Numerical Simulation Dynamics Research on Selective Reduction in Reaction Vessel of Fine Iron and Carbon Mixture

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Abstract

With the development of computer technology, computer numerical simulation has become one of the three major scientific methods in metallurgy field. Its basic idea is to achieve the simulation of metallurgical process and the design optimization through mathematical modeling, numerical dissertation and computer programming. Referring to the reaction model of theory of porous media within gas and solid, this research focuses on the selective reduction process in mixture vessel of fine iron and carbon, taking into consideration of heat transfer equation of porous medium, the rate equation of carbon gasified reaction, the equation of continuity, and the momentum equation and so on, and establishes a micro dynamics mathematical model of the selective reduction process of fine iron and carbon mixture under the non-uniform temperature and non-equal-pressure conditions. Based on this model, the analysis of micro-dynamics of selective reduction process can be conducted; it can be applied to analyses of the effects of mass transfer in gas phase, solid-state diffusion and surface chemical reaction to the selective reduction process, as well as the interaction between two different oxides and complex compounds; the enhance means of speed control can also be obtained.

Keywords: Numerical Simulation, Selective Reduction, Dynamics, Reaction Vessel

1. Introduction

Selective reduction is current research focus in the field of metallurgy. There are rich references from thermodynamics to the dynamics, from micro to macro dynamics, from experiment to mathematical models, from process research to microstructure observations, among which micro-dynamics studies have taken into account the factors such as porous media, heat transfer, quality, and interface and so on, and d some systemic researches have been conducted in dynamics experiments and mathematical models.

The computer numerical simulation research on selective reduction can have easy access to the relatively mature experimental data to change the related process parameters. Meanwhile, based on some original data which are closer to the primary state, the research makes use of mathematical model to calculate the variables related, such as heat transfer, mass transfer, and momentum transfer. In this way, the quantitative analysis of related variables can be finished before the start of the actual selective reduction process. Therefore, it is convenient to adjust the craft plan, optimize parameter, and guarantee the success rate. As a result, it is of vital importance in shortening the production cycle, reducing costs and improving economic efficiency.

2. The Experimental Device for Selective Reduction of Fine Iron and Carbon Mixture in Reaction Vessel

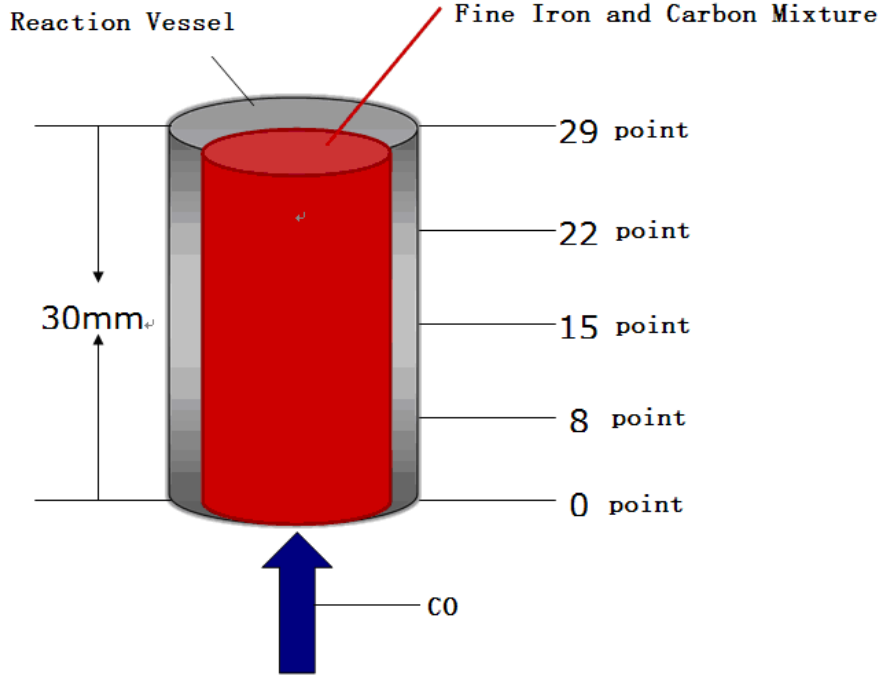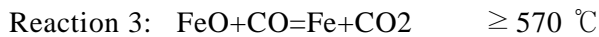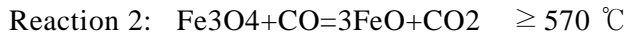The selective reduction device as shown in Figure 1:

