Problems of analysis of thermalphysic processes in a reaction zone of electrothermal reactor

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Analyzed are thermalphysic processes in an ore-smelting electrothermal reactor, which is a reaction bulk with different phase composition, where mechanisms of turbulent energy transfer act together with the physical-chemical target transformations proceeding. Chemical reduction processes proceed when isolating the gas phase, bubbling the melt and intensifying processes of the product making. Independent problems of analysis of thermalphysic processes in a near-electrode crucible reaction zone based on a two-dimensional model are considered. Analytical solutions for describing thermalphysic processes in a reaction zone which characterize conditions of the target product manufacturing are obtained. There are cited the data which define distributions of the Joule heat emission flux density for different modes as well as distribution of temperatures depending on different unit power values. Obtained are analytical solutions for energy metabolism problem under the change of phase condition in a slag tipping mode and equations of diffusion of the reagent being reduced in the area of physical-chemical transformations proceeding. Skull layer formation task is solved. Obtained solutions practically describe all the collection of processes in a reaction zone and can serve as a starting point for numerical approaches to analysis of reduction reactors operating modes. It is discovered that target processes are localized in a near-electrode zone with formation of the crucibles practically unrelated with each other. However, the energy transfer processes broaden an effective area of reactions and should be taken into account during designing and mode control. Neglecting heat efficiency may introduce considerable errors in analysis of the modes.

Key words: electrothermal reactor, thermalphysic process, mathematical model, mathematical physics equations, power distribution of the Joule heat sources, temperature distribution, concentration of reagent distribution over reactor volume, skull layer, near-electrode processes localization.

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Introduction

Electrothermal technology of reduction processes is topical in case of high-temperature conditions of reactions proceeding and requirements for absence of impurities affecting The purity of a reduction product. Processes of energy transfer to reacting components, proceeding within a high-temperature range, should be taken into account when analyzing operating modes of technological reactors. Difficulties of investigating the high-effective reduction modes lie in inaccessibility of a reaction zone and presence of high temperatures. In such conditions, mathematical simulation is almost sole method of analysis parallel with external survey of units operation, consisting in passive registration of control parameters and characteristics of efficiency [1–3]. In case of multiple-factor dependences, preference should be given to deterministic models. Mathematical models are also effectively used for plants of thermal preparation of the raw in the form of pellets and agglomerate [4, 5]. Modelling of electrothermal aggregates is realized in papers [6–12]. Problem solving in analytical form for the whole system of equations is not possible, but approximate analytical dependences may be obtained applying the successive approximations method, when separate equations may be considered to be "frozen" with the use of thermal and physical characteristics averaged over volume of a reaction zone.

The high-temperature reduction reaction zone consisting of a liquid reagent, solid reducing agent (carbon) and gas-core reaction products bubbling the liquid phase, is forming during operating. Rate and character of the reactions in a reaction zone proceeding, raw materials melting rate depend on the heat exchange processes intensity. Heat is supplied to a reaction zone from the working space of reactor owing to Joule heat generation.

In that case, the heat emission intensity mostly depends on the reaction zone heat resistance and heat perception surface evolution. Active liquid movement in a bath arising from bubbling by the evolved gas-core products leads to appearance of convective mechanism for temperature and concentrations equalization over thickness of layers. Enlargement of surfaces of reacting components, which in many respects depends on thermalphysic processes in reaction zone is of great importance for proceeding of reactions. The employed mathematical model is based on the transport coefficients representation in the form of generalized coefficients of heat conductivity and diffusion [13, 14].

Thermophysical processes in a bath of electrothermal reactor for reducing such products as phosphorus, calcium carbide, titanium carbide and the others proceed under the same conditions and are described by identical equations.

Analysis of distribution of energy-release power in a reaction zone of electrothermal reactor

Let us analyze computational model for describing heat emission in an area restricted by dimensions of the reaction zone of radius rp. If specific resistance value doesn't depend on temperature, the electric field potential distribution in the melt of a localized near-electrode zone will look like:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \varphi}{\partial r}\right)+\frac{\partial^2 \varphi}{\partial y^2}=0, \quad (1)$$

with the following boundary conditions:

$$\left.\frac{\partial \varphi}{\partial r}\right|_{r=r_p}=0 \ \ (y\in[0,\infty]);\ \left.\frac{\partial \varphi}{\partial r}\right|_{r=0}=0 \ (y\in[0,\infty]);$$

$$\left.\frac{\partial \varphi}{\partial y}\right|_{y=0}=\psi(r)\ \begin{cases}-\rho e_j & r\in[0,r_e];\\ 0 & r\in[r_e,r_p];\end{cases} \quad (2)$$

$$\bar{\varphi}=\frac{1}{\pi r_e^2}\int_0^{r_e}\varphi(r,0)2\pi r dr=0\ (y=0);$$

where j — density of electrode current; r_e — an electrode radius; r_ρ — the reaction zone radius.

