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MATHEMATICAL MODELING OF HEAT AND MASS TRANSFER IN A MELT DURING INTERACTION WITH JETS OF A CHEMICALLY ACTIVE GAS

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The temperature and concentration distributions of reacting components of a melt moving in an axisymmetric bath are obtained during interaction with jets of a gas injected on its surface.

The velocity distribution of a melt in an axisymmetric bath is found in [1] for the delivery of a gas jet to the free surface. It is possible to solve the problem of heat and mass transfer in a melt reacting with a gas jet for a known velocity field in order to obtain data on the characteristics of the process and on the efficiency of the reactor (oxygen converter, pyrolysis apparatus, etc.).

The physical model of jet interaction with a melt is represented in Fig. 1. There is a surface L on the lune on which the gas jet reacts with the melt. The heat being liberated is expended in heating and evaporating its components. Because of the formation of a high-temperature zone, the interface is heated to a temperature exceeding the temperature of the melt. The heated layer of the melt together with the oxides are transferred from the lune over the volume of the bath. As soon as the necessary thermodynamic state is achieved, reactions between the oxides and the melt components take place, including the appearance of gaseous interaction products. Therefore, the dimensions of the reaction surface, its temperature, and the concentration of the chemically active reaction products in combination with the hydrodynamic circumstances predetermine the rate of the processes in the bath.

In constructing the mathematical model, we assume that the purging mode does not change, and the motion is self-similar, i.e., with a turbulent analog for the Reynolds number not less than the limit value for the reactor [1]. Such an assumption permits considering the steady-state velocity field in the bath. The component concentrations in the melt and its temperature because of the chemical reactions are time dependent, hence the heat and mass transfer process is a nonstationary process.

The equation for the change in component concentration in a melt must be solved in conjunction with the energy equation governing the temperature change. These equations are written thus in the presence of chemical reactions [2]:

$$\frac{dm_n}{d\tau} = D_T \nabla^2 m_n + \Delta m_n;$$

$$\rho \frac{dh}{d\tau} = \lambda_T \nabla^2 T + D_T \operatorname{div}\left(\sum_n h_n \rho \operatorname{grad} m_n\right) + \Delta h.$$

The change in concentration of the n-th component because of chemical reactions is taken into account by Δm_n while Δh is the quantity of heat being liberated or absorbed per unit time. An assumption about the constancy of the turbulent analogs of the coefficients of diffusion and heat conduction over the volume of the path is introduced for the conditions of developed turbulent motion, which permitted it to be extracted outside the differentiation symbol. For

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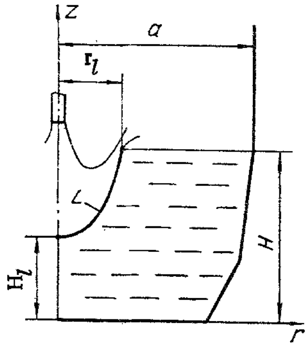

Fig. 1. Diagram of jet interaction with a melt.

axisymmetric motion, the equations are written in a cylindrical coordinate system after reduction to dimensionless form:

$$\frac{\partial m_n}{\partial \tau} + v_r \frac{\partial m_n}{\partial r} + v_z \frac{\partial m_n}{\partial z} = \frac{1}{\mathrm{Pe}_\mathrm{D}} \left(\frac{\partial^2 m_n}{\partial r^2} + \frac{1}{r} \frac{\partial m_n}{\partial r} + \frac{\partial^2 m_n}{\partial z^2} \right) + \Delta m_n \frac{a}{V};$$

$$\frac{\partial h}{\partial \tau} + v_r \frac{\partial h}{\partial r} + v_z \frac{\partial h}{\partial z} = \frac{1}{\mathrm{Pe}_T} \left(\frac{\partial^2 h}{\partial r^2} + \frac{1}{r} \frac{\partial h}{\partial r} + \frac{\partial^2 h}{\partial z^2} \right)$$

$$+ \frac{1}{\mathrm{Pe}_\mathrm{D}} \left(\frac{\partial}{\partial r} \sum_n h_n \frac{\partial m_n}{\partial r} + \frac{\partial}{\partial z} \sum_n h_n \frac{\partial m_n}{\partial z} \right) + \Delta h \frac{a}{V}.$$

