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DEM simulation and fractal analysis of particulate fouling on coal-fired utility boilers' heating surfaces

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ABSTRACT

The microstructure features of particulate fouling on convective heating surfaces play a dominant role on the deposition process in coal-fired utility boilers. Starting with the analysis of the main fouling mechanism, a particulate collision deposition numerical model based on the discrete element method is proposed in this paper. Applying the present method, the numerical simulation of the process of particulate deposition on a tube and a rectangular plate was carried out. The results show that simulated deposition can exactly reflect the microstructure characteristics of real fouling on boilers' heating surfaces, such as porous structure and porosity. The fractal features of the inner porous microstructure and surface morphology of the simulated deposition was further studied in this study. The investigation results indicate that the characteristics of the particle–pore interface and the surface topography, which are heterogeneous and anisotropy, can be quantitatively characterized by the fractural dimensions (FD) of pore contour and surface profile, respectively. The results of FD estimation using a box-counting method show that with decreasing porosity, the FD of pore contour increases and the FD of surface profile decreases. Additionally, particulate diameter plays a role on the fractal features of particulate deposition.

1. Introduction

Fouling on heating surfaces of coal-fired power plant boilers could lead to significant efficiency deterioration and costly unit outages. At the boiler backend, particulate fouling on convective tube surfaces form mainly by inertial collision deposition of fly ash particles, a loose granular material with many pores [1]. Similar to other porous materials, the physical properties of particulate fouling, such as the elastic modulus, structural strength and thermal conductivity are thought to be determined primarily by the deposit microstructure [2]. It has been shown that studies on the deposit structure contribute to the understanding of the deposition process and to develop countermeasures to the problem of particulate fouling [3–5].

During the past years, many studies on the deposit structure of coal-fired boiler fouling have been carried out and some useful achievements have been obtained. Kweon et al. [3] researched the interconnected structure of ash deposits formed under different temperature conditions. Baxter et al. [2] studied deposit bulk porosity and the relationship between bulk porosity and transport property of boiler ash deposits. Zhang et al. [5] studied the effects of the porosity structure of the deposition on coal-fired boiler heating surfaces. Rushdi et al. [6] developed an experimental approach to measure the changes in deposit bulk porosity at elevated temperatures and investigated the deposit porosity of Australian bituminous coal ash deposits. Xiang et al. [7] studied the mean porosity of fine particle packing material and the effect of different forces on the packing structures. All of these researches have focused on the quantitative description of the deposit structure, in terms of porosity, through the analysis on X-ray microtomography, scanning electron microscopy, laser scanning, and other optical techniques on ash samples obtained from experimental setups or actual coal-fired utility boilers. However, characterization of deposit pore structure only by porosity, which statistically describes the area extent or volume fraction of the pore phase, using traditional Euclidean geometry measurement, is not enough for clear digital expression of all geometric structure features generally [8]. New methods that offer a detailed quantitative description of the deposit geometrical microstructures, such as particle–pore interface and surface topography, which are especially important to the physical and mechanical properties of the deposit [9] are required.

It has been reported by Ref. [9] that the microstructure of particulate deposit on boiler convective tubes, which is greatly irregular and complex, has obvious self-similar features and could be studied with fractal theory. Due to the difficulty to obtain the deposit microstructure in situ and in real time, while using imaging techniques [3], researchers have used numerical simulation to get an inside into the fouling

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microstructures. For example, Kweon et al. [3] and Mendes et al. [10] analyzed fractal features of simulated particulate deposits using a ballistic deposition model. Gomatam and Mulholland studied fractal structure and thermal conductivity of deposits simulated with the shuffled Sierpinsk carpets model [9]. Filippov et al. [11] and Zhang et al. [12] studied the relationship between the fractal dimension (FD) of the deposit structure and its thermal conductivity, based on Rayleigh–Debye–Gans and renormalization group models, respectively. Refs. [13,14] reported the fractal structure and the permeability of deposits simulated with a Monte Carlo model. Also, Li et al. [15] analyzed deposit structure and fouling prevention with a cluster aggregation simulation model. Although these studies have contributed to providing theoretical foundations and technical means for deposit structure modeling, fouling simulated by those models cannot present the structural features and their changes in three-dimensional space of the real fouling. As the effects of the deposit structure relate largely to the phases present in the deposit and the extent of contact between individual particles [6], a new more reasonable model that accurately describes the contact between individual particles and the microstructures of particulate deposition on boiler convective tubes needs to be proposed.

In this paper, a new discrete element method (DEM)-based numerical model for particulate inertial impact deposition on boiler convective heating surfaces is proposed. This model can be applied into the numerical calculation of every individual particulate motion. A numerical simulation of the process of particulate deposition on a tube and a rectangular plate was then performed to demonstrate the validity of the present model. Based on a box-counting method, the fractal analysis of the simulated deposition was implemented to calculate the fractal dimension of pore interface and surface profile. The relationship between the fractal features, and deposit height and porosity was concluded from the results of the study.

