

## NUMERICAL SIMULATION OF MAGNESIUM PRODUCTION BY THE PIDGEON PROCESS PART II: COUPLING OF THE MAGNESIUM REDUCTION IN THE RETORTS WITH THE SURROUNDING THERMAL-FLOW FIELDS IN A COAL-FIRED FURNACE

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### ABSTRACT

The magnesium reduction process occurring in a retort as described in Part I is carried out in a refractory brick coal-fired furnace. It is considered that the thermal-flow inside the furnace has an important effect on the heat transfer and reduction of the reactive compound in the retort. In this paper, a comprehensive two-dimensional unsteady model was developed in combination of the magnesium reduction model put forward in Part I with the conventional gas-particle turbulent flow and combustion models. The set of equations was solved by the time-marching method. The prediction revealed the flow characteristics and temperature distribution in the furnace, and the magnesium reduction rate distribution in the retort. Variation of the total magnesium reduction rate with the time was also presented, which is useful for the design and operation of the magnesium reduction system.

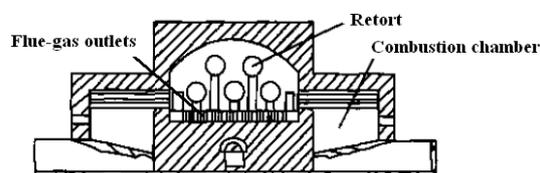
### NOMENCLATURE

$c_p$	Effective specific heat capacity of the reactant
$C_p$	Coal particle specific heat capacity
$F_d$	Drag force
$F_g$	Gravitational force
$m_p$	Coal particle mass
$Q_c$	Convective heat transfer between particle and gas phase
$Q_m$	Coal combustion heat
$Q_r$	Radiative heat transfer between particle and gas phase
$S_r$	Reaction source term
$S_\phi$	Source term in Eq. (4)
$S_{\phi p}$	Source term representing the interaction between coal particle and gas phase in Eq. (4)
$T_p$	Coal particle mass
$u_p$	Coal particle velocity
$u$	Gas velocity
$\rho$	Effective density
$\lambda$	Effective thermal conductivity
$\phi$	Universal variable in Eq. (4)
$\Gamma_\phi$	Generalize diffusion coefficient in Eq. (4)

### INTRODUCTION

The magnesium production process is carried out in a traditional coal-fired furnace, as shown in Figure 1 (Xu, 2003). Several retorts(5~11) are horizontally placed in the upper and lower rows with a staggered layout in the refractory brick furnace, which are heated by high temperature flue gas(1200~1250°C) from the combustion

chamber arranged symmetrically on two sides of the furnace. The magnesium reduction process occurs in the retort. The high temperature flue gas flows out via the outlets at the bottom of the furnace to preheat the inlet air.



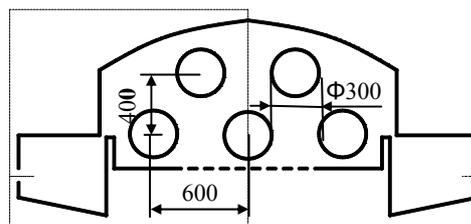
**Figure 1:** Cross-section schematic diagram of coal-fired furnace for magnesium production

In Part I (Li et al., 2009), we established the magnesium reduction model in the retort according to the actual physical process, and analyzed in detail the behavior of performance of the magnesium reduction process, such as temperature distribution, magnesium reduction rate and heat absorption power, with the time. The influence of heating temperature on the magnesium reduction rate and the heat absorption power was also investigated. However, the heat transfer occurred on the surface of the retort placed in the furnace involves not only the heat conduction but also the convective and radiative heat transfer. Therefore, the objective of this paper is to develop a comprehensive unsteady model in combination with the magnesium reduction model put forward in Part I and with the conventional coal combustion models, and to investigate the effect of thermal-flow field on the performance of the magnesium reduction process in terms of temperature and reduction rate profiles in the retort, and the variation of total reduction rate with the time.