Figure 1. Selective Reduction Device

The selective reduction device is a reaction vessel containing iron ore with the height 30mm, which is evenly divided into 5 points. CO is input from the bottom of the reaction vessel, with heating temperature at 1000 ° c at the bottom. CO_2 is output from the top of the vessel, with the temperature at the top of and the component of carbon monoxide and carbon dioxide having no boundary effect. The chemical reaction equation is:

Reaction 1: Fe3O4+4CO=3Fe+4CO2   <570 ℃

Reaction 2: Fe3O4+CO=3FeO+CO2   ≥ 570 ℃

Reaction 3: FeO+CO=Fe+CO2   ≥ 570 ℃

Three reactions are carried out in the order of reaction 1, reaction 2, and then the reaction   3.
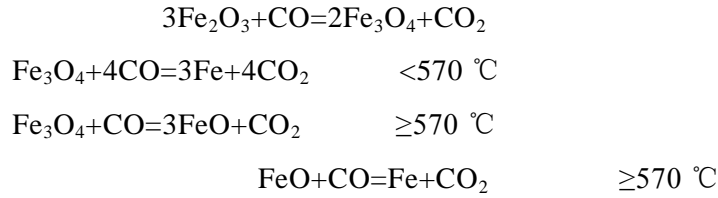
3. Mathematical Model

（1）Internal heat transmission equation porous medium

$$\frac{\partial}{\partial t}\left(\rho_m C_{pm} T\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\left(\rho_g V_0 C_{pg} T - K_{effm}\frac{\partial T}{\partial r}\right)\right) = -\sum_i \dot{R}_i \Delta H_i$$

（2）Dynamics equation of chemical reaction out of phase

Reduction of iron-oxide compounds

With CO as the reducing agent, reducing reaction is as follows:

$$3Fe_2O_3+CO=2Fe_3O_4+CO_2$$

$$Fe_3O_4+4CO=3Fe+4CO_2 \qquad <570 \ ℃$$

$$Fe_3O_4+CO=3FeO+CO_2 \qquad \geq 570 \ ℃$$

$$FeO+CO=Fe+CO_2 \qquad \geq 570 \ ℃$$

With CO as the reducing agent, the equation of the reaction rate is as follows:

$$\dot{R}_i^{CO} = S_{fi} n_i 4\pi \bar{r}_i^2 k_i^{CO} \left(C_{CO} - \frac{C_{CO_2}}{K_{Ei}^{CO}} \right)$$

$$k_i^{CO} = k_{i0}^{CO} \exp\left(\frac{-\Delta E_{iCO}^*}{RT} \right)$$

With H_2 as the reducing agent, the reducing reactions and rate equation are similar to the above.

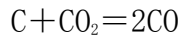Total reaction rate of iron oxide reduction is calculated as follows:

$$\dot{R}_i = \dot{R}_i^{CO} + \dot{R}_i^{H_2}$$

Volatilization of coal

$$Coal \rightarrow C + volatile$$
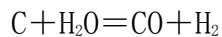
$$\dot{R}_{vi} = k_{vi0} \exp\left(\frac{-\Delta E_{vi}^*}{RT} \right) W_{vi}$$
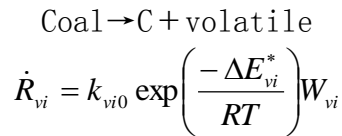
Gasification of carbon

The gasification reaction is as follows：

$$C+CO_2=2CO$$

The reaction rate equation of carbon gasification:

$$\dot{R}_c^{CO_2} = S_c n_c 4\pi \bar{r}_c^2 k_c^{CO_2} \left(C_{CO_2} - \frac{C_{CO}^2}{K_{Ec}^{CO_2}} \right)$$

$$k_c^{CO_2} = k_{c0}^{CO_2} \exp\left(\frac{-\Delta E_{cCO_2}^*}{RT} \right)$$

Water gas reaction is as follows:

$$C+H_2O=CO+H_2$$

Water gas reaction rate equation:

$$\dot{R}_c^{H_2O} = S_c n_c 4\pi \bar{r}_c^2 k_c^{H_2O} \left(C_{H_2O} - \frac{C_{CO} \times C_{H_2}}{K_{Ec}^{H_2O}} \right)$$

Total gasification reaction rates are calculated as follow:

$$\dot{R}_c = \dot{R}_c^{CO_2} + \dot{R}_c^{H_2O}$$

Size changes of pulverized coal particles in the heating process are as follows:

$$\bar{r}_c = \bar{r}_c^0 \left(1 + \gamma \times \exp\left(\frac{-(T-650)^2}{2 \times 300^2} \right) \right)$$

