Thermalphysic processes in a reaction zone of electrothermal ore-smelting reactor

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Considered are the features of hydrodynamics and heat and mass transfer during the reduction reaction proceeding in a coke zone of electrothermal ore-smelting reactor, when the process is complicated by gas phase evolving, which bubbles the melt. The gas bubbles provides conditions for intense immixture, which for it’s turn intensifies target reduction processes. The peculiarity of the reacting lies in the fact that an active reagent on mixing transfers the reduction process into kinetic area. In that case, the temperature of a reaction zone and reagent concentration in a volume are the governing factors, so the reduction reaction and gas bubbles evolving influence on development of convection currents is thought of as influence of temperature and reagent concentration. Hydrodynamics of the bubbles and liquid interconnection has its peculiar features like a local Influence over liquid by means of added mass for example. The effect strength is in direct relation of the gas content gradient. It is shown that the chemical reduction reaction rate determines gas content and hence, an extent of influence on immixture. The effective criteria, which characterize the chemical reaction influence by means of heat and concentration effect, have been introduced as a measure of the gas phase impact on hydrodynamics in filter equation. The coefficients, considering the chemical reaction influence on hydrodynamics of the system are well greater than the influence parameters of free and concentration convection, which actually determines the melt behaviour in a reaction zone. In that case, the problem is reduced by structure to an estimation of influence of the temperature and concentration small perturbations on hydrodynamics of the melt being filtered in a coke layer.

It is deduced that in a reduction process there takes place the formation of dissipative hydrodynamic structures, which determine thermophysical behaviour of a reaction zone, including temperature and reagent concentrations. Synergetic behaviour features of a reaction bulk provide conditions and possibilities of control. It is precisely the situation that should be taken into account when organizing the operating mode of electrothermal ore-smelting reactor.

Key words: electrothermal ore-smelting reactor, reaction zone, layer of disperse particles, filter equations, heat and mass transfer equations, bubbling of gas bubbles, dissipative structures.

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Introduction

Obtaining calcium carbide or phosphorus sublimation in electrothermal ore-smelting reactors, the reduction reactions on carbon particles take place in high-temperature melt with evolving gaseous carbon oxide which bubbles the melt. Rising gas bubbles set up the conditions for intensive liquid immixture. Strengthening of the processes of chemical response is mainly determined by processes of heat and mass transfer, which form temperature condition of the reactor and ensure supply of reagent. Direct experimental study of electrothermal processes is impeded by high temperature and a reaction zone which is difficult of access, etc. Therefore, one should be content with fixing parameters, which are accessible outside on inspecting of operating modes of reactors [1–5] or by investigating the low-temperature zones only. The papers, devoted to computational simulation of the processes in such reactors are few in number [6–9, 13]. Preliminary analytical estimation of the phenomenon, accompanying target processes is of value for computational simulation. These supporting estimations have been implemented in the papers [10–12]. The present work contains their advancement with more careful taking into account both thermal and hydrodynamic behaviour of reagents.

As for reduction processes with evolving gas-core products into liquid, the hydrodynamic state of a reaction space is often determined by chemical reactions. Below are considered conditions of responding multiple-phase medium, where rate of the energy exchange processes is in many respects determined by the bubbling reaction products in gaseous form.

The qualitative theoretical analysis of hydrodynamic features of a reaction zone of technological reactor with the melt of reagent, which is bubbled by reaction products, is based on the hydrodynamic and heat transfer equations sets.
The simulator of thermophysical processes in a reaction zone of electrothermochemical reactor

It is thought that the movement of a liquid phase is provoked by difference between the liquid densities owing to temperature, reagent concentration and presence of the gas phase in the form of bubbles. The system being analysed is a two-dimensional structure of height \( H \) and width \( L \), filled by dispersed material with percentage of voids \( \varepsilon \) and by liquid.

The paper is aimed to detection of convection currents, stipulated by density changes, and their influence on the system characteristics.

