

Mathematical modeling of non-stationary heat and mass transfer in disperse systems

L A Ermakova, S Y Krasnoperov and S N Kalashnikov

Siberian State Industrial University, 42 Kirova Street, Novokuznetsk, 654007, Russia

E-mail: ermakova@sibsiu.ru

Abstract. The work describes mathematical model of non-stationary heat and mass transfer processes in dispersed environment, taking into account the phase transition; presents the results of numeric modelling for conditions of direct reduction in high-temperature reducing atmosphere, corresponding to the direct reduction in the jet-emulsion unit according to the principles of self-organization. The method was developed for calculation of heat and mass transfer of the aggregate of iron material particles in accordance with the given distribution law.

1. Introduction

Today, the most urgent task in the development of metallurgy technology is to obtain the metal by direct reduction directly from fine-disperse materials, including wastes from metallurgical production (scale, sludge, flue dust). These technologies have a number of important advantages: solution of environmental problems through recycling of wastes from metallurgical production, a significant acceleration of reduction due to the large reaction surface of fine materials, reduction of costs and energy consumption by eliminating the stage of pre-processing and pelletizing materials. One of the variants of such processes is the process for producing metal from dispersed materials in the jet-emulsion unit having a reaction chamber and the refining sump [1, 2].

During development of technologies for production metals in the units of a jet-emulsion type, an important task is to determine the feeding mode of charging the main reactors of the unit with iron ore materials, oxygen, fuel and reductants. The solution of this problem requires the creation of appropriate models and techniques allowing the heat and mass transfer processes in disperse systems to be calculated. In this paper we carry out the mathematical modeling of heat and mass transfer of particles with regard to phase transition. On its bases we developed the method of calculation of heating, melting and reduction of the aggregate of particles in the iron ore materials under the given boundary conditions.

2. Calculation of numerical characteristics of raw materials

When calculating the numerical characteristics of dispersed materials it was assumed that the particles have a spherical shape, and the initial experimental data for quantitative description of density of particles distribution according to their diameters in the interval (d_{\min} , d_{\max}) are the weight fractions, obtained by sieving processing of charge materials on the row of standard sieves. For description we used such characteristics as the density of particles distribution by their quantity $f_n(d)$, surface $f_s(d)$ and



the mass $f_m(d)$, as well as the respective distribution functions $F_n(d)$, $F_s(d)$, $F_m(d)$. By $\tilde{f}_n(d)$, $\tilde{f}_s(d)$, $\tilde{f}_m(d)$ we denote the corresponding normalized density distribution, and by $\tilde{F}_n(d)$, $\tilde{F}_s(d)$, $\tilde{F}_m(d)$ – normalized distribution function. Assessment for $\tilde{f}_m(d)$ was performed in the class of regular distributions in the interval (d_{\min}, d_{\max}) in the form of a lognormal law, taking into account the minimum and maximum diameters of particles d_{\min} и d_{\max} [3-4].

$$\tilde{f}_m(d) = \frac{d_{\max} - d_{\min}}{(d_{\max} - d)(d - d_{\min})\sigma\sqrt{2\pi}} e^{-\frac{\left(\ln\left(\frac{d_{\max}-d}{d-d_{\min}}\right) - \ln a\right)^2}{2\sigma^2}} \quad (1)$$

Specific type $\tilde{f}_m(d)$ is determined by the values of the parameters a^* and σ^* that minimize the functional.

$$\Phi(a, \sigma) = \min_{a, \sigma} \sum_{i=1}^{N_f} \left(\int_{d_{i-1}}^{d_i} \tilde{f}_m(\xi) d\xi - \frac{M_i}{M} \right)^2 \quad (2)$$

where N_f – the number of fractions; d_i – the maximum diameter of particles in the i -th fraction; M_i mass of i -th fraction.

As a result of the processing of experimental data we obtained and adopted in the simulation the following values a^* and σ^* of parameters of the distribution laws and the corresponding values of the numerical characteristics of the dispersed charge materials shown in Table 1.

Table 1. Numerical characteristics of dispersed materials.

