+ = 0.057 \text{Sc}^{-2/3} + 4.5 \times 10^{-4} \tau_p^{+2} \qquad \tau_p^+ < 10$$
 (8)

Sc is Schmidt number, which is given by:

$$Sc = \frac{v}{D_{bf}} = \frac{3\pi v d_p \mu}{C_c \kappa_b T}$$
⁽⁹⁾

Where D_{bf} is Brownian particle diffusivity, κ_b is Boltzmann constant. From equations (2)~(9), particle arriving rate *J* and particle arriving efficiency η_{imp} can be computed.

2.2.2 Sticking efficiency of particles

The net rate of deposition depends on both the arriving rate of particles and their ability to stick to wall. The sticking efficiency is used to describe this ability, which is:

$$f_{dep} = \frac{J_{dep}}{J} \tag{10}$$

Where J_{dep} is the deposition mass rate of particles, J is the arriving mass rate of particles. Walsh [8] thinks that the viscosities of particle and deposition surface are the most important factors that can affect the particle's sticking. For this, he used particle's viscosity to describe the sticking probability:

$$p_{i}(T_{p}) = \frac{\mu_{ref}}{\mu_{p}} \qquad (\mu_{p} > \mu_{ref})$$

$$p_{i}(T_{p}) = 1 \qquad (\mu_{p} \le \mu_{ref})$$
(11)

Where $p_i(T_p)$ is the sticking probability of particles of composition *i*, T_p is the particle temperature while impacting, μ_{ref} is critical viscosity with the value $10^5 \cdot 10^8$ Pa.s commonly and with the value 10^3 Pa.s while existing molten slag layer [9]. μ_p is particle's viscosity with the temperature dependence described by Urbain model [10].

Considering the properties of particle and deposition surface, sticking efficiency can be regarded as:

$$f_{dep} = p_i(T_p) + \left[1 - p_i(T_p)\right] p_{sur}(T_s) - k_e \left[1 - p_i(T_p)\right] \left[1 - p_{sur}(T_s)\right]$$
(12)

Where $p_i(T_p)$ stands for the sticking probability of particles of composition *i* at the particle's temperature and $p_{sur}(T_s)$ stands for the sticking probability of the deposition surface at surface's temperature. k_e is the erosion efficiency of dry ash towards its own deposition, which contributes negatively to the particle sticking.

Basing on equations $(10)\sim(12)$, the deposition mass rate of particles can be computed and that will provide the basis for the following wall burning model.

2.3 Wall burning model

In pulverized coal-fired furnace or combustor, especially in liquid-bath furnace or combustor, the particle whose size less than 1mm is at the state of intenerating or melting while depositing, so once they are captured by deposition surface, it is very difficult for them to go back to spatial space and be carried by gas again. Only a few particles with big size more than several millimeters keep its rigidity while depositing, these particles are likely to be carried into gaseous field time after time. In pulverized coal-fired boilers, the size of most particles is less than 1mm, so the hypothesis that the particles cannot go back to spatial space once depositing is reasonable.

Following the hypothesis, if there is combustible matter (volatile, char) not being consumed up yet while depositing, the particles will stick to the wall and continue to burn, as shown in Fig.3. The burning characteristics of single particle on the molten slag layer depend on contact radius a to a great extent. Johnson *et al.* [11] developed *JKR* model that included the effect of adhesion force on the deformation of an elastic sphere in contact radius is given as:

$$a^{3} = \frac{R}{K} \left[P + 3\pi\gamma R + \sqrt{6\pi\gamma RP + (3\pi\gamma R)^{2}} \right]$$
(13)

$$K = \frac{4}{3} \left[\frac{(1 - v_{particle}^2)}{E_{particle}} + \frac{(1 - v_{slag}^2)}{E_{slag}} \right]^{-1}$$
(14)

Here *R* is the particle radius, *K* the elastic constant, *P* external force applied on the particle, γ the surface energy, *E* elastic modulus and *v* Poisson ratio. If setting *P* = 0 in equation (13), the corresponding contact radius is:

$$a = \left(\frac{6\pi\gamma R^2}{K}\right)^{1/3} \tag{15}$$

For plastic deformation, equation (13) should be modified. But in our present computing work, the result from equation (15) is adopted without considering the plastic deformation of particles yet.



Fig.3. The diagram of particle burning on molten slag layer

The effective surface area S_{eff} and effective volume V_{eff} , which is exposed to the gas, are:

$$S_{eff} = 2\pi R(R + \sqrt{R^2 - a^2})$$
 (16)

$$V_{eff} = \frac{4}{3}\pi R^3 - \frac{1}{6}\pi (R - \sqrt{R^2 - a^2}) \left[3a^2 + (R - \sqrt{R^2 - a^2})^2 \right] (17)$$

The effective diameter d_{eff} is defined as:

$$d_{peff} = \sqrt{\frac{S_{eff}}{\pi}} \tag{18}$$

The effective temperature of the particle on the molten slag layer is defined as:

$$T_{eff} = [T_p V_{eff} + T_{slag} (V - V_{eff})]/V$$
(19)

Where, T_p is particle temperature while impacting,

 T_{slag} is surface temperature and V is particle's volume. The effective diameter, effective surface area, effective volume, effective temperature and the content of combustible matter in the particle computed from above equations will help to gain the char consumption rate q_c and volatile pyrolysis rate q_v . Accordingly, the heat production of char combustion, CO production and volatile production in the time duration t_d will be known. Integrating with all other depositing particles, the total source term produced from solid-phase will be simulated reasonably.