The dimensionless form of equations describing the filtered liquid movement as well as mass, heat and gas phase transfer in a form of bubbles is written as follows:

\[
\nabla \bar{v} = 0, \quad \frac{1}{\sigma Pr} \frac{\partial \bar{c}}{\partial t} = -\nabla \bar{p} + (Ra_0 \theta + Ra_c \bar{c} + Ra_q \bar{q}) \bar{\nabla}^2 \bar{c} - \bar{v} + \frac{Fs}{Pr_p} \bar{v} |\bar{v}|, \\
\frac{1}{\sigma} \frac{\partial \theta}{\partial t} = -\bar{v} \theta c + \frac{Le}{k} \theta c^2 + D\alpha \theta (c, \theta), \\
\frac{\partial N}{\partial t} = -\bar{v} \bar{N} + D_N \Delta N + \omega_R(c, \theta) \theta cl / (p_g V_g),
\]

Where \( c \) is fractional conversion \((c = 1 - C' / C'_0)\) with initial and end concentrations \( C' \) and \( C'_0 \), respectively; \( t \) is dimensionless time \((t = t' / H^2 \sigma)\), \( t' \) is time; \( \dot{c} \) is temperature conductivity, \( \dot{m}^2 / s; \sigma \) is a heat capacity ratio \( \sigma = 1 + (\rho c' \rho_c (1 - \varepsilon)) / (\rho c \rho_c \varepsilon); \rho_c \rho_g \) are densities of solid and liquid carrier; \( C_p' \rho_c, C_p \rho_g \) are heat capacities of solid and liquid carrier; \( \varepsilon \) is percentage of voids; \( Le \) is the Lewis’ criterion \((Le = Dc / \dot{c}; Dc \) is an effective diffusion coefficient); \( Da \) is the Damkhler criterion: \( Da = (k_0 \exp(-\gamma) L^2 / C'_0)^{\nu_0} / (\dot{c} \dot{a}) \). \( k_0 \) is a preexponential, \( \gamma = E / RT_0 \) is a dimensionless activation energy, \( T \) is temperature, \( R \) is absolute gas constant, “0” index refers to initial values, \( n \) is the reaction order; \( \theta \) is dimensionless temperature; \( \theta = \gamma(T - T_0) / T_0 \); \( B \) is a dimensionless calorific effect of the reaction, an adiabatic temperature rising:

\[
B = Q_k C_g \dot{c}^2 / (\rho c T_0); \quad N \text{ is a number of bubbles; } D_N \text{ is the \( \dot{c} \) diffusion coefficient; } V_g \text{ is \( \dot{c} \) volume of bubbles; } \rho = \rho' k'(1 / \mu a'), \rho' \text{ denotes pressure, } Pa; \text{ } k' \text{ is a permeability ratio; } \mu \text{ denotes the liquid dynamic viscosity, } Pa s; \text{ } Pr^* = \mu H^2 / (k a'); \rho' \text{ denotes the Darcy’s criterion; } Ra_0 = \beta_g k H (T_0) / (\mu a'); \text{ } Ra_c = \beta_g k H (\nu a'); \text{ } Ra_q = \beta_g k H (va'); \text{ } \beta_g, \beta_c, \beta_q \text{ are mass, thermal and gas-phase expansivenesses (density changes due to gas presence).}
\]

With boundary condition as follows:

\[ c = 0 \text{ at } y = 0, \quad n \nabla c = n \nabla \theta = 0 \text{ at all boundaries, where } n_0 \text{ near side wall.} \]

\[ \text{At } y = 0, \, \nu_z = -Pe; \, y = 1, \, \nu_z = -Pe. \quad \text{(2)} \]

Taking into account smallness of the bubbles diffusion coefficient \( D_b \) and gradient \( \nabla N \), the transport equation for a gas phase one can rewrite as follows:

\[
\frac{\partial N}{\partial t} = \omega_R(c, \theta) \gamma cl / (p_g V_g), \quad N = \int \omega_R(c, \theta) \gamma cl / (p_g V_g) dt. \quad \text{(3)}
\]

Whence \( \phi_g = \omega_R \gamma \tau \tau_R / p_g \tau_R \) is a duration of the bubbles being in a layer.

\[
\omega_R(c, \theta) = \frac{\partial c}{\partial t} = k_0 \exp\left( -\frac{\theta}{1 + \theta / \gamma} \right) \quad \text{(4)}
\]

Further we consider the first-order reaction. Let us decompose the exponent into a series up to first order.

\[
\omega_R(c, \theta) = \frac{\partial c}{\partial t} = k_0 \exp\left( -\frac{\theta}{1 + \theta / \gamma} \right) = k_0 \exp\left( -\frac{\theta}{1 + \theta / \gamma} \right), \quad \text{(5)}
\]

Then \( \phi_g = (k_0 \gamma S \tau_R / p_g) (a - ac + b \theta - bc \theta). \)

Solving such a problem even numerically presents certain difficulty.