γ is constant, value is 0.18

（3）gaseous phase conservation equations

in the gaseous phase, these components are CO、CO$_2$、H$_2$、H$_2$O、CH$_4$、Tar etc, for each component continuity equations were established as follows：

$$\frac{\partial}{\partial t}(\phi \rho_j) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\left(V_0 \rho_j - \frac{\phi}{\tau} D_{effj} \frac{\partial \rho_j}{\partial r} \right) \right) = -\sum_i \dot{N}_{ij} M_j$$

Formula for calculating the effective diffusion coefficient of j in the gas mixture components:

$$D_{effj} = (1 - y_j)\left(\sum_{\substack{i=1 \\ i \neq j}} \frac{y_i}{D_{ij}} \right)^{-1}$$

（4）Continuity equation

Gas-phase continuity equation is as follows:

$$\frac{\partial}{\partial t}(\phi \rho_g) + \frac{1}{r}\frac{\partial}{\partial r}(r V_0 \rho_g) = -\sum_j \sum_i \dot{N}_{ij} M_j$$

（5）Momentum equation

Vapor-momentum equation is as follows

$$\frac{\partial}{\partial t}\left(\rho_g \frac{V_0}{\phi} \right) = -\frac{\partial P}{\partial r} - \alpha \mu V_0$$

Where in：

$$\alpha = 150 \frac{(1-\phi)^2}{\phi^3 (S_{fa} d_p)^2}$$

$$\mu = \frac{\sum\limits_{j} M_j^{1/2} y_j \mu_j}{\sum\limits_{j} M_j^{1/2} y_j}$$

（6）The ideal gas equation

In the context of the given temperature and pressure, gas can be considered to be incompressible and meets the ideal gas equation of State

$$P = \frac{\rho_g}{M_g} RT$$

4. Discrete Solutions

(1) Discretization of heat transmission equation in porous medium

$$\frac{\partial}{\partial t}\left(\rho_m C_{pm} T\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\left(\bar{\rho}_g V_0 C_{pg} T - K_{effm}\frac{\partial T}{\partial r}\right)\right) = -\sum_i \dot{R}_i \Delta H_i$$

With S_T as the source item, $S_T = -\sum_i \dot{R}_i \Delta H_i$

$$\frac{\partial}{\partial t}\left(\rho_m C_{pm} T\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\left(\rho_g C_{pg} V_a T - K_{effm}\frac{\partial T}{\partial r}\right)\right) = S_T$$

For internal nodes p, integration in the body under its control points

$$\int \frac{\partial}{\partial t}\left(\rho_m C_{pm} T\right) dV + \int \frac{1}{r}\frac{\partial}{\partial r}\left(r\left(\rho_g C_{pg} V_a T - K_{effm}\frac{\partial T}{\partial r}\right)\right) dV = \int S_T dV$$

Where in：

$$\int \frac{\partial}{\partial t}\left(\rho_m C_{pm} T\right) dV = \frac{\rho_m^1 C_{pm}^1 T_P^1 - \rho_m^0 C_{pm}^0 T_P^0}{\Delta \tau} \Delta V$$

$$\int S_T dV = S_T^0 \Delta V$$

$$\int \frac{1}{r}\frac{\partial}{\partial r}\left(r\left(\rho_g C_{pg} V_a T - K_{effm}\frac{\partial T}{\partial r}\right)\right) dV = J_e^0 A_e - J_w^0 A_w$$

$$J_e^0 = \left(\rho_g C_{pg} V_a T - K_{effm}\frac{\partial T}{\partial r}\right)_e^0 = \left(\rho_g C_{pg} V_a\right)_e T_P^0 - \frac{\left(\rho_g C_{pg} V_a\right)_e}{\exp(P_e) - 1}\left(T_E^0 - T_P^0\right)$$

$$J_w^0 = \left(\rho_g C_{pg} V_a T - K_{effm}\frac{\partial T}{\partial r}\right)_w^0 = \left(\rho_g C_{pg} V_a\right)_w T_P^0 - \frac{\left(\rho_g C_{pg} V_a\right)_w \exp(P_w)}{\exp(P_w) - 1}\left(T_P^0 - T_W^0\right)$$

$$\Delta V = r\Delta r$$

$$A_e = r_e, \quad A_w = r_w$$

hypothesis：

$$F_e = \left(\rho_g C_{pg} V_a\right)_e A_e, \quad F_w = \left(\rho_g C_{pg} V_a\right)_w A_w$$