2. The numerical simulation model

2.1. Mathematical model

A discrete element method, which represents the characteristics of the entire flow field through a composite of the numerical calculation of every interior individual element's motion using Newton's second law, has been applied successfully in particulate system simulation in many engineering fields, such as fluidized bed [16], particle deposit in vertical containers [17], and fine particulate packing [7,18]. Particulate fouling on boiler backend convective tube surfaces consists of many particulate elements of different sizes. Each element, either a single particle or a cluster of micro-particles, is independent and would collide with its neighbors. Therefore, this loose fouling can be thought as a dense particle system and, hence, the movement and microstructure of the fouling can be simulated with DEM.

At the boiler backend, fly ash particles with size distribution mainly in the range from 10 to 200 μm are transformed primarily by inertial forces. The density ratio of the flue gas to particles is about 0.001–0.0001. Thus, the following assumptions are valid:

(1) The influence of the gas phase on particulate movement is negligible. The forces acting on the fly ash particles, viz., the electrophoretic force, the Brownian motion force and the Van der Waals force, can be ignored [19,20];
(2) The temperature factor can also be neglected, which means that neither phase changes, nor heat transfer occurs in the flow field during the particle deposition process;
(3) Fly ash particles, which have the same chemical composition, can be considered as solid spheres and distributed uniformly along the flow field;
(4) Particles can be modeled as soft spheres, and the contact force between collision particles obeys the spring-damping rule, which evaluates the energy loss during the particulate collision phase by adjusting its damping coefficient.

Based on the theory of DEM, a mathematical model can then be established for every particulate element. Contact and separation are the two relationships between particles. The impact motion of particles is divided into two types: one is the impact between two particles; and the other one is between a particle and a wall, where the wall is treated as a special particle with zero velocity and infinite size. Applying the Hertz's contact theory and the spring-damping rule, the contact force between particle i and particle j can be calculated as:

$$\mathbf{F}^c_{n,ij} = \left(-k_n\delta_n^{3/2} - \eta_n \mathbf{v}_{ij}\mathbf{n}_{ij}\right)\mathbf{n}_{ij} \tag{1}$$

$$\mathbf{F}^c_{t,ij} = -k_t\delta_t\mathbf{t}_{ij} \tag{2}$$

where subscripts n and t present the normal and tangential components, respectively; k is the elasticity coefficient; η is the damping coefficient; δ is the particulate deformation at the contact point; $\mathbf{n}_{ij}$ and $\mathbf{t}_{ij}$ are the normal and tangential unit vector linking the centers of particle i and particle j, respectively; and $\mathbf{v}_{ij}$ is the relative velocity of particle i to particle j, $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$.

The normal and tangential components of the elasticity coefficient can be defined respectively as:

$$k_n = \frac{4}{3}\left(\frac{R_iR_j}{R_i+R_j}\right)^{1/2}\left(\frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j}\right)^{-1} \tag{3}$$

$$k_t = 8\delta_n^{1/2}\left(\frac{R_iR_j}{R_i+R_j}\right)^{1/2}\left(\frac{1-\nu_i^2}{G_i} + \frac{1-\nu_j^2}{G_j}\right)^{-1} \tag{4}$$

where R is particulate radius, E is the elastic modulus, G is the shear modulus and v is the Poisson's ratio.

The damping coefficient is a function of the critical damping coefficient, c_{cri}, and can be written as:

$$\eta = \beta c_{cri} = 2\beta\sqrt{mk} \tag{5}$$

where β is a constant determining the energy loss during the impact phase.

If $|\mathbf{F}^c_{t,ij}| > \mu|\mathbf{F}^c_{n,ij}|$, slipping between the impact particles occurs with the velocity, $\mathbf{v}_{ct}$, as:

$$\mathbf{v}_{ct} = \mathbf{v}_{ij} - \left(\mathbf{v}_{ij}\cdot\mathbf{n}_{ij}\right)\mathbf{n}_{ij} + R_i\boldsymbol{\omega}_i\times\mathbf{n}_{ij} + R_j\boldsymbol{\omega}_j\times\mathbf{n}_{ij} \tag{6}$$

where $\boldsymbol{\omega}_i$ and $\boldsymbol{\omega}_j$ are the angle velocities of particles i and j, respectively. And the contact force in the tangential direction would be changed as:

$$\mathbf{F}^c_{t,ij} = -\mu\left|\mathbf{F}^c_{n,ij}\right|\frac{\mathbf{v}_{ct}}{|\mathbf{v}_{ct}|} \tag{7}$$

where μ is the coefficient of static friction.

When the target particle i is impacted with several other particles simultaneously, the total contact force, F_c, acting on the particle can be expressed as:

$$\mathbf{F}_c = \sum_j\left(\mathbf{F}^c_{n,ij} + \mathbf{F}^c_{t,ij}\right). \tag{8}$$

And the moment of contact forces is written as:

$$\mathbf{M}_c = \sum_j\left(R_i\mathbf{n}_{ij}\times\mathbf{F}^c_{t,ij}\right). \tag{9}$$