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]:

\[
\frac{dm_n}{d\tau} = D_T \nabla^2 m_n + \Delta m_n; \\
\rho \frac{dh}{d\tau} = \lambda_T \nabla^2 T + D_T \nabla \left( \sum_n h_n \rho \nabla m_n \right) + \Delta h.
\]

The change in concentration of the n-th component because of chemical reactions is taken into account by \(\Delta m_n\) while \(\Delta h\) 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
axisymmetric motion, the equations are written in a cylindrical coordinate system after reduction to dimensionless form:

\[
\begin{align*}
\frac{\partial m_n}{\partial \tau} + v_r \frac{\partial m_n}{\partial r} + v_z \frac{\partial m_n}{\partial z} &= \frac{1}{Pe_D} \left( \frac{\partial^2 m_n}{\partial r^2} + \frac{1}{r} \frac{\partial m_n}{\partial r} + \frac{\partial^2 m_n}{\partial z^2} \right) + \frac{\Delta m_n}{V} ; \\
\frac{\partial h}{\partial \tau} + v_r \frac{\partial h}{\partial r} + v_z \frac{\partial h}{\partial z} &= \frac{1}{Pe_T} \left( \frac{\partial^2 h}{\partial r^2} + \frac{1}{r} \frac{\partial h}{\partial r} + \frac{\partial^2 h}{\partial z^2} \right) \\
&+ \frac{1}{Pe_D} \left( \frac{\partial}{\partial r} \sum_n h_n \frac{\partial m_n}{\partial r} + \frac{\partial}{\partial z} \sum_n h_n \frac{\partial m_n}{\partial z} \right) + \frac{\Delta h}{V} .
\end{align*}
\]

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

\[
Pe_D = \frac{V a}{D_T} = Re_T Pr_D ; \quad Pe_T = \frac{V a}{a_T} = Re_T Pr_T
\]

depend on the turbulent analog of the Reynolds number [1] and the Prandtl numbers \( Pr_D = \nu_T / D_T \) and \( Pr_T = \nu_T / a_T \). 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

\[
\alpha A + \beta B \rightarrow \gamma C + \delta D
\]

\[
\Delta m_n = \mu_n \Delta M, \quad \Delta M = k M_A^\alpha M_B^\beta,
\]

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

\[
h = h^{298} + \frac{T}{c_p} \int_{298}^{T} dT
\]

depends on the heat of formation \( h^{298} \) and the specific heat \( c_p \). Its temperature dependence in the form \( c_p = a + b T + c T^{-2} \) 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.