$$D_e = \frac{(K_{effm})_e}{(\delta r)_e} A_e, \quad D_w = \frac{(K_{effm})_w}{(\delta r)_w} A_w$$

$$P_e = \frac{F_e}{D_e}, \quad P_w = \frac{F_w}{D_w}$$

$$a_E = \frac{F_e}{\exp(P_e)-1}, \quad a_W = \frac{F_w \exp(P_w)}{\exp(P_w)-1}$$

then：

$$\frac{\rho_m^1 C_{pm}^1 \Delta V}{\Delta \tau} T_P^1 = a_E T_E^0 + a_W T_W^0 + \left(F_w - F_e - a_E - a_W + \frac{\rho_m^0 C_{pm}^0}{\Delta \tau} \Delta V \right) T_P^0 + S_T^0 \Delta V$$

(2) Discretization of gas-phase equations

$$\frac{\partial}{\partial t}\left(\phi \overline{\rho}_j\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\left(V_0 \overline{\rho}_j - \frac{\phi}{\tau} D_{effj} \frac{\partial \overline{\rho}_j}{\partial r} \right)\right) = -\sum_i \dot{N}_{ij} M_j$$

Can be written as:

$$\frac{\partial}{\partial t}\left(\rho_g Y_j\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\left(\rho_g V_a Y_j - \Gamma_j \frac{\partial Y_j}{\partial r} \right)\right) = S_j$$

For internal nodes p, integration in the body under its control points

$$\int \frac{\partial}{\partial t}\left(\rho_g Y_j\right) dV + \int \frac{1}{r}\frac{\partial}{\partial r}\left(r\left(\rho_g V_a Y_j - \Gamma_j \frac{\partial Y_j}{\partial r} \right)\right) dV = \int S_j dV$$

Where in：

$$\int \frac{\partial}{\partial t}\left(\rho_g Y_j\right) dV = \frac{\rho_g^1 Y_{jP}^1 - \rho_g^0 Y_{jP}^0}{\Delta \tau} \Delta V$$

$$\int S_j dV = S_j^0 \Delta V$$

$$\int \frac{1}{r}\frac{\partial}{\partial r}\left(r\left(\rho_g V_a Y_j - \Gamma_j \frac{\partial Y_j}{\partial r} \right)\right) dV = J_e^0 A_e - J_w^0 A_w$$

hypothesis：

$$J_e^0 = \left(\rho_g V_a Y_j - \Gamma_j \frac{\partial Y_j}{\partial r} \right)_e^0 = \left(\rho_g V_a\right)_e Y_{jP}^0 - \frac{\left(\rho_g V_a\right)_e}{\exp(P_e)-1}\left(Y_{jE}^0 - Y_{jP}^0 \right)$$

$$J_w^0 = \left(\rho_g V_a Y_j - \Gamma_j \frac{\partial Y_j}{\partial r}\right)_w^0 = \left(\rho_g V_a\right)_w Y_{jP}^0 - \frac{\left(\rho_g V_a\right)_w \exp(P_w)}{\exp(P_w)-1}\left(Y_{jp}^0 - Y_{jw}^0\right)$$

$$\Delta V = r\Delta r, \quad A_e = r_e, \quad A_w = r_w$$
$$F_e = \left(\rho_g V_a\right)_e A_e, \quad F_w = \left(\rho_g V_a\right)_w A_w$$

$$D_e = \frac{(\Gamma_j)_e}{(\delta r)_e} A_e, \quad D_w = \frac{(\Gamma_j)_w}{(\delta r)_w} A_w$$

$$P_e = \frac{F_e}{D_e}, \quad P_w = \frac{F_w}{D_w}$$

$$a_E = \frac{F_e}{\exp(P_e)-1}, \quad a_W = \frac{F_w \exp(P_w)}{\exp(P_w)-1}$$

then：

$$\frac{\rho_g^1 \Delta V}{\Delta \tau} Y_{jP}^1 = a_E Y_{jE}^0 + a_W Y_{jW}^0 + \left(F_w - F_e - a_E - a_W + \frac{\rho_g^0 \Delta V}{\Delta \tau}\right)Y_{jP}^0 + S_j^0 \Delta V$$

（3）Discretization of continuity equations

$$\frac{\partial}{\partial t}\left(\phi \overline{\rho}_g\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r V_0 \overline{\rho}_g\right) = -\sum_j \sum_i \dot{N}_{ij} M_j$$