### PHYSICAL MODEL

#### Geometrical model

A 2-D geometrical model suitable for simulation is



**Figure 2:** Geometrical model

established in Figure 2 referring to Figure 1, and the main geometrical sizes are also marked. Half of the model is taken out as the computational domain due to the symmetry of the model, which is indicated by dashed line.

### Mathematical model

The phenomenon occurring in the furnace can be taken as a fluid-solid coupling problem, and the physical processes involve three main parts: 1) magnesium reduction process in the retort, 2) coal combustion and gas turbulent flow, and 3) radiative heat transfer. Different models are used to describe the three processes and numerical details are presented below. The set of equations is solved using the commercial CFD code, FLUENT (Fluent 6.3 Documentation, 2006) via a user-defined function (UDF).

### Magnesium reduction

The 2-D time-dependent magnesium reduction model was established in Part I, the equation to describe this process in the Cartesian coordinate is expressed as,

$$\frac{\partial}{\partial t}(\rho c_p T) = \nabla \cdot \lambda \nabla T + S_r \quad (1)$$

where  $S_r$  is the magnesium reduction reaction heat which was derived and calculated in Part I and is added to Eq. (1) as source term via UDF.

### Coal combustion and gas turbulence flow

The conventional gas-particle turbulent flow and combustion model is used to simulate coal combustion occurring in the furnace (Zhou, 1994). In this model, the coal particle is modeled as a discrete phase in a Lagrangian reference frame, the trajectory of the coal particle is calculated by,

$$m_p \frac{d\mathbf{u}_p}{dt} = F_d + F_g \quad (2)$$

The total heat transfer equation for the coal particle is calculated by,

$$m_p C_p \frac{dT_p}{dt} = Q_c + Q_m + Q_r \quad (3)$$

The gas phase is modeled in an Eulerian reference frame. The reactions between coal and gas phase are modeled using the simplified PDF model (Zhou, 1994). The standard  $\kappa$ - $\epsilon$  turbulent model is employed for gas turbulence. The control equations for the gas phase can be written in a generalize form in the Cartesian coordinates as follows,

$$\frac{\partial}{\partial t}(\rho \phi) + \nabla \cdot (\rho \mathbf{u} \phi) = \nabla \cdot (\Gamma_\phi \nabla \phi) + S_\phi + S_{\phi p} \quad (4)$$

where  $\phi$  represents any quantity of mass, velocity components, gas enthalpy, turbulent kinetic energy and its dissipation rate, mixture fraction and its variance.

### Radiative heat transfer model

The P-1 radiation model is used to model the radiative heat transfer between coal particles, gas phase and retort walls (Siegel and Howell, 1992). The emissivity of the furnace wall and retort wall are set to 1.0 and 0.8, respectively. The absorption coefficient of gas phase is calculated by the Weighted-Sum-of-Gray-Gases Model (WSGGM) (Coppalle and Vervisch, 1983).

### Simulation procedure

In the actual industrial operation, the retorts without the briquette were firstly heated. When the retorts outer wall temperature approached to 1150°C, the briquettes were then charged.

For simulation, we divided this process into two ones.

Firstly, a steady state process was solved to make the temperature in the retort region be greater than 1250°C and be also uniform by adjusting the flowrates of coal and air. Once the briquettes (300 K) were charged, the retorts outer wall temperature would decrease because of the heat conduction and reaction. The higher temperature was to guarantee the required outer wall temperature of the retorts (around 1150°C) in subsequent process (unsteady state calculation) and to focus on discussing the influence of the thermal flow. Additionally, we assumed the retorts to be filled with the briquettes without reaction. Such deal does not affect the calculation results from Eq. (1).

When the steady state process was finished, the reaction heat  $S_r$  was then added as source term and the temperature of the briquette in the retorts was simultaneously initialized to be the charging temperature, 300 K. The time-marching method was used to solve the unsteady process (Tao, 2001). The time step was set to 60s, and interphase coupling iterations were performed to get a convergent solution at each time step.