To make an analytical investigation, let us do some simplification. We consider a layer between horizon planes with temperatures \( T_0 \) and \( T_1 \). We believe the problem two-dimensional and stationary and the liquid seepage velocities low; we also neglect non-linearity in the equation of motion. We consider small deviations of all quantities, involved in the equations:

\[ \nu = \nu_0 + \nu_1, \theta = \theta_0 + \theta_1, \varepsilon = \varepsilon_0 + \varepsilon_1, \text{ in which connection we suppose } \nu = 0 \text{ in equilibrium.} \]

The filter equation may be written as:

\[
0 = -\nabla p + (Ra_0 \theta + Ra_c \bar{c} + Ra_q(k_0 S \tau \tau_R / p_g) \times (a - ac + b \theta - bc \theta)) \varepsilon^2 - \bar{v},
\]

Or by using the perturbed and linearized forms:

\[
0 = -\nabla p_1 + ((Ra_0 + Ra_c \phi(k_0 S \tau \tau_R / p_g) \omega_0) \theta_1 + (Ra_c + Ra_q(k_0 S \tau \tau_R / p_g \omega_c) c_1) \varepsilon^2 - \bar{v}. \quad \text{(6)}
\]

Applying operator \( rot \) to the equation of motion in the medium equilibrium conditions, when velocity equals to zero, one can show that the temperature and concentration distribution are one-dimensional along the y axis. The tempe-
nature and concentration distribution in equilibrium turns out an exponential one, within the temperature range from \( T_0 \) to \( T_1 \). The temperature and concentration field in tranquillity we approximate by linear dependence; for temperature, as an example, we have: \( T = T_1 - \beta y \), \( \beta = (T_1 - T_0)/H \).

Following the use of perturbed components, the linearized equations become:

\[
\nabla v = 0
\]

\[
0 = -\nabla p_1 + ((R_{a_0} + R_{a_0} R_{q_0} \omega_0) \theta_1 + (R_{a_0} + R_{a_0} R_{q_0} \omega_0) c_1) \nabla^2 v_1
\]

\[
0 = -\nabla v_1 \nabla v_0 + \nabla^2 v_0 + (Fk/B)(\omega_0 \theta_1 + \omega_0 c_1)
\]

Following the use of perturbed components, the system of equations becomes:

\[
R_q = (K_0 \gamma \frac{\tau}{\rho_0} \gamma), \quad \omega_0, \quad \omega_c \text{ are coefficients of expansion in a series.}
\]

**Method of solution of the problem**

Let us define the flow function \( \psi \) as follows:

\[
v_x = \frac{\partial \psi}{\partial y}, \quad v_y = -\frac{1}{\alpha} \frac{\partial \psi}{\partial x},
\]

The simplified form of the motion equations will be written in the following form:

\[
\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} = 0,
\]

\[
\frac{\partial p}{\partial x} = v_x = 0,
\]

\[
\frac{\partial p}{\partial y} + ((R_{a_0} + R_{a_0} R_{q_0} \omega_0) \theta_1 + (R_{a_0} + R_{a_0} R_{q_0} \omega_0) c_1) - v_y = 0,
\]

And upon eliminating the pressure, the system of equations will be presented in the following form:

\[
\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{1}{\alpha} \left((R_{a_0} + R_{a_0} R_{q_0} \omega_0) \frac{\partial \theta_1}{\partial x} + (R_{a_0} + R_{a_0} R_{q_0} \omega_0) \frac{\partial c_1}{\partial x}\right) + (R_{a_0} + R_{a_0} R_{q_0} \omega_0) \frac{\partial \psi}{\partial x} = 0,
\]

\[
\frac{\partial^2 \theta_1}{\partial x^2} + \frac{\partial^2 \theta_1}{\partial y^2} - \frac{1}{\alpha} \frac{\partial \psi}{\partial x} + Fk(\omega_0 \theta_1 + \omega_0 c_1) = 0,
\]

\[
\frac{\partial^2 c_1}{\partial x^2} + \frac{\partial^2 c_1}{\partial y^2} - \frac{1}{Le \alpha} \frac{\partial \psi}{\partial x} + (Fk/LeB)(\omega_0 \theta_1 + \omega_0 c_1) = 0.
\]