Calculations according to the proposed model show an acceptable qualitative and quantitative conformity of results obtained on the base of mathematical simulation and experimental data [6, 15]. Fig. 1, 2 represent dependences of energy-release power in the reaction zone volume. The process is characterized by sharp decrease of the evolved power subject to distance from electrode, which bring with it localization of target processes in the near-electrode areas.

The obtained distribution of bulk power possesses a reaction capacity stabilization property, which becomes apparent in a distinctive displacement of the volumetric capacity fractions towards an electrode as an rp reaction crucible radius increases. Consequently, on skull growing in melt on the bath walls which is equivalent to rp decrease, there is realized a potential distribution promoting more intense heat emission at crucible borders and preventing from further decrease of reaction space.

An exponential dependence of heat emission over depth of reaction zone takes place. In the general way, the heat emission is localized nearby an electrode. This gives grounds to believe that electrical fields of electrodes in a smelt bath of three-electrode ore-smelting furnaces are slightly interconnected.

Specific electrical resistance of slag differs from that of a coke layer. Analysis shows that heterogeneousness of such a type has slight influence upon the heat sources distribution.

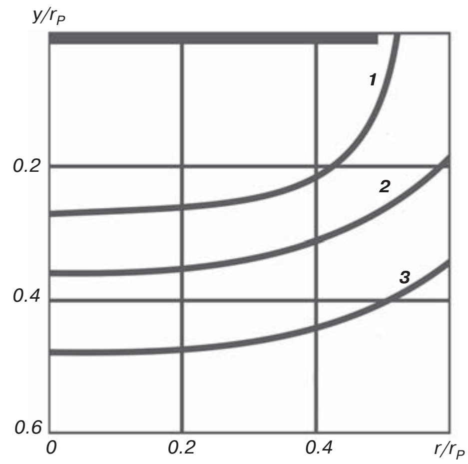

Fig. 1. Distribution of heat emission $qv/(r_e j^2)$ in a reaction zone of the furnace when an electrode radius and a reaction zone radius are in the 0.5 relationship to each other:
1 — 0.4; *2* — 0.2; *3* — 0.1

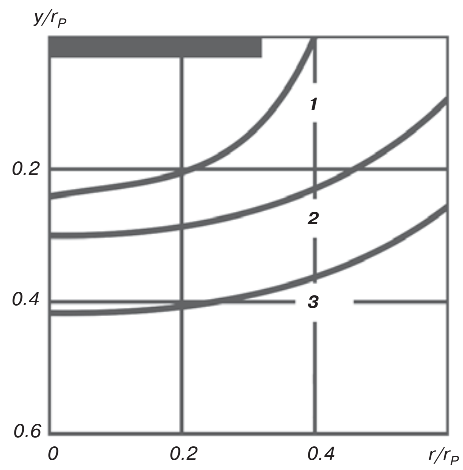

Fig. 2. Distribution of heat emission $qv/(r_e j^2)$ in a reaction zone of the furnace when an electrode radius and a reaction zone radius are in the 0.35 relationship to each other:
1 — 0.2; *2* — 0.1; *3* — 0.05

Analysis of temperature fields in an under-electrode area (coke zone)

Approximate evaluation of temperature fields in a chemical reaction zone is possible with some assumptions of the constancy of reagent concentrations in a reaction volume, of the processes in the melt stationarity and of the heat emission and heat transmission processes independence.

Let us write an equation of heat exchange taking into account the considered assumptions:

$$\lambda_{tr}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)+\lambda_{ty}\frac{\partial^2 T}{\partial y^2}-\rho_l c_l v_l\frac{\partial T}{\partial y}-$$

$$-q_R K_0 \Delta C\frac{f_k}{V_\ell}\exp(-E/RT)+q_{v\ell}=0. \qquad (3)$$

Boundary conditions are as follows:

$$r=0,\ \partial T/\partial r=0;\ y\in[0,h_P];\ r=r_P,$$

$$-\lambda_{tr}(\partial T/\partial r)=\alpha(T-T_L);\ y\in[0,h_P];$$

$$y=0,\ \lambda_{ty}(\partial T/\partial y)=0;\ y=h_P,$$

$$-\lambda_{ty}(\partial T/\partial y)=\rho_g c_g v_g T;\ r\in[0,r_P], \qquad (4)$$

where T — temperature in a reaction zone; λ_{tr} — radial component of anisotropic turbulent thermal conductivity; λ_{ty} — vertical components of anisotropic turbulent thermal conductivity; ρ_l, c_l, v_l, ρ_g, c_g, v_g — density, heat capacity and rate of liquid and gas phase; h_P — height of a reaction zone; S_k — reaction surface.