The bath radius a, the characteristic velocity V [1], the time a/V, and the initial specific heat content of the melt h_0 are taken as scales. The turbulent analogs of the Peclet diffusion and thermal numbers

$$\mathrm{Pe}_\mathrm{D} = \frac{Va}{D_T} = \mathrm{Re}_T \mathrm{Pr}_\mathrm{D};\ \mathrm{Pe}_T = \frac{Va}{a_T} = \mathrm{Re}_T \mathrm{Pr}_T$$

depend on the turbulent analog of the Reynolds number [1] and the Prandtl numbers $\mathrm{Pr}_\mathrm{D} = \nu_\mathrm{T}/D_\mathrm{T}$ and $\mathrm{Pr}_\mathrm{T} = \nu_\mathrm{T}/a_\mathrm{T}$. At this time, the independence of Pr_T = 0.7-0.8 from the physical Prandtl number has been established experimentally [3]. The question of Pr_D remains open. There is hence no foundation for taking it equal to Pr_T because of the difference in the mass diffusion and heat transmission mechanisms in vortices generated by a turbulent flow.

The source term in the mass transfer equation is governed by the chemical kinetics relationships. For a reaction of the form

$$\alpha A + \beta B \rightleftarrows \gamma C + \delta D$$

$$\Delta m_n = \mu_n \Delta M,\ \Delta M = k M_A^\alpha M_B^\beta,$$

where the reaction rate constant k depends on the temperature and activation energy of the reacting components.

The quantity of heat being liberated $\Delta h = \Delta H \cdot \Delta M$ is taken with the plus sign and the quantity absorbed with a minus sign:

$$\Delta H = \alpha h_A + \beta h_B - \gamma h_C - \delta h_D.$$

The total specific enthalpy of the n-th component in the melt

$$h = h^{298} + \int_{298}^{T} c_p dT$$

depends on the heat of formation h^{298} and the specific heat c_p. Its temperature dependence in the form $c_p = a + bT + cT^{-2}$ J/mole·deg with known coefficients [4] can be used in the computations.

The initial conditions are determined by the temperature and concentration of the components in the melt, which should be known in the whole range of solution of the problem.

The boundary conditions are given for the domain boundary defined by the bottom, the walls of the bath, and the free surface with the lune. The axis of symmetry of the melt volume agrees with the bath axis for an axisymmetric disposition of the blowing unit.

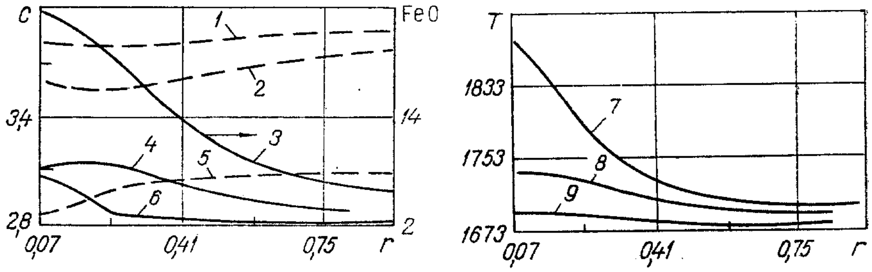

Fig. 2. Temperature and concentration distributions in the melt (τ = 3 min): 1) z = 0.15; 2) 0.29; 3) 0.52; 4) 0.29; 5) 0.52; 6) 0.15; 7) 0.52; 8) 0.29; 9) 0.15.

In the absence of mass elimination through the bottom and walls, we have:

$$z=0\quad \frac{\partial m_n}{\partial z}=0;\ r=1\quad \frac{\partial m_n}{\partial r}=0.$$

In the general case, the chemical interaction between the melt components and the wall can be taken into account. Heat elimination from the melt through the bottom and walls is inevitable. Then, for

$$z=0\quad -\frac{\partial T}{\partial z}=\frac{q_1}{\lambda};\ r=1\quad -\frac{\partial T}{\partial r}=\frac{q_2}{\lambda}.$$

From the axisymmetry condition, on the bath axis for

$$r=0\quad \frac{\partial m_n}{\partial r}=\frac{\partial h}{\partial r}=0.$$

The concentration and temperature on the free surface and in the lune are given as a function of the problem to be solved.