Taking into account that perturbations are damping on borders and don’t penetrate outside the area, the boundary conditions may be written as:

\[
\begin{align*}
\bar{x} &= 0, \quad 0 < y < 1, \quad \theta_1 = 0, \quad c_1 = 0, \quad \psi = 0; \\
\bar{y} &= 1, \quad 0 < x < 1, \quad \theta_1 = 0, \quad c_1 = 0, \quad \psi = 0; \\
\bar{x} &= 0, \quad 0 < x < +1, \quad \theta_1 = 0, \quad c_1 = 0, \quad \psi = 0; \\
\bar{y} &= 1, \quad 0 < x < +1, \quad \theta_1 = 0, \quad c_1 = 0, \quad \psi = 0.
\end{align*}
\]

Let us study the behaviour of solutions of the system (8) with respect to small perturbations. We will look for a solution, which meets boundary conditions in the form as follows:

\[
\psi = \sum_{n=1}^{\infty} \psi_n \sin n \pi y, \quad \theta_1 = \sum_{n=1}^{\infty} \theta_n \sin n \pi y,
\]

\[
c_1 = \sum_{n=1}^{\infty} c_n \sin n \pi y,
\]

where \( \psi_n, \theta_n, c_n \) are the functions of \( x \).

Substituting the expressions (10) into equations (8), we obtain:

\[
\begin{align*}
\frac{d^2 \psi_n}{dx^2} - n^2 \pi^2 \psi_n + \frac{1}{\alpha} \left((R_{a_0} + R_{a_0} R_{q_0} \omega_0) \frac{d\theta_n}{dx} + (R_{a_0} + R_{a_0} R_{q_0} \omega_0) \frac{d\psi_n}{dx}\right) &= 0; \\
\frac{d^2 \theta_n}{dx^2} - n^2 \pi^2 \theta_n - \frac{1}{\alpha} \frac{d\psi_n}{dx} + Fk(\omega_0 \theta_n + \omega_0 c_n) &= 0; \\
\frac{d^2 c_n}{dx^2} - n^2 \pi^2 c_n - \frac{1}{Le \alpha} \frac{d\psi_n}{dx} + (Fk/LeB)(\omega_0 \theta_n + \omega_0 c_n) &= 0.
\end{align*}
\]

With the boundary conditions

\[
\begin{align*}
\psi_n(0) &= \psi_n(1) = 0; \\
\theta_n(0) &= \theta_n(1) = 0; \\
c_n(0) &= c_n(1) = 0.
\end{align*}
\]

Let us form a differential equation of the forth order relative to \( \psi_n \) out of initial system of equations (11). For that, the first equation of the system (11) we will differentiate on \( x \) twice and obtain:

\[
\begin{align*}
\frac{d^4 \psi_n}{dx^4} - n^2 \pi^2 \frac{d^2 \psi_n}{dx^2} + \frac{1}{\alpha} \left((R_{a_0} + R_{a_0} R_{q_0} \omega_0) \frac{d^3 \theta_n}{dx^3} + (R_{a_0} + R_{a_0} R_{q_0} \omega_0) \frac{d^3 \psi_n}{dx^3}\right) &= 0; \\
\frac{d^4 \theta_n}{dx^4} - n^2 \pi^2 \theta_n - \frac{1}{\alpha} \frac{d\psi_n}{dx} + Fk(\omega_0 \theta_n + \omega_0 c_n) &= 0; \\
\frac{d^4 c_n}{dx^4} - n^2 \pi^2 c_n - \frac{1}{Le \alpha} \frac{d\psi_n}{dx} + (Fk/LeB)(\omega_0 \theta_n + \omega_0 c_n) &= 0.
\end{align*}
\]