Dispersed material	d_{\min} , mm	d_{\max} , mm	$d(\max f_m)$, mm	$d(\max f_s)$, mm	$d(\max f_N)$, mm	Distribution options		m_{Σ} , kg	S_{Σ} , m ²	$N_{\Sigma} \cdot 10^{-6}$
						a	σ			
Iron ore concentrate	0.025	1.0	0.60	0.49	0.20	0.80	0.79	1.0	5.2	11.9
Sludge	0.025	1.0	0.13	0.08	0.05	3.85	1.00	1.0	16.2	537.4
Scale	0.025	3.0	0.94	0.61	0.23	1.76	0.78	1.0	1.2	1.2
Manganese concentrate	0.03	1.0	0.26	0.21	0.14	2.55	0.64	1.0	16.9	122.3
Coxlittle	0.025	5.0	0.10	0.02	0.02	4.93	1.42	1.0	17.2	444.7
Cox	5.0	50.0	1.24	1.11	0.95	0.65	3.88	1.0	5.5	1.2
Lime	0.05	3.0	0.07	0.04	0.03	4.04	1.64	1.0	18.6	1079.2

3. The mathematical model of heat and mass transfer process of particles with phase transition

The study of the processes in the jet-emulsion unit, when fine materials are used as a charge, showed that heat and mass transfer processes occur in the turbulent environment and have a very high intensity [1]. This allows to pose the problem of mathematical modeling of heat and mass transfer processes based on the solution of internal tasks, taking into account the external conditions of processes [5-6].

Therefore, the process of unsteady heat and mass transfer was described by the equation of heat conduction and molecular diffusion for particles of spherical shape with the boundary conditions of the 3 kind.

The obtained system of equations and the boundary conditions for the dimensionless relative temperature and concentration have the form [7]:

$$\left\{ \begin{array}{l} \frac{\partial \tilde{C}}{\partial Fo_{dif}} = \frac{1}{\tilde{r}^2} \frac{\partial}{\partial \tilde{r}} \left(\tilde{r}^2 \frac{\partial \tilde{C}}{\partial \tilde{r}} \right) \\ \frac{\partial \Theta}{\partial Fo_{dif}} = \frac{1}{Lu \tilde{r}^2} \frac{\partial}{\partial \tilde{r}} \left(\tilde{r}^2 \frac{\partial \Theta}{\partial \tilde{r}} \right) \\ \tilde{C}|_{Fo_{dif}=0} = 0 \quad \Theta|_{Fo_{dif}=0} = 0 \\ \left. \frac{\partial \tilde{C}}{\partial \tilde{r}} \right|_{\tilde{r}=0} = 0 \quad \left. \frac{\partial \Theta}{\partial \tilde{r}} \right|_{\tilde{r}=0} = 0 \\ \left. \frac{\partial \tilde{C}}{\partial \tilde{r}} \right|_{\tilde{r}=1} = Bi_{dif} (1 - \tilde{C}) \quad \left. \frac{\partial \Theta}{\partial \tilde{r}} \right|_{\tilde{r}=1} = Bi(1 - \Theta) \end{array} \right. \quad (3)$$

where $\tilde{C} = \frac{C - C_0}{C^* - C_0}$ – dimensionless relative concentration; C_0 – initial concentration of the considered element in the particle; C^* – concentration of this element in the environment;

$\Theta = \frac{t - t_0}{t_{en} - t_0}$ – dimensionless relative temperature; t_0 – initial temperature of the particle; t_{en} – ambient

temperature; R – radius of the particle; $\tilde{r} = \frac{r}{R}$ – dimensionless radius; $Lu = \frac{D}{a}$ – Lewis number;

$Fo_{dif} = \frac{D\tau}{R^2}$ – diffusion Fourier number; $Bi_{dif} = \frac{\beta R}{D}$ – diffusion Bionumber; $Bi = \frac{\alpha R}{\lambda}$ – Bionumber;

D – diffusion coefficient, m^2/c ; β – coefficient of mass transfer, m/c ; a – thermal diffusivity of particles, m^2/c ; λ – coefficient of thermal conductivity of particles, $W/(m \cdot K)$; α – the heat transfer coefficient, $W/(m^2 \cdot K)$; τ – time, sec.

The process of phase transition for spherical particles with a diameter of $0.025 \cdot 10^{-3} \div 3 \cdot 10^{-3} m$, where the criterion Bio is changed in the range of $0,1 \div 10$ is described by the ratio of the form [8]:

$$Fo - Fo_0 = \frac{Ko}{Bi} (\delta - \delta_0) + \frac{1}{n} \left(\frac{1}{n+1} + \frac{Ko}{2} \right) (\delta^2 - \delta_0^2) \quad (4)$$

where $Fo = \frac{a\tau}{R^2}$; $Fo_0 = \frac{a\tau_0}{R^2}$ – Fourier number; τ_0 – time of particles heating up to the melting temperature, c; τ – heating time, c; $Ko = L_{mel} / c \cdot (t_{sur} - t_{mel})$ – number of Kossovich; t_{sur} – surface temperature, $^{\circ}C$; t_{mel} – temperature of melting, $^{\circ}C$; L_{mel} – latent heat of phase transition, kJ/kg ; $\delta = \xi / R$; $\delta_0 = \xi_0 / R$; ξ_0 – thickness of the molten crust during τ_0 , m; $\xi = \xi(\tau)$ – law of displacement of the flat front of the melt; n – indicator of the parabolic law of temperature distribution.