Fig.4. Computation frame for coal combustion considering the deposition and wall-burning of particles

3 Computational frame

Using above numerical models, the whole burning characteristics near the wall in the combustor will be known. In fact, the process of ash deposition is relevant to deposition time steps: at the initial time, particles will deposit on the clean wall. Then with the time increasing, the depositing particles will cumulate on the wall and the thickness of slag layer will increase. Basing on the heat transfer mechanism, the temperature of layer will continue to increase till it is higher than the fusion temperature of bulk ash. At this time, the thickness of slag layer will not change and the process of deposition is regarded as stable. The steady-state computational frame is given in Fig. 4. From this frame, it should be paid attention to that the transient changing of slag layer thickness has not been considered at present. So for steady-state computation, it is supposed that there has been molten slag layer existing on the wall and the computational "wall" is the molten slag layer actually. In the computation case, the temperature of external wall and average heat resistance basing on the experimental test will be given in order to compute the heat flux through the wall. SIMPLE algorithm is used for p-v correction, and TDMA algorithm is used to solve the discretisation equations line by line.

4 Computational cases

The computational grid of a liquid-bath combustor is shown in Fig. 5. The secondary air is ejected into the combustor chamber through the annular vane with 30mm width at the position between r =200mm~230mm. The primary air with coal particles is ejected into the place very near the secondary air, which will make the primary air gain the largest tangential momentum. The external wall surface is cooled by water steam with 373K temperature, the average heat resistance of water steam, steel tube, flame retardant coating and slag layer is $0.03m^2$ K/W basing on hot test, the initial particle mass rate J_0 is 0.0279kg/s, the average size of particles d_p is 0.075mm and the stoichiometric ratio is 1.03. Other inlet conditions are shown in Table 1.



Fig.5 Computational grid (Unit: mm)

Table 1. Air inlet conditions

Primary air				Secondary air			
Axial velocity (m/s)	Radial velocity (m/s)	Tangential velocity (m/s)	Inlet temperature (K)	Axial velocity (m/s)	Radial velocity (m/s)	Tangential velocity (m/s)	Inlet temperature (K)
10.74	0	0	293	10.74	0	102.18	580

For the simulation of interaction between particle and wall in liquid-bath combustor, there is about three kinds of methods: (1) elastic impingement between particle and wall without considering particle deposition mechanism; (2) partially non-elastic or totally non-elastic impingement without considering particle deposition mechanism; (3) Partially non-elastic impingement with considering particle deposition and wall burning mechanism, which is shown in this paper.

Fig. 6 shows all particles' information just when the deposition phenomenon happens. These information include volatile mass rate, char mass rate, ash mass rate, etc. From the information, it is known that volatile has emitted from coal particle during the process of spatial combustion, so there is almost no volatile content at the time of deposition. But char is burning so slowly that there is much char content in particles during deposition process. If the temperature of molten slag layer is high enough to capture these particles, the char will continue to burn on the layer. Fig. 7 gives the comparison of "wall" temperature calculated from above three methods. It should be noticed that the "wall" temperature is the temperature of slag layer actually. Calculating with method (1), computational temperature is too low for steady burning and the results is wrong; calculating with method (2), the results depend on the coefficient of restitution, e. some researchers [12] hypothesis of totally used the non-elastic impingement, which means, e = 0. This hypothesis adapts to the condition that the whole wall is covered by molten slag layer includes the place which is very near the air inlet. By experimental probe, the temperature at the position near the air inlet is not high enough to make slag melt and the temperature of particles is low too, which will make the particle hardly stick to the wall. In that place, the coefficient of restitution e cannot be regarded as zero. Reflected from the calculation result, using method (2), the wall temperature near the air inlet is something high; calculating with method (3),

particle deposition and wall burning mechanism are combined with partially non-elastic impingement condition with e = 0.5. From the computational result, it is known that there is an obvious wall-burning region from 0.14m to 0.65m and the



5 Conclusion

For the simulation of liquid-bath combustor, it is the key point that how to analyze burning characteristics near the wall properly. In this paper, a new wall-burning model from the true physical phenomenon of coal particle deposition is developed and the total computational frame is given. Compared with other simulation methods, this computational idea is more reasonable. But some hypothesis in the paper should be modified further:

(1) Once the thickness changing of slag layer will affect the total heat transfer, it should be noticed more thoroughly. Though the transient program can compute this process more properly, it will take more computational CPU time. So the quasi steady-state program is the better choice, as discussed in [1].

(2) When particles deposit on molten slag layer, it will move together with the slag flow. The hypothesis that particles should be fixed in the deposition place will make the local temperature high. Slag flow model should be added in next work.

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temperature is high because of the wall-burning mechanism. From the head of the combustor to 0.14m, the temperature is low because of the cooling by inlet air and external water steam.



i ig., wan temperature of compastor

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