## RESULTS AND DISCUSSION

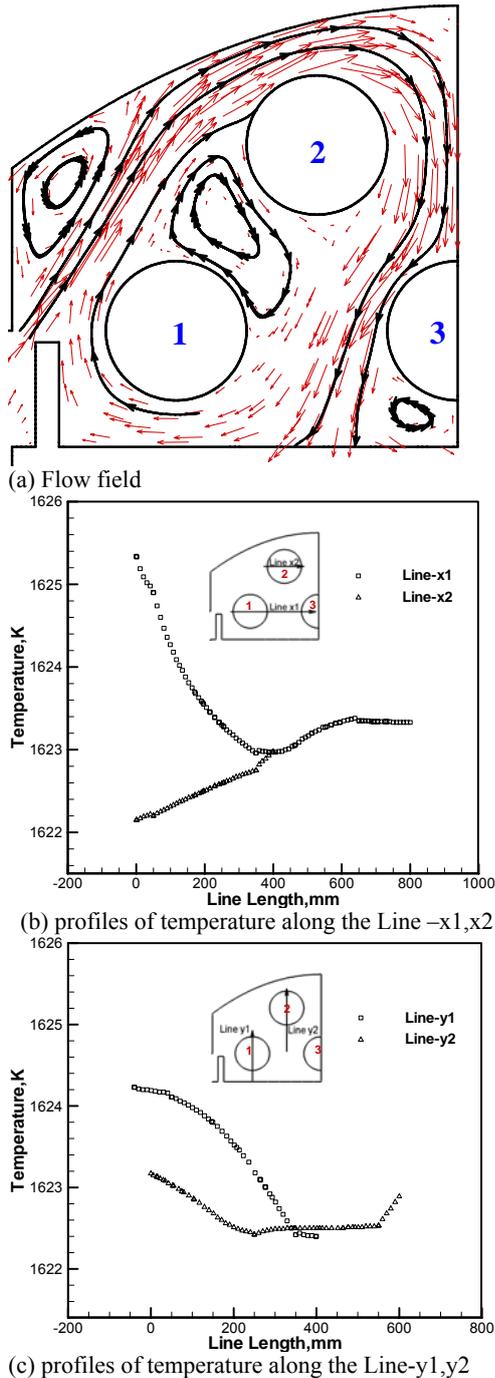
### Flow field and temperature distributions in the furnace in the steady state process

The steady state flow and heat transfer was firstly solved to obtain the initial flow field for solving the magnesium reduction process in the furnace. The necessary heating temperature and gas flow velocity in the retort region are obtained by adjusting the flowrates of coal and air.

Figure 3(a), (b) and (c) show the flow field and temperature distributions in this process. The high temperature flue-gas is introduced into the furnace from the chamber, flows around the retorts and then flows out via the outlet. Recirculation zones are formed in the furnace corner adjacent to the inlet and in between the retorts. In addition, there is a large difference of velocity magnitude around the retorts. The velocity in the recirculation zone is much smaller. Investigation of temperature distribution in the retort region is realized by illustrating the variation of the temperature along several typical lines shown in Figure 3(b) and (c). Lines x1 and x2 are horizontal lines passing through the circle center of the retort 1 and 3 and that of the retorts 2, respectively, while lines y1 and y2 are vertical lines passing through the circle center of the retort 1 and that of the retort 2, respectively. Generally, the temperature distribution is uniform with a maximum temperature difference of 3 K. However, the profiles of temperature show a concave shape along Line x1 and Line y2, and a lower temperature at the left part of Line x2 and the top part of Line y1. The low temperature on the four lines corresponds to the recirculation region in the furnace.