In that way the heat exchange in anisotropic system with thermal conductivity coefficients differing in vertical and radial directions is analyzed. It is approximately accepted that heat exchange at radial borders of reaction zone is carried out under conditions of skull formation, lower border is insulated, while the heat exchange at the upper border is determined by kiln gases leaving the melt. Estimations show that the heat carry-over with gases considerably exceeds the heat flow by thermal conductivity throw electrode and burden. Heat emission localization in an under-electrode zone enables to approximate a thermal source function as a function of a form close to stepped in radial direction. Moreover, the analysis enables to represent heat generation capacity in a volume unite qve in factorized form, in other words as a product of functions each of which depends only of one coordinate. Since heat exchange in the considered zone is very intensive due to agitation, temperature deviations from some average value should be insignificant. That fact serves as a ground for using a reaction constant decomposition to the Taylor's series with keeping decomposition members of the first order only:

$$a\exp(-E/RT)\approx a\exp(-E/RT_\bullet)\,(1-E/RT)+$$

$$+\,a(E/RT_\bullet^2)\exp(-E/RT_\bullet)T,$$

where $a=q_R k_0 c_\ell(S_k/V_\ell)$; $T_\bullet$ — a carry-over temperature, as which a melting temperature T_L may be used.

Taking into account the accepted assumptions, let us write a heat transmission equation in a dimensionless form in the following way:

$$\frac{\partial^2\theta}{\partial y^2}+\frac{1}{\bar r}\frac{\partial}{\partial \bar r}\left(\bar r\frac{\partial\theta}{\partial \bar r}\right)-Pe\frac{\partial\theta}{\partial y}-\bar b\theta+\bar a+$$

$$+\,\bar q_v\sigma_1(\bar r)\sigma_2(\bar y)=0; \qquad (5)$$

Boundary conditions are as follows:

$$r=0,\ \partial\theta/\partial r=0;\ r=r_P,\ \frac{\partial\theta}{\partial \bar r}=-Bi\theta$$

$$\bar y=0,\ \partial\theta/\partial\bar y=0;\ \bar y=1,\ \partial\theta/\partial\bar y=-Pe_g(\theta+1), \qquad (6)$$

where $\bar y=y/h_P$; $Pe=\rho_l c_l v_l h_P/\lambda_{ty}$; $Bi=\alpha h_P\sqrt{\lambda_{tr}/\lambda_{ty}}/\lambda_{tr}$

$$\bar r=r/(h_P\sqrt{\lambda_{ty}/\lambda_{tr}});\ \bar y=y/h_P;\ Pe_g=\rho_g c_g v_g h_P/\lambda_{ty};$$

$$\bar q v=q_v h_P^2/\lambda_{ty}T_L;\ \theta=(T-T_L)/T_L;$$

$$\bar a=q_{xp}k_0(S_k/V_\ell)c_\ell^{P_2O_5}\exp(-E/RT_L)^2 h_P/(\lambda_{ty}T_L);$$

$$\bar b=\bar a(E/RT_L).$$

Heat generation function dependence of y is expressed in the following way:

$$\sigma_2(\bar y)=\exp[-f(1-\bar y)]=\exp(-f)\exp(f\bar y),$$

where f is an empirical coefficient.

Boundary value problem has been solved by method of finite integral transformations.

Method of finite integral transformations with the use of Hankel transform $\bar\theta=\int_0^1\bar r J_0(\mu_k\bar r)\theta(\bar r,\bar y)d\bar r$, where μ_k — the roots of equation $\mu J_1(\mu)+BiJ_0(\mu)=0$ ($\mu_k>0$), is assumed to be the most effective method of solution for problems with the source in general and dependent on a radial coordinate all the more.