The second-order equations for \( \theta_n \) and \( c_n \) of the system (11) we differentiate on \( x \):
\[
\frac{d^4 \psi_n}{dx^4} - n^2 \pi^2 \frac{d^2 \psi_n}{dx^2} + \frac{1}{\alpha} \left( (R_0 - R_a) \psi_\omega \right) \frac{d^2 \psi_n}{dx^2} + 
\]
\[
\times \left( \frac{R_0 + R_a \psi_\omega}{\frac{d\theta_n}{dx} + \frac{dc_n}{dx}} \right) = 0.
\]

We put the expressions of derivatives of the third order to the equation for flow function (13):

\[
\frac{d^4 \psi_n}{dx^4} - n^2 \pi^2 \frac{d^2 \psi_n}{dx^2} + \frac{1}{\alpha} \left( (R_0 + R_a \psi_\omega) \frac{d^2 \psi_n}{dx^2} + 
\]
\[
\times \left( \frac{R_a + R_q \psi_\omega}{\frac{d\theta_n}{dx} + \frac{dc_n}{dx}} \right) + 
\]
\[
+ (F_k/Le_B) \left( \frac{d\theta_n}{dx} + \frac{dc_n}{dx} \right) = 0.
\]

Or uniting the factors, we obtain:

\[
\frac{d^4 \psi_n}{dx^4} - n^2 \pi^2 \frac{d^2 \psi_n}{dx^2} + \frac{1}{\alpha} \left( (R_0 + R_a \psi_\omega) \frac{d^2 \psi_n}{dx^2} + 
\]
\[
+ \frac{1}{\alpha} \left( (R_a + R_q \psi_\omega) \frac{d\theta_n}{dx} \right) + 
\]
\[
+ \frac{1}{\alpha} \left( (R_0 + R_a \psi_\omega) \frac{d^2 \psi_n}{dx^2} \right) \frac{d\theta_n}{dx} + 
\]
\[
+ \left( \frac{1}{\alpha} \left( R_0 + R_a \psi_\omega \right) \right) n^2 \pi^2 - 
\]
\[
- \frac{1}{\alpha} \left( R_0 + R_a \psi_\omega \right) F_k \omega_\theta - 
\]
\[
- \frac{1}{\alpha} \left( R_a + R_q \psi_\omega \right)(F_k/Le_B) \omega_\theta - 
\]
\[
- \frac{1}{\alpha} \left( R_a + R_q \psi_\omega \right)(F_k/Le_B) \omega_\theta \right) \frac{d\theta_n}{dx} + 
\]
\[
+ \left( \frac{1}{\alpha} \left( R_a + R_q \psi_\omega \right) \right) n^2 \pi^2 - 
\]
\[
+ \frac{1}{\alpha} \left( R_0 + R_q \psi_\omega \right) F_k \omega_\theta - 
\]
\[
- \frac{1}{\alpha} \left( R_0 + R_q \psi_\omega \right) F_k \omega_\theta - 
\]
\[
- \frac{1}{\alpha} \left( R_a + R_q \psi_\omega \right)(F_k/Le_B) \omega_\theta \right) \frac{dc_n}{dx} = 0.
\]

In this system, let us single out the coefficients

\[
a_{11} = \frac{1}{\alpha} \left( R_0 + R_q \psi_\omega \right) n^2 \pi^2 - 
\]
\[
- \frac{1}{\alpha} \left( R_a + R_q \psi_\omega \right) F_k \omega_\theta - 
\]
\[
- \frac{1}{\alpha} \left( R_0 + R_q \psi_\omega \right) F_k \omega_\theta - 
\]
\[
- \frac{1}{\alpha} \left( R_a + R_q \psi_\omega \right)(F_k/Le_B) \omega_\theta = 0.
\]

As a result, we have the system of linear second-order equations with respect to derivatives \( \frac{d\theta_n}{dx} \), \( \frac{dc_n}{dx} \).

