

## A NUMERICAL MODEL FOR CHEMICAL REACTION ON SLAG LAYER SURFACE AND SLAG LAYER BEHAVIOR IN ENTRAINED-FLOW GASIFIER

by

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*The paper concerns with slag layer accumulation, chemical reaction on slag layer surface, and slag layer flow, heat and mass transfer on the wall of entrained-flow coal gasifier. A slag layer model is developed to simulate slag layer behaviors in the coal gasifier. This 3-D model can predict temperature, slag particle disposition rate, disposition particle composition, and syngas distribution in the gasifier hearth. The model is used to evaluate the effects of O<sub>2</sub>/coal ratio on slag layer behaviors.*

Key words: *deposition, reaction on slag layer surface, slag layer behavior*

### Introduction

Entrained-flow coal gasification is characterized by operating at a temperature higher than melting point of coal ash slag. The char/slag particles collide with wall under the effect of turbulent gas flow, form a liquid slag layer on the wall, and then leave gasifier through slag tapping hole at the bottom of gasifier as molten slag. Entrained flow coal gasifiers have been on commercial operation for nearly 30 years, but slag layer behavior characteristics have not been revealed yet. Slag blocking is still a problem that exists in the operation of entrained-flow coal gasifier.

Reid and Cohen [1] consider molten slag as a Newtonian fluid above the temperature of critical viscosity  $T_{cv}$ , and as a plastic fluid below  $T_{cv}$ ; the slag flow in plastic region is neglected owing to the very high viscosity. Seggiani [2] proposed a simplified model to describe the slag building behaviour in water wall entrained-flow gasifier. The thickness of slag layer is calculated by mass conservation. The motion of liquid slag layer is treated as Newtonian fluid, and the flow of slag layer is simplified as falling film along a vertical wall. Linear temperature profile is assumed in slag layer (including liquid slag layer and solid slag layer), and Fourier law is adopted to calculate heat transfer across slag layer. Temperature of critical viscosity  $T_{cv}$  is treated as the solidification temperature of slag. This model was adopted to detect slag layer behaviors in entrained-flow coal gasifiers by Seggiani, [2] Benyon *et al.* [3], Benyon [4], and Zhou *et al.* [5], respectively.

In the slag layer model of Seggiani, some factors, which have significant effects on slag layer behaviors, were ignored, such as particle deposition, chemical reaction on slag layer surface, gas flow and so on. In this work, the slag layer behavior is critically analyzed, and a more precise slag layer model is proposed. The influences of particle deposition, chemical reaction on slag layer surface, and gas flow are involved in this model.

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## Mathematical model

Coal particles experience a series of processes such as devolatilization, combustion, gasification and so on before they deposit on the wall or flow out with syngas. Simulations of entrained-flow coal gasifier can be divided into two parts, one is the behaviors of gas and particle in hearth includes devolatilization, combustion, gas-solid flow, heat and mass transfer and so on; the other is behaviors of slag layer. These two parts can give an integrated description of entrained-flow gasifier through providing boundary conditions for each other. In this paper, the work is mainly carried out on the behaviors of slag layer.

### Particle capture

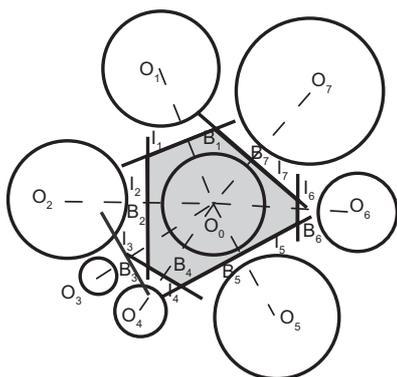
The capture efficiency of impacting particles is calculated with viscosity model [6]. The operation temperature of entrained-flow coal gasifier has to be higher than  $T_{cv}$ , to ensure liquid slag tapping. So the slag layer and deposit particles are all in molten state which means all the particles collide with slag layer surface are captured.