### Performance of magnesium reduction process in the retort

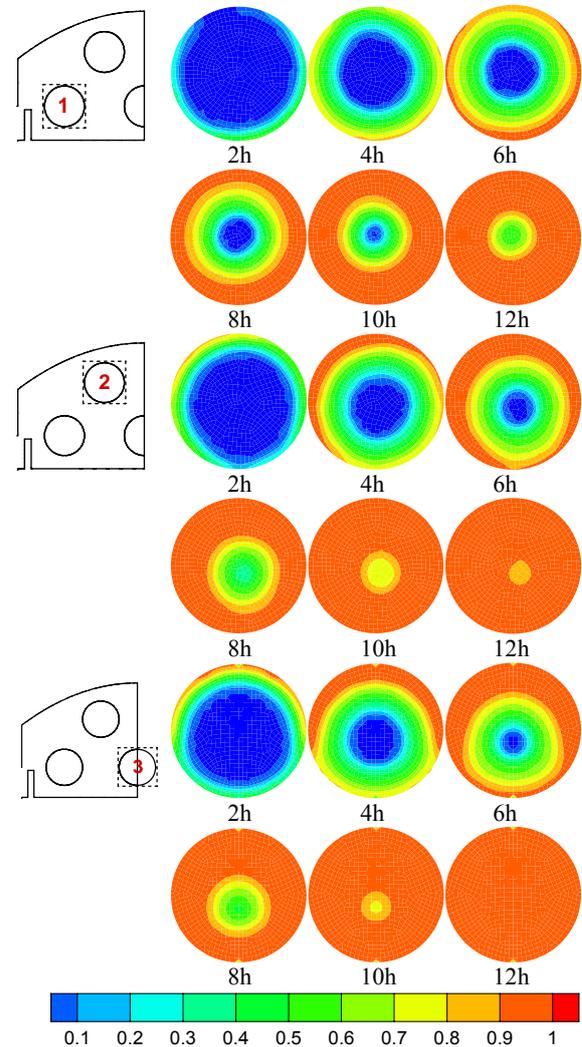
Figure 4 shows the reduction rate distribution in each



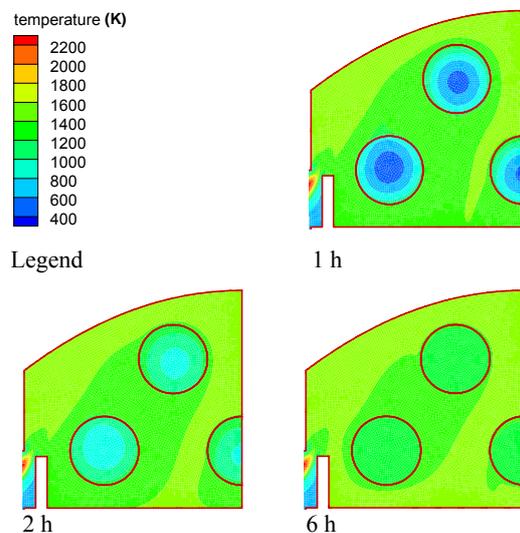
**Figure 3:** Flow field and temperature distribution in the furnace in the steady state process

retort with the time. The reduction regions and reduction rates increase with time due to the continuous heat absorption. However, there is an obvious asymmetry of the reduction in these retorts. The reduction reaction occurs firstly in a certain region of the retorts, and then expands to other regions. Besides, this region keeps a higher reduction rate than other regions during the entire reaction time. Figure 5(a) shows the temperature distribution at a certain time in the furnace and retorts. Quantitatively, we extract the data of temperature along the wall of the retort 1 and the velocity along a circle 5 mm away from the retort wall to try to explain the phenomenon. Figure 5(b) shows the variation of the temperature and the velocity along the circles at a fixed time (6h). It shows clearly that