Can be written as:

$$\frac{\partial}{\partial t}\left(\rho_g\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r \rho_g V_a\right) = S$$

hypothesis：

S as the source item, $\quad S = -\sum_j \sum_i \dot{N}_{ij} M_j \quad$, then：

$$\int \frac{\partial}{\partial t}\left(\rho_g\right)dV + \int \frac{1}{r}\frac{\partial}{\partial r}\left(r \rho_g V_a\right)dV = \int S dV$$

Where in：

$$\int \frac{\partial}{\partial t}\left(\rho_g\right)dV = \frac{\rho_g^1 - \rho_g^0}{\Delta \tau}\Delta V$$

$$\int \frac{1}{r}\frac{\partial}{\partial r}\left(r \rho_g V_a\right)dV = \left(\rho_g V_a\right)_e A_e - \left(\rho_g V_a\right)_w A_w = F_e - F_w$$

$$\int S dV = S^0 \Delta V$$

then：

$$\frac{\rho_g^1 - \rho_g^0}{\Delta \tau} \Delta V + F_e - F_w = S^0 \Delta V$$

（4）Discretization of momentum equation

$$\frac{\partial}{\partial t}\left(\overline{\rho}_g \frac{V_0}{\phi}\right) = -\frac{\partial P}{\partial r} - \alpha \mu V_0$$

make：

$$\alpha' = 150 \frac{(1-\phi)^2}{\phi^2 (S_{fa} d_p)^2}$$

then：

$$\frac{\partial}{\partial t}\left(\overline{\rho}_g V_a\right) = \frac{\partial P}{\partial r} - \alpha' \mu V_a$$

For internal nodes p, integration in the body under its control points

$$\int \frac{\partial}{\partial t}\left(\overline{\rho}_g V_a\right) dV = \int \left(\frac{\partial P}{\partial r} - \alpha' \mu V_a\right) dV$$

then：

$$\frac{\overline{\rho}_g^1 \Delta V}{\Delta \tau} V_{aP}^1 = P_e A_e - P_w A_w + \left(\frac{\overline{\rho}_g^0}{\Delta \tau} \Delta V - \alpha' \mu \Delta V\right) V_{aP}^0$$

The result can be obtained with discrete staggered grid solution.

5. Calculation Results

Based on the mathematical model above, the research developed a calculation program with Visual C++ and a preliminary simulation was conducted in the fine iron reducing process under the one-way heating condition. The whole procedure is shown in Figure 2:
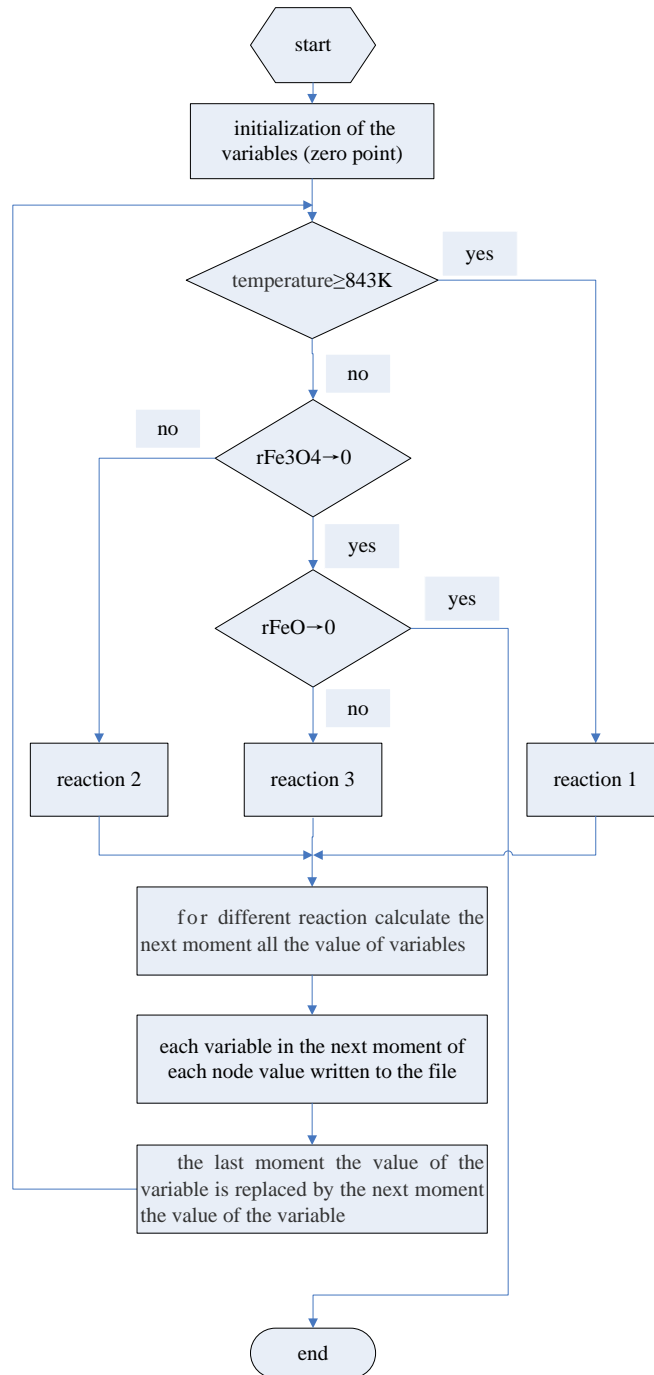
Figure 2. Computation procedure of the model