### Chemical reaction on slag layer surface

Carbon in deposit particles will keep on reaction after they deposit on slag layer surface, as long as they stay on the surface [7]. The model of chemical reaction on slag layer surface proposed in this paper assumes that particles on slag layer surface are pushed into inner part of slag layer after new particles deposit on the surface, and these particles will stop reacting. Therefore the residence time of particles on slag layer surface and char chemical reaction kinetics are the basic elements in detecting the influences of reaction on slag layer.

### Particle distribution on slag layer surface

The residence time of particles on slag layer surface is calculated through deposit particle rate and particle distribution on slag layer surface. Particle distribution on slag layer surface is described from the projections of deposit particles on slag layer surface in this model. For the operation temperature of entrained-flow gasifier is above the flow temperature (FT) of slag; deposit particles are treated as sphere in this model. The area occupied by a particle on slag layer surface includes the area of its projection and the area between its projection and neighbor projections, as can be seen in fig. 1.



**Figure 1. Particle distribution on slag layer surface**

Circle  $O_0$  is the projection of a certain deposit particle on slag layer surface; point  $O_0$  is the center of circle  $O_0$ . Circle  $O_1, \dots, O_7$  are its neighbor projections, point  $O_1, \dots, O_7$  are the center of each circle. Here 7 neighbor projections are around projection 1, but there may be more or less than 7 projections in actual situation. Draw line  $O_0O_1, \dots, O_0O_7$ , respectively. Separate line  $O_0O_1, \dots, O_0O_7$  into two parts according to the ratios of radiuses of circle  $O_0$  and circle  $O_1, \dots, O_7$ , respectively, and separated points are  $B_1, \dots, B_7$ , respectively. Draw perpendicular line  $l_1, \dots, l_7$  of line  $O_0O_1, \dots, O_0O_7$ , through points  $B_1, \dots, B_7$ , respectively. If line  $l_i$  intersects with its neighbor lines  $l_{i-1}$  and  $l_{i+1}$ , at each side of line  $O_0O_i$ , respectively, then circle  $O_i$  is assumed to relate to circle  $O_0$ , or circle  $O_i$

is assumed to have nothing to do with circle  $O_0$ . So, circle  $O_1$ , circle  $O_2$ , circle  $O_4$ , circle  $O_5$ , circle  $O_6$  and circle  $O_7$  relate to circle  $O_0$ , while circle  $O_3$  does not relate to circle  $O_0$ . The polygon constituted by line  $l_1, l_2, l_4, l_5, l_6$ , and  $l_7$  is the area occupied by circle  $O_0$ .

When the distribution of particles on slag layer surface is deserved, the slag layer surface can be divided into two parts, one is covered by particles containing carbon, the other is covered by slag particles (without carbon) based on particle content.

#### *Kinetics of chemical reaction on slag layer surface*

Devolatilization takes place as soon as coal particles enter into gasifier because of the high operation temperature. If deposit particle contains carbon, the particle will be treated as char particle, or the particle will be treated as slag particle. Here, reaction on slag layer surface means the reaction between carbon in particles on slag layer surface and gas which surrounds the particles. Since entrained-flow coal gasifier operates at a critical condition with elevated temperature and pressure, the char reaction kinetics under high temperature and pressure proposed by Hurt and Calo [8], Liu and Niksa [9] is chosen to describe the reaction on slag layer surface. In this char chemical reaction mechanism, char reaction are divided into combustion and gasification, and the total reaction rate is:

$$R = R_{C-Com} + R_{C-GAS} \quad (1)$$

details of this char reaction kinetics can be seen in [8, 9].

#### ***Slag layer flow, heat and mass transfer, and phase change model***

The viscosity of slag layer is as high as several Pa·s in entrained-flow gasifier. For the high viscosity, slag layer thickness increase gradually as it flows down. The gasifier is divided into several cells, the thickness of slag layer and deposition rate are treated as uniform in each cell. Slag layer flow, heat and mass transfer, and phase change behaviors are critical analyzed in each cells, respectively.