On the basis of equation (4) we calculated the time of particles melting, which was taken into account in the calculation of heat transfer process.

The boundary value problem was solved by separation of variables using a rapidly converging series. The peculiarity of the solution method consists in the construction of a calculation scheme, which allows the results to be obtained, that characterize the relationship between the determining parameters of the problem in any given interval of variables, presented in the criterion and dimensional physical forms. This technique is described in detail in [6].

4. The results of mathematical modelling

In the numerical realization of the method the change in the system parameters during the phase transition was taken into account as follows. At each iteration, first, by the composition we determined the melting temperature, then counted the current temperature, according to which determined the diffusion coefficient taking into account the phase state of the particle. Then, on the next iteration the new thermophysical material parameters with regard to the obtained composition and phase state were determined.

In the study accepted: the range of sizes variation for materials $0.025 \div 3$ mm; the temperature of the environment in accordance with the conditions of liquid-phase reduction $1400 \div 1600$ °C; thermophysical parameters and diffusion coefficients, which are given in [8-12].

Figure 1 and Figure 2 show the results of heat exchange process at a temperature of gas medium $t = 1500$ °C for a process time $0.3 \div 0.6$ s.

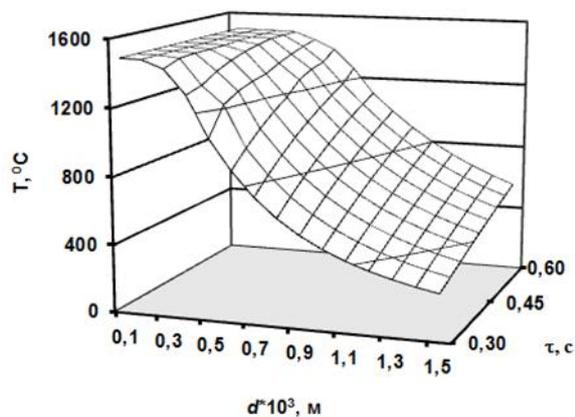


Figure 1. Dependence of the heating temperature of particles on the particle diameter and process time at a temperature of 1500 °C environment.

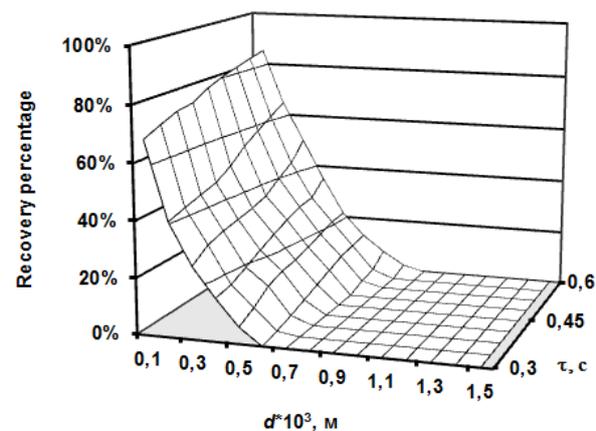


Figure 2. Dependence of the recovery of the particles on the particle diameter and process time at a temperature of 1500 °C environment.

As can be seen from figures 1 and 2 that with the duration of the process $0.3 \div 0.6$ s particles with a diameter up to $0.5 \cdot 10^{-3}$ m manage to get heated and start melting initiating the reduction processes. The particles of a larger size do not have time to get heated to the phase transition temperature and are not reduced.

Thus, the developed model of heat and mass transfer allows the temperature and composition of particles or droplets at any point of time to be determined which are in the high-temperature reducing environment. This model served as a basis for the methods of calculation of heat and mass transfer of an aggregate of dispersed particles.

5. The calculation method of heat and mass transfer of the aggregate of dispersed particles

To calculate the heat exchange process of the aggregate of dispersed particles of the given distribution law on the basis of the equations (3)-(4) we used the following method: set of initial conditions

(process time, ambient temperature, division of the size interval into a number of ranges, so that all particles within one range would have the same size); calculation of heat and mass transfer processes for particles of the selected range, calculation of the fraction and composition of phases according to the results of heat and mass transfer; determination of costs of heat required for heat and mass transfer of all particles of the current range; definition of the integral values of masses, phase composition and costs for heating, melting and reduction; analysis of material and heat balances.

