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Modeling of ash deposition in a pulverized-coal boiler by direct simulation Monte Carlo method

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HIGHLIGHTS

- A dynamic mechanistic model of ash deposit formation was developed.
- Particle collision was modeled using a direct simulation Monte Carlo method.
- Fine particles were selectively captured during the initial deposition stage.
- Results are consistent with the morphology of ash deposit determined by SEM.

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ABSTRACT

In this paper, a mathematical model of the fly ash deposition in a 660 MW supercritical once-through boiler was developed. The mechanism of particle-particle and particle-wall collisions has been considered. Particle collision is modeled by a direct simulation Monte Carlo (DSMC) method. Three sub-models (impaction, thermophoresis, and sticking) were included in the mathematical model. In the ash deposition model, the critical velocity model was used to calculate the ash sticking rate during initial deposition, and the viscosity model was used for the outer layer deposition. An ash deposition probe was inserted into the peephole and ash deposits were collected. The morphology of these samples was analyzed using SEM. The deposit thickness and the distributions of adhesion particle size were obtained by mathematical model. The mean deposit thickness calculated by the DSMC method agreed with the value measured by the ash deposition probe with the relative error within 3.79%. The simulation results show that the deposition inner layer consists of fine particles less than 10 μm in size and sticky fine particles were selectively captured during the initial deposition stage. The DSMC method may be a practical alternative for studies of ash deposit formation.

1. Introduction

Fly ash formed during fuel combustion and sticking on boiler tube, may seriously reduce the heat transfer ability and cause the corrosion of the boiler. Ash deposition is a function of a number of chemical and physical processes. Many studies have examined ash deposition during the past few decades [1–4]. Two main processes are involved in ash deposition: ash particles impacting on deposit surfaces and sticking on surfaces [5].

In recent years, some studies have investigated on the growth of ash deposits by the numerical simulation and experimental. For instance, Richards et al. [6] simulated ash deposition rate, porosity and temperature of the deposit as a function of time. Allan et al. [7] developed the slagging and fouling submodels to calculate the ash impacting efficiency in a utility boiler. Zhou et al. [8] proposed a digital image technique to observe the ash deposits growth in a vertical furnace.

For analysis of the ash deposition process, the calculation of impact and sticking efficiency of particles is the principal problem [9]. Wood [10] calculated the particle impact rate by a free-flight model. Guha [11] and Baxter and DeSollar [12] presented a unified theory of ash deposition based on a turbulent impaction mechanism. Generally, the particle impacting efficiency mainly determined by Stokes number [13]. For calculating the sticking rate, Walsh et al. [14] developed a viscosity model and the particle sticking probability is determined by the ratio between the predicted impacting particle viscosity and the critical viscosity. However, the particle sticking probability predicted by these viscosity models only considered effects of temperature and ash

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Nomenclature

$\bar{c}$	mean speed of gas molecules, m/s
d	particle diameter, m
E	Young's modulus
f	friction factor
f_{dep}	capture efficiency
F_d	drag force, N
F_{th}	thermophoretic force, N
g	acceleration of gravity, m/s^2
g_0	radial distribution function
J	impulse, kg m/s
k_B	Boltzmann constant
m	mass, kg
n	local particle number
N	number of simulated particles
p_i	sticking probability
P	collision probability
q	local heat flux rate, W/m^2
R	particle radius, m
t	time, s
T	temperature, K
u	fluid velocity, m/s
v	particle velocity, m/s
W	Wadhesion energy

Greek symbols

α	function of degree of consolidation
δ	thickness, m
κ_{tr}	gas thermal conductivity, W/(m K)
λ	thermal conductivity, W/(m K)
μ	viscosity, Pa·s

composition [15]. Then, a critical velocity model was proposed [16] that considered effects of van der Waals force [17]. In this model, the incoming velocity of the particle is compared to the critical velocity, and the particle will adheres on the surface when the critical velocity is larger than the particle normal impact velocity.