Mass conservation is used to calculate the thickness of slag layer in each cell. For  $i^{\text{th}}$  cell, mass changes of slag layer in a time step include particle deposit rate  $q_{m,in,i}$ , mass rate flowing in from the  $i-1^{\text{th}}$  cell  $q_{m,out,i-1}$ , mass rate flowing out the  $i^{\text{th}}$  cell  $q_{m,out,i}$ , and mass rate consumed in the chemical reaction on slag layer surface  $q_{m,r,i}$ . So the change of slag layer thickness  $\Delta\delta_i$  is:

$$\Delta\delta_i = \frac{q_{m,in,i} + q_{m,out,i-1} - q_{m,out,i} - q_{m,r,i}}{A_i\rho} \quad (2)$$

where  $\delta_i$  is the thickness of slag layer in the  $i^{\text{th}}$  cell, m;  $q_{m,in,i}, q_{m,out,i-1}, q_{m,out,i}, q_{m,r,i}$  [ $\text{kg}\cdot\text{s}^{-1}$ ].

In each cell, the slag layer behaviors are described with Navier-Stokes equation:

$$\frac{\partial\rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = \dot{m}_{in} - \dot{m}_r \quad (3)$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \mu \frac{\partial u_i}{\partial x_j} - \overline{\rho u_i' u_j'} \right) + \rho g + \Phi_u \quad (4)$$

$$\frac{\partial(\rho H)}{\partial t} + \frac{\partial(\rho u_j H)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_T} \right) \frac{\partial T}{\partial x_j} \right] + \dot{m}_{in} H_{in} + \dot{m}_r Q_r \quad (5)$$

where  $\dot{m}_n$  [ $\text{kgm}^{-3}\text{s}^{-1}$ ] is the particle deposit rate,  $\dot{m}_r$  [ $\text{kgm}^{-3}\text{s}^{-1}$ ] – the mass consumed in chemical reaction on slag layer surface,  $\Phi_u$  – the source term in momentum equation introduced by particle deposition, chemical reaction on slag layer surface, surface tension and shear force;  $H_{in}$  – the enthalpy of deposition particles, and  $\dot{m}_r Q_r$  – the source induced by the reaction on slag layer surface.

### Simulation tests

Slag layer simulation was carried out with a certain pulverized coal entrained flow gasifier (fig. 2). Boundary conditions were obtained from the simulation of multiphase flow,

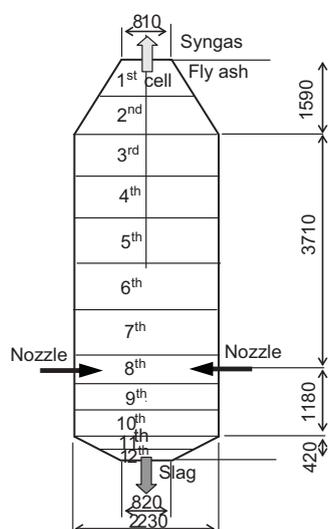


Figure 2. Schematic diagram of the gasifier

heat and mass transfer and chemical reaction in the hearth, (figs. 3 and 4). The properties of the slag are  $\rho = 2650 \text{ kg/m}^3$ ,  $\lambda = 1.33 \text{ W/mK}$ ,  $C_p = 1120.0 \text{ kJ/kgK}$ ,  $T_{cr}$  is 1550 K, and the viscosity is in tab. 1.

Table 1. Viscosity of the slag samples

	1920 K	1860 K	1750 K	1650 K	1630 K	1600 K	1580 K	1550 K
Viscosity [ $\text{Pa}\cdot\text{s}^{-1}$ ]	1.2	2.2	7.7	23.9		42.2	52.9	115.2

$\text{O}_2/\text{coal}$  ratio is one of the most important factors in entrained-flow gasifier, which affects operation temperature, carbon conversion rate, syngas composition, etc. Three cases were carried out to study the effects of  $\text{O}_2/\text{coal}$  ratio, as can be seen in tab. 2, and results are given in figs. 5-7.

Table 2. Cases of different  $\text{O}_2/\text{coal}$  rates

Case	Case 1	Case 2	Case 3
$\text{O}_2/\text{coal}$ rates	0.77	0.82	0.9

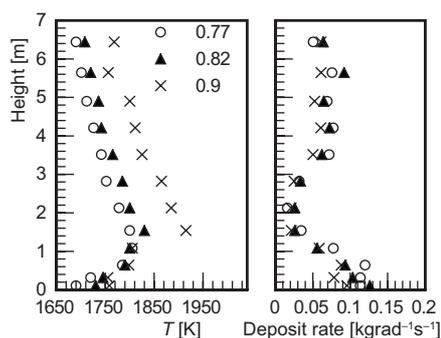


Figure 3. Temperature of hearth and particle deposit rate

2, while liquid slag layer of case 3 is 14% thinner than that of case 2.