Figure 3 shows the simulation results of heat and mass transfer processes for 1 kg of the iron-containing material ($\sigma = 1.01$ and $a = 4.92$) at the environment temperature 1550°C . The dependence of fractions is shown here: solid heated charge material (CH_s^h), in which each range of particle sizes has its own temperature; melted charge material (CH_m), the droplets of which have a temperature above the melting temperature; charge material is melted and recovered (CH_m^r).

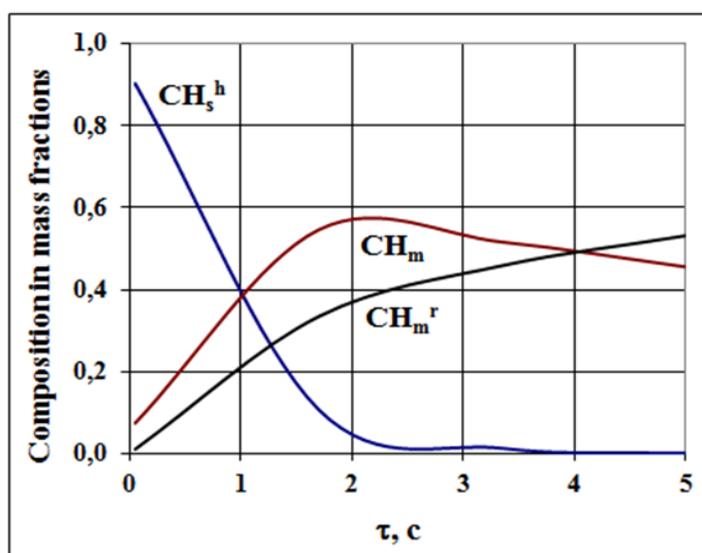


Figure 3. The results of simulation of heat and mass transfer processes of particles aggregate in the iron-containing materials at a ambient temperature 1550°C .

As it can be seen from Figure 3 the whole process can be divided into two periods. The first period lasts $2 \div 3$ seconds, and this time is sufficient for complete melting of the dispersed material and reduction of small particles with sizes up to $1 \cdot 10^{-3}$ m, which is 40% by weight of the total mixture. The duration of this period is comparable to the residence time of the materials in the reaction chamber of the jet-emulsion unit. In the second

period the reduction of already molten particles of larger size takes place, it requires several minutes, which might be provided by the design and modes of phases interaction in the emulsion reactor of a column type.

6. Conclusions

A mathematical model of heat and mass transfer of particles with phase transition in the form of a joint system of equations of heat conduction and molecular diffusion with boundary conditions of the 3 kind was offered. The method of modeling heat and mass transfer processes of particles aggregate of iron ore material of the given distribution law was developed. The proposed method allows the heat exchange process of the aggregate of the dispersed iron-bearing particles of the given distribution law to be calculate, and can be used for calculation of processes occurring in the reactors of jet-emulsion units.

7. References

- [1] Tsymbal V P, Kozhemyachenko V I et al 2015 *Steel in Translation* **45** (8) 550–554
- [2] Ermakova L A and Mochalov S P 2004 *Izvestiya Vysshikh Uchebnykh Zavedenij. Chernaya*

- Metallurgiya* **10** 48–51
- [3] Nichiporenko O S, Naida Y I and Medvedsky A B 1980 *Atomized Metal Powders* (Kiev: Naukova Dumka) p 239
 - [4] Dityatky Y F, Klyachko L A et al 1977 *Spraying Liquids* (M.: Mashinostroenie) p 263
 - [5] Kalashnikov S N, Ermakova L A and Mochalov S P 2001 *Izvestiya Vysshikh Uchebnykh Zavedenij. Chernaya Metallurgiya* **6** 67–71
 - [6] Kalashnikov S N, Mochalov S P, Ermakova L A and Krasnoperov S Y 1999 *Steel in Translation* **29** (10) 19–23
 - [7] Telegin A S, Shvydky V S and Yaroshenko Yu G 1995 *Heat and Mass Transfer* (M.: Metallurgy) p 440
 - [8] Mastryukov B S 1996 *Thermal Physics of Metallurgical Processes* (M.: MISiS) p 271
 - [9] Krivandina V A 1986 *Metallurgical Heat Engineering* (M.: Metallurgiya) vol 1, 2
 - [10] *Thermophysical Properties of Fuels and Charge Materials of Ferrous Metallurgy. Reference Book* 1982 (M.: Metallurgy) p148
 - [11] Kafarov V V and Glebov M B 1991 *Mathematical Modeling of Basic Processes of Chemical Productions* (M.: Higher school) p 400
 - [12] Kamkina L V, Yakovlev Yu N et al 1995 *Izvestiya Vysshikh Uchebnykh Zavedenij. Chernaya Metallurgiya* **2** 8–10