Improved methods have been developed to calculate the ash deposition rate by the numerical simulation of ash transport and sticking [18]. The first dynamic simulation of particle deposition was carried out by Li and Marshall [19] using a discrete-element method (DEM). The DEM was then used to simulate the ash deposition process in a down-fired furnace by Li et al. [20,21]. However, the particle-particle collisions were not examined in these studies [18–21]. Recently, a discrete particle motion-collision decoupled model [22,23] was developed by DSMC method [24]. In this method, the trajectories of a fraction of the existing particles, are calculated. The particle number existing in the calculation region may be very large if the particle size is small, so computation based on the behavior of each particle is difficult and the DSMC method can solve this problem [25].

In this paper, the detailed process of ash deposition was simulated in a 660 MW supercritical once-through boiler. Particle collision was modeled using the DSMC method. A mathematical model includes three submodels (impaction, thermophoresis, and sticking) was proposed. To complement the simulation data, the morphology of ash deposit samples was analyzed by SEM. The deposit thickness and the distributions of adhesion particle size were obtained. The calculated results were compared with the experiments. This predictive model provides a reference for the future development and improvement of ash deposition models.

2. Mathematical model

2.1. DSMC method

In the DSMC, the particle motion is separated by the two processes of movement and collision. The detailed computation can be described by: First, the particle-particle collisions were neglected and particle position is calculated by the motion equation in a small time step Δt. Then, the Monte-Carlo method was used to calculate the particle-particle collision and the post-collision velocities of particles are calculated by the Eqs. (7) and (8). At last, the particle velocities are updated and without changing the particles positions [22,24].

The collision probability of particle i in a time step Δt can be written as [24,25]:

$$P_i = \sum_{j=1}^{N} P_{ij} \tag{1}$$

$$P_{ij} = \frac{n}{N}\pi d^2 g_0 v_{ij}\Delta t \tag{2}$$

where N is the simulated particles number in the grid, n is the local particle number, v_{ij} is the relative velocity between particle i and j.

The collision pairs searching is the key problem in the calculation of particle-particle collision. Some methods [22] have been proposed using a Monte Carlo simulation, and the modified Nanbu method was used in this study.

2.2. Particle motion model

The equation describing the particle movement can be obtained by:

$$m_i\frac{d\boldsymbol{v}_i}{dt} = m_i g + \boldsymbol{F}_d + F_{th} \tag{3}$$

The drag force $\boldsymbol{F}_d$ can be written as:

$$\boldsymbol{F}_d = -3\pi d\mu_g(\boldsymbol{v}-\boldsymbol{u})f \tag{4}$$

where μ_g is the gas viscosity and f is a drag force coefficient that used to revise the Stokes expression and $f = 1$ in this study.

The thermophoretic force is given by Waldmann [26]

$$\boldsymbol{F}_{th} = -\frac{32}{15}\frac{\kappa_{tr} r^2}{\bar{c}}\nabla T \tag{5}$$

where ∇T is the temperature gradient and κ_{tr} is the gas thermal conductivity. The mean speed $\bar{c}$ of gas molecules is given by

$$\bar{c} = \sqrt{\frac{8k_B T}{\pi m_g}} \tag{6}$$

After the particle position was determined, the particle post-collision velocities are calculated by the collisional dynamics. To reduce the complexity of particle collision analysis, some assumptions are made: interaction forces are impulsive and other forces are not considered during collision. The equation describing the particle collision can be written as [22,27]:

$$m_i(v_{i,1} - v_{i,0}) = J \tag{7}$$

$$m_j(v_{j,1} - v_{j,0}) = -J \tag{8}$$

where $v_{i,0}$ and $v_{i,1}$ are the pre-collisional and post-collisional velocities of particle i, and $v_{j,0}$ and $v_{j,1}$ are the pre-collisional and post-collisional velocities of particle j.