The carbon contents of deposit particles decrease from case 1 to case 3. About 31.1% carbon in deposit particles is consumed in reaction on slag layer surface in case 1,

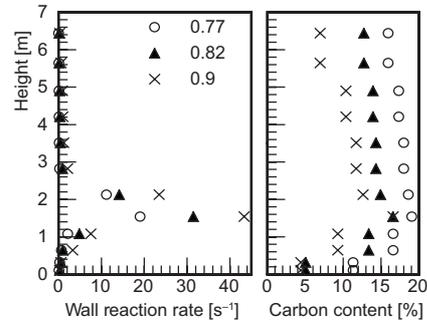
Water wall is adopted in pulverized coal gasifier. As slag layer flows down, slag is cooled by water wall, average temperature of slag layer decreases, thicknesses of solid slag layer and liquid slag layer increases. Carbon content of slag layer decreases in up cells, for chemical reaction on slag layer surface rate increases from cell 1 to cell 8, and reaches the lowest value at 9<sup>th</sup> cell.

Case 1 has the thickest solid slag layer and liquid slag layer, and the lowest average temperature while case 3 has the thinnest solid slag layer and liquid slag layer, and highest average temperature. The results of case 2 are between case 1 and case 3. The liquid slag layer of case 1 is 18% thicker than that of case 2,

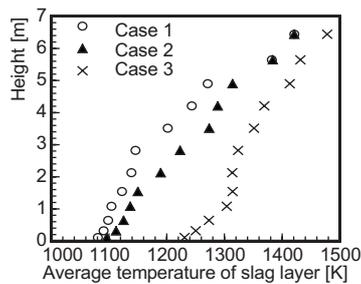
about 58.4% in case 2, and about 81.7% in case 3. Carbon consumed in reaction on slag layer surface occupies 1.5-3% of the carbon in feed coal. Carbon content of 12<sup>th</sup> cell in case 1 to case 3 is 11.2%, 5.1%, and 1.3%, respectively. Carbon content of slag is around 2% in commercial operation gasifier, simulation result of this model has a good accordance with operation data.

### Conclusions

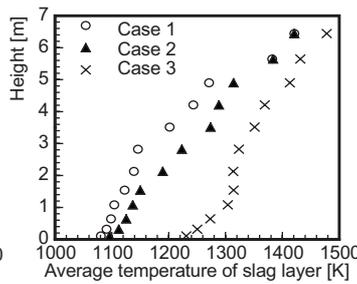
A model for slag particle capture, chemical reaction on slag layer surface, and slag layer flow, heat and mass transfer, phase change has been proposed in this paper. Simulations were carried out with a certain pulverized coal entrained flow coal gasifier.



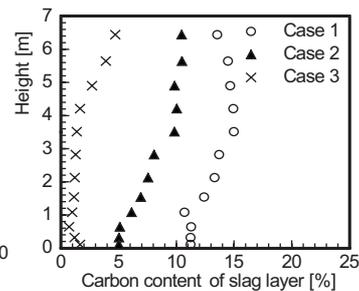
**Figure 4. Chemical reaction on slag layer rate and deposit particle carbon content**



**Figure 5. The thickness of slag layer**



**Figure 6. Average temperature of slag layer**



**Figure 7. Carbon content of slag layer**

About 50% carbon in deposit particles is consumed in chemical reaction on slag layer surface. Carbon content in 12<sup>th</sup> cell is 1.3-11.2% in these cases. The carbon content in case 2 is 5.1%, which is close to the carbon content of slag in commercial gasifier. Thickness of solid slag layer and liquid slag layer increase, while average temperature and carbon content of slag layer decrease from top to bottom of gasifier. Thickness and carbon content of slag layer decrease, while average temperature of slag layer increase with the increase of O<sub>2</sub>/coal ratio.

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