For a numerical solution, the system of equations and the boundary conditions are reduced to the finite-difference form

$$m_{i,j,k}=D_1m_{i,j+1,k}+D_2m_{i,j-1,k}+D_3m_{i+1,j,k}+D_4m_{i-1,j,k}+D_5m_{i,j,k-1}+D_6,$$

where

$$D_1=\frac{1}{\varkappa}\left(\frac{1}{\Delta r^2\mathrm{Pe}}+\frac{1}{2r_j\Delta r\mathrm{Pe}}-\frac{v_{r\,i,j}}{2\Delta r}\right);$$

$$D_2=\frac{1}{\varkappa}\left(\frac{1}{\Delta r^2\mathrm{Pe}}-\frac{1}{2r_j\Delta r\,\mathrm{Pe}}+\frac{v_{r\,i,j}}{2\Delta r}\right);$$

$$D_3=\frac{1}{\varkappa}\left(\frac{1}{\Delta z^2\mathrm{Pe}}-\frac{v_{zi,j}}{2\Delta z}\right);$$

$$D_4=\frac{1}{\varkappa}\left(\frac{1}{\Delta z^2\mathrm{Pe}}+\frac{v_{zi,j}}{2\Delta z}\right);$$

$$D_5=\frac{1}{\varkappa}\Delta\tau;\quad D_6=\frac{1}{\varkappa}\Delta m_{\,i,j,k}\frac{a}{V};$$

$$\varkappa=\frac{1}{\Delta\tau}+\frac{2}{\Delta r^2\,\mathrm{Pe}}+\frac{2}{\Delta z^2\,\mathrm{Pe}}.$$

For the energy conservation equation

$$D_6=\frac{1}{\varkappa}\left[\Delta h\frac{a}{V}-\frac{1}{\mathrm{Pe}_\mathrm{D}}\left(\frac{Q^1_{i+1,j,k}-Q^1_{i-1,j,k}}{2\Delta z}-\frac{Q^2_{i,j+1,k}-Q^2_{i,j-1,k}}{2\Delta r}\right)\right],$$

where

$$Q^1_{i,j,k}=\sum_n h_n\frac{m_{n\ i+1,j,k}-m_{n\ i-1,j,k}}{2\Delta z};$$

$$Q^2_{i,j,k}=\sum_n h_n\frac{m_{n,i,j+1,k}-m_{n\ i,j-1,k}}{2\Delta r}.$$

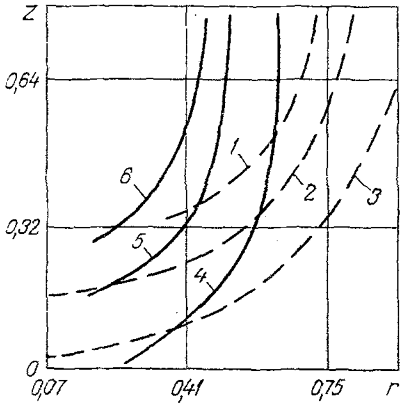

Fig. 3

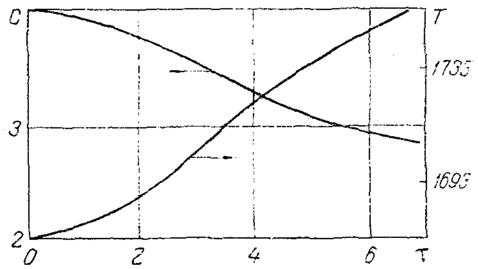

Fig. 4

Fig. 3. Lines of constant temperature and concentration in the melt (τ = 7 min): 1) C = 2.3%; 2) 2.6; 3) 2.8; 4) T = 1690°K; 5) 1710°K; 6) 1730°K.

Fig. 4. Change in the mean mass temperature T, °K, and concentration C, % carbon, in time τ, min.

The temperature is evaluated by means of the formula

$$T_{i,j,k} = T_{i,j,k-1} + \frac{1}{c_{p\,i,j,k-1}}(h_{i,j,k} - h_{i,j,k-1}),$$

where

$$c_{p\,i,j,k} = \sum_n c_{p\,n\,i,j,k} m_{n\,i,j,k};\quad h_{i,j,k} = c_{p\,i,j,k} T_{i,j,k}.$$

Computations of the process of decarburization of cast iron in an oxygen converter according to the velocity field obtained in [1] were performed as an illustration of the application of the mathematical model.

It was assumed in the computation scheme that iron on the reaction surface is oxidized to FeO and then is oxidized by the carbon in the melt according to the reaction

$$[\mathrm{FeO}] + [\mathrm{C}] \rightleftarrows [\mathrm{Fe}] + \{\mathrm{CO}\}$$

with CO being liberated in the gas phase.