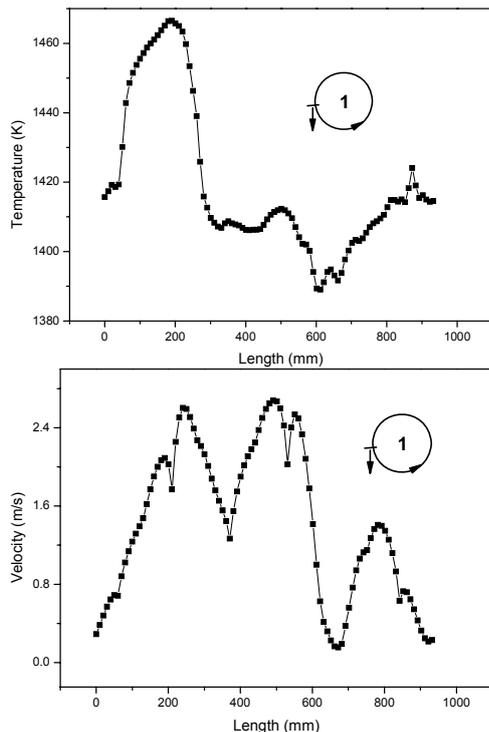
there is a larger fluctuation temperature and velocity along the circles, a higher temperature and velocity in the third and fourth quadrants of the circle, lower in the other two quadrants, which leads to the asymmetry distributions. The other retorts have the similar conclusion.



**Figure 4:** Reduction rate distribution with the time



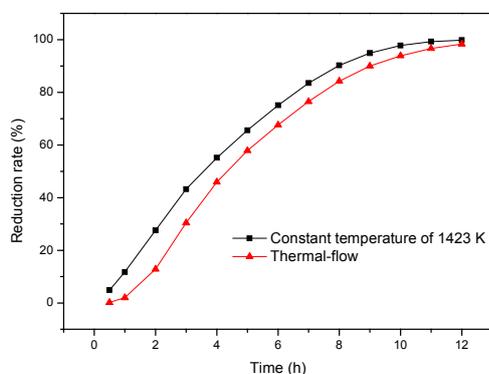
(a) Temperature distribution at a certain time in the furnace



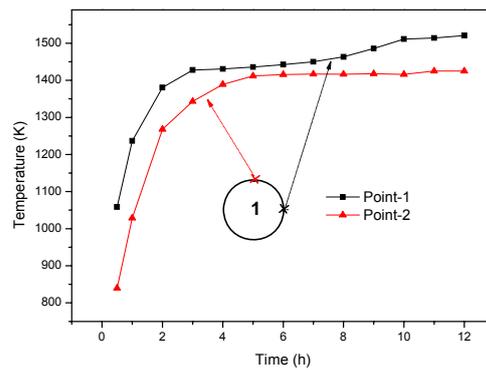
(b) Profiles of temperature and velocity along the specified circle

**Figure 5:** Temperature and velocity distribution

Figure 6 shows the total magnesium reduction rate under the heating condition by a thermal-flow field in the furnace. The result at a constant wall temperature (1423 K) obtained from the Part I was also shown for comparison. In Figure 6, the total reduction rate increases rapidly at first and then slows with time. However, at any time, the value for the thermal-flow field case is lower than that for the constant wall temperature case. This is because there is a long time during which the retort wall temperature is lower than the constant temperature of 1423 K. Figure 7 shows the variation in the temperature at two selected points of the retort wall with time. We can see that, in the initial heating stage, the retort wall temperature is lower than 1423 K, which prolongs the time of reaching the onset temperature for the reaction of the compound, and thus influences the reduction rate. The time delay can not be made up even though the heating temperature is higher than 1423 K at the subsequent stage.



**Figure 6:** Performance of magnesium reduction process



**Figure 7:** Retort wall temperature versus time

## CONCLUSION

A comprehensive 2-D unsteady mathematical model was developed in combination of the proposed magnesium reduction model with conventional coal combustion model to describe the magnesium production process in a coal-fired furnace. The influence of thermal-flow on the performance of the magnesium reduction process in the retort was investigated, and the following conclusions can be drawn.

- 1) The reduction characteristic in the retort under the thermal-flow heating condition is different from that under the constant heating temperature condition, showing an asymmetric distribution of temperature and reduction rate. The new design of furnace guaranteeing the uniform thermal-flow field is needed.
- 2) Variation in the total magnesium reduction rate with time under the thermal-flow field case showed a similar trend with that under the constant wall temperature, but the former had a lower reduction rate than the latter at a fixed time.

## ACKNOWLEDGEMENT

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