Calculated parameters are as follows: the thickness of iron ore is 30mm, and its particle sizes, density, heat capacity, thermal conductivity coefficient parameters are shown previously; reducing agent is CO, not involved in H_2.

Initial conditions: the layer temperature is 300K, gas is 100%CO.

Boundary conditions:

(1) hot end: temperature is 1273K; reducing agent is 100%CO;

(2) cold end: thermal boundary is adiabatic boundary, one-way, no effect on gas export boundaries.

In the computation process, the spatial length of stride is 0.001m, the time length of stride is 0.001s, and the total overall reaction will not be finished until the computation carries on for 55s. The results are shown from Figure 3 to Figure 7.
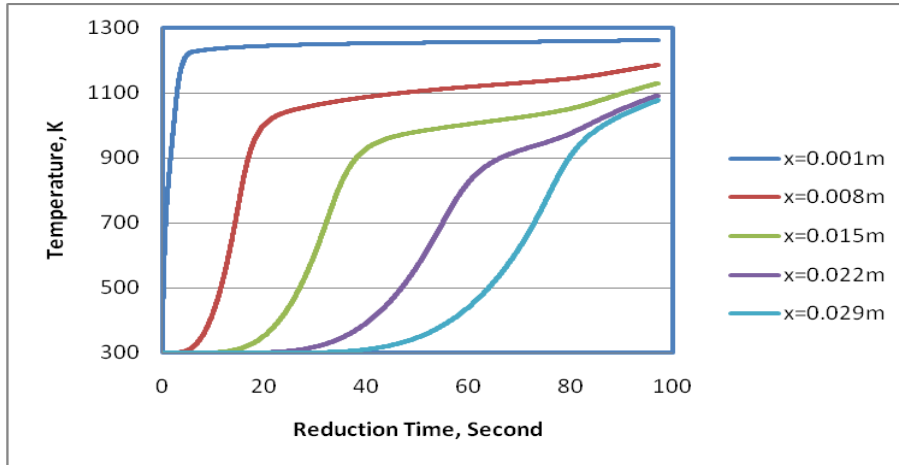

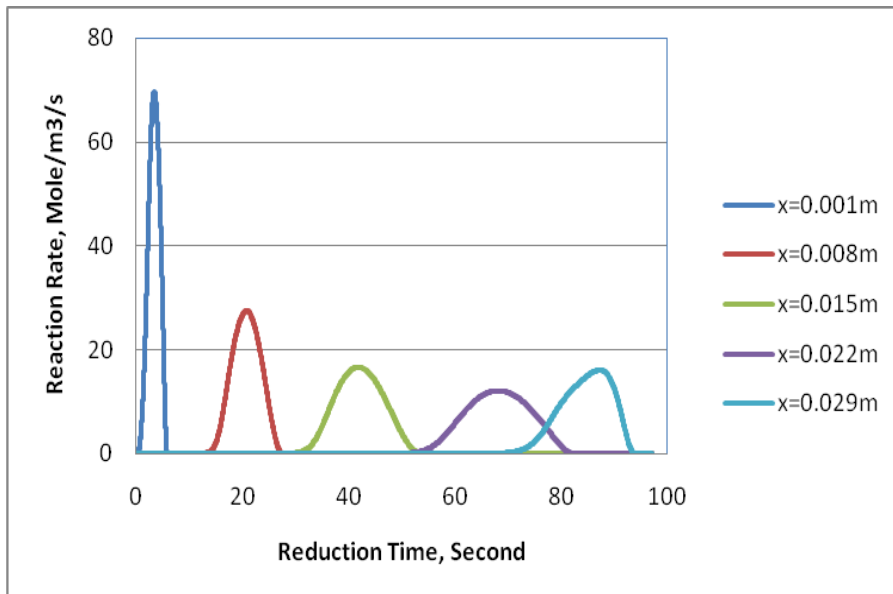**Figure 3. Relations between layer temperature and time**