The reaction rate constant is calculated by means of the formula [5]

$$k = 11.73 \exp\left(-\frac{4900}{T}\right),$$

and the rate of change of the molar concentration

$$\Delta M = \mathrm{k} M_{\mathrm{FeO}} M_{\mathrm{C}}.$$

The initial composition of impurities in the melt is the following: C 4%, 0.71% Si, 0.91% Mn, 0.043% S, and 0.13% P. Since the major part of the impurities (except carbon) is oxidized at the beginning of the purging, then the total quantity of heat being liberated, evaluated according to the data [6], is taken into account in the initial heat content h_0 of the melt. The initial temperature of the interface is 2373°K, and the component composition in the slag being formed on the free surface is taken on the basis of tests [7]. The computation is performed for the Peclet number $\mathrm{Pe_T}$ = 0.75, and $\mathrm{Pe_D}$ = 11, taken from the data [8].

Taking this into account, the boundary conditions are written thus in difference form:

$$\tau = 0,\ 0 \leqslant r_j \leqslant 1,\ 0 \leqslant z_i \leqslant H \quad T_{i,j,1} = 1673\,°\mathrm{K}$$

$$m^{\mathrm{Fe}}_{i,j,1} = 0.92,\ m^{\mathrm{C}}_{i,j,1} = 0.04,\ m^{\mathrm{FeO}}_{i,j,1} = 0;$$

$$\tau > 0,\ 0 < r_j < r_l,\ z_{in} = H_l \quad T_{in\,j,k} = 2373\,°\mathrm{K}$$

$$m^{\mathrm{Fe}}_{in,j,k} = 0,\ m^{\mathrm{C}}_{in,j,k} = 0,\ m^{\mathrm{FeO}}_{in,j,k} = 0.89;$$

$$r_l < r_j < 1,\quad z_{in} = H \quad T_{in,j,k} = T_{in-1,j,k},$$

$$m^{\mathrm{Fe}}_{in,j,k} = 0, \quad m^{\mathrm{C}}_{in,j,k} = 0, \quad m^{\mathrm{FeO}}_{in,j,k} = 0.1;$$

$$0 < r_j < 1, \quad z_1 = 0 \quad T_{2,j,k} = T_{1,j,k}, \quad m_{n2,j,k} = m_{n1,j,k};$$

$$r_1 = 0, \quad r_{jn} = 1, \quad 0 < z_i < H \quad T_{i,2,k} = T_{i,1,k},$$

$$m_{ni,2,k} = m_{ni,jn-1,k}, \quad m_{nj,jn,k} = m_{ni,jn-1,k}.$$

Because of the interdependence of the heat and mass transfer processes in the bath, the computation is performed in the following sequence: the reaction rate constant and the source terms $\Delta m_{\mathrm{FeO}} = -72\Delta M$, $\Delta m_{\mathrm{C}} = -12\Delta M$, $\Delta m_{\mathrm{Fe}} = 56\Delta M$ are determined for the known temperature, after which the distribution of the concentrations, the heat content, and the temperature field are found and the reaction rate constants for the next time interval are determined. The calculations are carried out in the direction from the free surface to the bottom and from the bath axis to the wall. For each time the iteration process is continued until a given error, calculated at the mesh nodes, is reached. The mesh is selected analogous to that in [1].

The concentration distribution of C, FeO, and the temperature over the bath volume in a 3-min purging is shown in Fig. 2, and the isotherms and lines of equal concentration of C and FeO are represented in Figs. 3. Changes in the temperature and carbon concentration in the melt, averaged with respect to the mass, are shown in Fig. 4.

It follows from the figures that supersaturation of the iron oxide occurs in the zone of the lune in the dynamic mode, which is adequate for seeding the gas phase and boiling of the melt in the bath volume. The shape of the isotherms and the lines of constant concentration is determined by the lune profile and varies under the influence of the temperature and composition of the slag on the free surface. The growth rates of the mean mass temperature of ∼12°/min and of carbon burn-up 0.18%/min are similar to those known for a 130-ton oxygen converter [9]. Thus, for a 2.6 $\mathrm{m}^3/\mathrm{ton\cdot min}$ blowing intensity, the mean rate of decarburization is ∼0.20%/min.

A rise in the accuracy of the boundary conditions and obtaining reliable data on the diffusion transport of the substance during chemical reactions is the fundamental direction of research on a further improvement in the adequacy of the mathematical model for heat and mass transfer in a reactor.

NOTATION

r, z, coordinates; v, velocity; h, heat content; T, temperature; m, concentration; ρ, density; c_p, specific heat; τ, time; μ, molecular mass; M, molar concentration; D_T, λ_T, a_T, ν_T, turbulent analogs of the diffusion, heat conduction, thermal diffusivity, and viscosity coefficients; *l*, lune; i, j, mesh nodes; in, jn, boundary nodes of the domain; n, melt component.

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