In such a way, two considered equations allow to obtain expressions for first derivatives of temperature and concentration, which being substituted for example into the first equation for flow function will produce the differential equation of the fourth order of the flow function, giving an indication of the behaviour of the flow function of \( x \) and \( y \).

\[
\frac{d^4 \psi_n}{dx^4} + f_1 \frac{d^2 \psi_n}{dx^2} + f_2 \psi_n = 0.
\]

Presenting solution (15) as \( \psi_n = e^{\rho x} \), we will get the characteristic equation in the following form:

\[
p^4 + f_1 p^2 + f_2 = 0.
\]
Thus, partial solutions in the form of harmonic functions are true for the flow function.
Let us write down the solution for $\psi$ as:

$$\psi = C \sin(\pi x) \sin(\pi ny),$$  \hfill (16)

where $C$ is a constant.

**Analysis of hydrodynamic conditions of a reaction zone of the reactor**

With definitions for flow function, we find the expressions for velocity component:

$$\nu_x = \frac{\partial \psi}{\partial y} = \pi n C \sin(\pi ny),$$  \hfill (17)

$$\nu_y = -\frac{\partial \psi}{\partial x} = -p C \cos(\pi x) \sin(\pi ny).$$  \hfill (18)

Movement of a separate gas element is described by trajectories, mathematical representation of which have the following form:

$$\frac{dx}{dy} = \frac{\pi n C}{p C} \tan(\pi x),$$  \hfill (19)

Solution of the last equation gives:

$$\sin(\pi x) \sin(\pi ny) = Tr,$$  \hfill (20)

where $Tr$ is the constant, defined by initial conditions.

The lines for which $Tr = 0$ are of particular importance. Position of these lines is characterized by the equations

$$\frac{ny}{H} = \frac{m_2}{m_1}, \quad \frac{H}{n} = \frac{x}{L} = \frac{m_2}{m_1},$$  \hfill (21)

where $m_1$, $m_2$ are whole numbers.

These straight lines divide the reaction zone into separate cells. The liquid moves inside the cells, not exceeding their bounds, since normal components of velocity at cell bounds equal to zero, i.e. the liquid doesn’t overstep the limits (Fig. 1). Such cells are analogues to the Bénard ones.

Inside each cell, an element of the liquid moves over closed trajectory around the centre, where the liquid is at rest. Such approximate description of the liquid movement in a reaction zone of technological reactor allows qualitatively describe an appearance of hydraulic dissipative structures and dependences for estimating modes of operation, which form vortical structures, arising on impact of gas bubbles, bubbling the liquid phase medium of the reaction zone. Formation of circulation cells provides an intensive immixture of the liquid and hence intensifies mass exchanged processes and chemical response. In that case, diffusion is not an inhibitory factor in the response process, and the assumption of the first order of a reaction is quite sound. The higher is vortex frequency, the better is immixture quality.

**Conclusion**

It has been obtained that additional factors appear in the reaction zone of reduction reactor owing to formation of a gas phase. They are influencing on the liquid phase density change and modifications of an Archimedean constituent, the value of which is vastly superior to the concentration and temperature ones. Since the rate of bubbles formation and their number depend on temperature and concentration, the immixture and energy exchange processes are interrelated. Immixture is a way of the reagent mass supply and enhancement of the target processes efficiency. Hence, providing conditions for micro-vortex formation is just the way to intensification of mass exchange and target physical and chemical processes.

As equivalent Rayleigh numbers rise, new types of convective movement are developing. This leads to violation of well-ordered stream movement during convection and finally makes convectional liquid movement unsteady, which cause confused or turbulent nature of the liquid movement even with the system placed in a closed space. Taking into consideration the synergetic possibilities in such systems allow to programme control action and more correctly guarantee an effective impact on target processes.

**Resume:**

1. Showed is a mechanism of affecting the reaction zone hydrodynamics by the bubbles of the gas phase, arising on the reduction reaction proceeding.
2. The reaction rate for linearized exponent, presented for the perturbed components, brings the
resulting action to a sum of the temperature and concentration actions.

3. It is ascertained that the gas phase impact is reduced to the temperature and concentration influence, but that is much more effective.

4. It has been analytically demonstrated an existence of hydrodynamic dissipative structures, which provides the reacting melt immixture in a reaction zone.

5. Consequently, an intensifying effect on the mass transfer processes lies mainly in the reduction reaction itself, so given mechanism of affecting, there is a possibility to efficiently control such processes.

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References