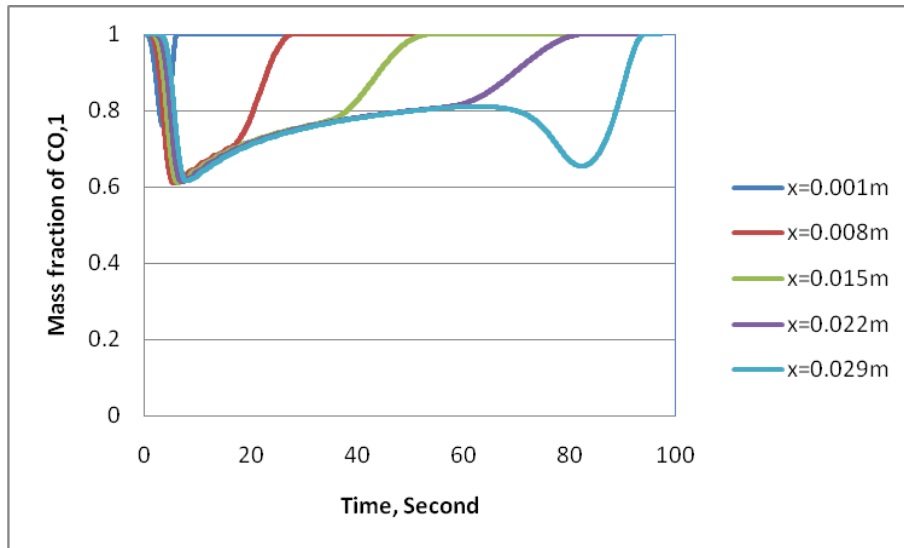**Figure 4. The curve of reduction rates changing with reduction time**

Figure 5. The curve of CO Component variation changing with reduction time

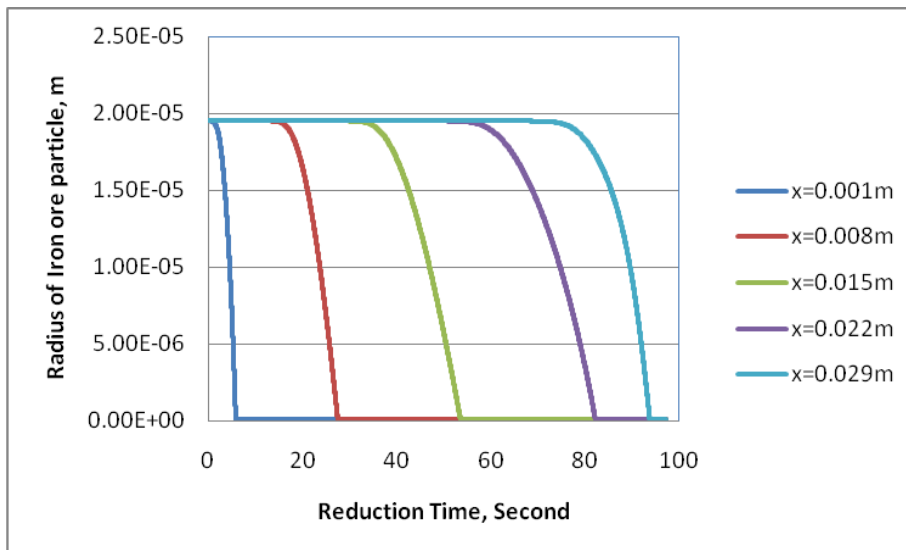

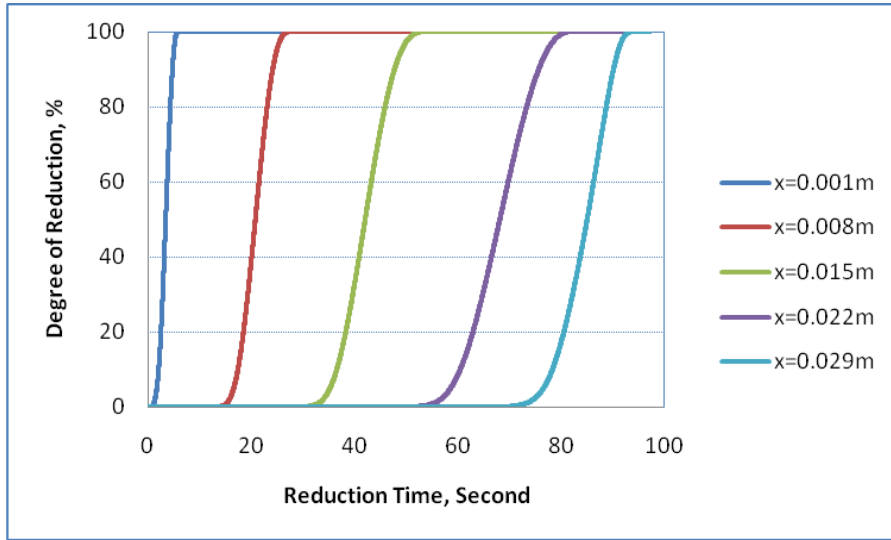**Figure 6. Size Changes of Mineral powder particles with reaction time**

Figure 7. The curve of reduction degree changing with reduction time

6. Conclusion

According to the experimental research illustrated from Figure 3 to Figure 7, this research focuses on the selective reduction process of fine iron in reaction vessel, taking into consideration of following equations, such as heat transfer equation of porous medium, the rate equation of carbon gasified reaction, the equation of continuity, and the momentum equation and so on, and it establishes a micro dynamics mathematical model of the selective reduction process of fine iron and carbon mixture under the non-uniform temperature and non-equal-pressure conditions. Meanwhile, its results are reasonable, which confirms that the model can be applied to the simulation of reduction process of fine iron ore.

Acknowledgements

Nomenclature

T : temperature （ K)

ρ_m : density of mixture （ $kg \cdot m^{-3}$)

ρ_g : density of gas （ $kg \cdot m^{-3}$)

C_{pm} : specific heat of solid mixtures （ $J \cdot kg^{-1} \cdot K^{-1}$)

C_{pg} : specific heat of gases （ $J \cdot kg^{-1} \cdot K^{-1}$)

V_0 : superficial gas velocity （ $m \cdot s^{-1}$)

V_a : average velocity of gas fiow in the interstices of the packed bed $(m \cdot s^{-1})$

K_{effm} : effective thermal conductivity of the mixture $(W \cdot m^{-1} \cdot K^{-1})$

$\dot{R}_i$: rate of chemical reaction i $(mol \cdot m^{-3} \cdot s^{-1})$

ΔH_i : heat of chemical reaction i $(J \cdot mol^{-1})$

S_f : shape factor of particles

n_i : number of particles of solid reactant for reaction i in the mixture (m^{-3})

$\bar{r}_i$: average radius of particle for reaction i (m)

k_i : rate constant for reaction i $(m \cdot s^{-1})$

k_{i0} : Pre-exponential constant in rate constant for reaction i

K_{Ei} : equilibrium constant for reaction i

ΔE_i^* : 'activation energy' of reaction i $(J \cdot mol^{-1})$

R : gas constant $(8.314 J \cdot mol^{-1} \cdot K^{-1})$

C_{CO} : concentration of CO $(mol \cdot m^{-3})$

C_{CO_2} : concentration of C02 $(mol \cdot m^{-3})$

C_{H_2} : concentration of H2 $(mol \cdot m^{-3})$

C_{H_2O} : concentration of H2O $(mol \cdot m^{-3})$

W_{vi} : un-evolved portion of volatile component i $(kg/kg-coal)$

D_{ij} : binary diffusivity in the gaseous phase (m2/s)

y_j : mole fraction of species j in the gaseous phase （%）

ϕ : void fraction of the packed bed

ρ_j : density of gaseous species j $(kg \cdot m^{-3})$

$\dot{N}_{ij}$: net rate of gaseous species j consumed/generated by chemical reaction i （ $mol \cdot s^{-1} \cdot m^{-3}$ ）

M_j : molecular weight of the gaseous species j ($kg \cdot mol^{-1}$)

τ : tortuosity factor

μ : viscosity of fluid ($kg \cdot m^{-1} \cdot s^{-1}$)

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Author

Lan Xiaowen received the BS in computer science from Inner Mongolia University, China, in 2001, and received the MS in computer science from Chengdu University of Technology, China, in 2008. Currently, his research interests include embedded system and scheduling techniques and parallel algorithms for clusters, and also multi-core processors and numerical simulation.