Inversion operation allows us to write a task solution in the following form:

$$\theta=2\sum_{k=1}^{\infty}\frac{\mu_k^2 J_0(\mu_k\bar r)}{(Bi^2+\mu_k^2)J_0^2(\mu_k)}\{c_1\exp[k_1\bar y]+$$

$$+\,c_2\exp[k_2 y]+c_3\exp[fy]\}, \qquad (7)$$

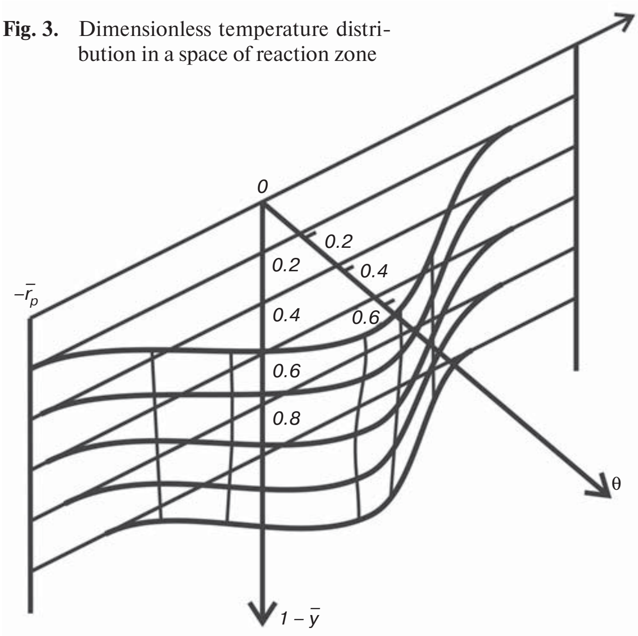

Fig. 3. Dimensionless temperature distribution in a space of reaction zone

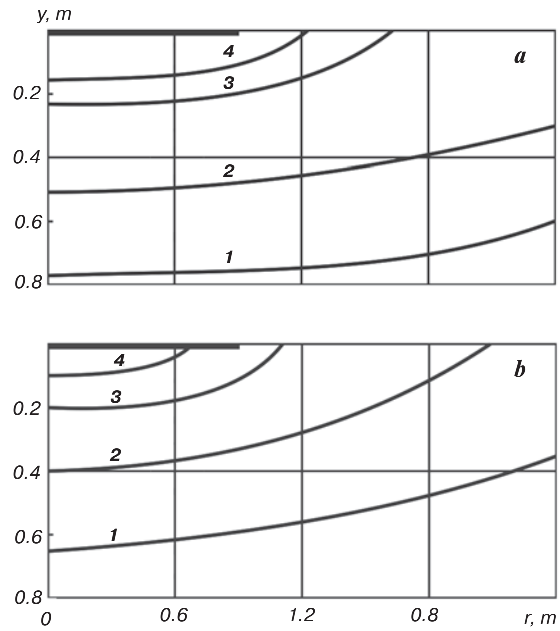

Fig. 4. Temperature field $t(r, y)$ in smelt:
a — furnace power – 72 MW; *b* — 54 MW;
1 — 1570 °C; *2* — 1600 °C; *3* — 1700 °C; *4* — 1900 °C

where $k_{1,2} = 0.5Pe \pm\sqrt{(0.25Pe^2 + \mu_k^2 + b)}$; $c_3 = -\ B/(fPe - f^2 + \mu_k^2 + b)$ — coefficient, which can be found by substituting partial solution into governing equation; $\bar{B} = \bar{q}_v \exp(-f)\int_0^{\bar{r}_P} \bar{r}\, J_0(\mu_n \bar{r}/r_P)\sigma_1(\bar{r})\,d\bar{r}$ — coefficient, which characterized an influence of the thermal source distribution over radius.

The c_1 and c_2 coefficients can be found from boundary conditions.

Temperature distribution over the reaction zone volume is presented in Fig. 3.

For partial modes, under conditions of closed notches and perfectly insulated side lining, the task is reduced to the more simple earlier examined setting.

Calculation results in the form of isotherms for different proportions of electrode and reaction zone dimensions are put in Fig. 4. Shape and location of isotherms qualitatively comply with the results of paper [3].

Heat exchange conditions in the process of skull layer formation in the bath

Deterioration of graphite lining of a furnace is one of important factors affecting reliability characteristics. To protect the graphite lining in the bath, a skull layer is forming. Its thickness is determined by the furnace operation mode that is by heat exchange between the melt and skull film. The skull layer thickness dependence on operating parameters makes it possible to select an operating mode of the furnace, which provides a reliable protection of lining.

Simulation of a skull layer formation at the boundary of the reaction zone process is based on equations of heat transmission in smelt with condition of melting at one of the boundaries.

It is approximately accepted that heat exchange at the boundaries of the reaction zone come from convection with the boundary having melting temperature. It is supposed that the boundary is practically immovable. This allows to intertwine solutions of heat transmission equations written down for distinct areas of the furnace bath without essential distortions of the energy exchange process.

Heat balance at the skull layer melting front can be written in a quasione-dimensional setting, in which a heat-conducting flow through the furnace lining is directed in a radial way only, while heat from the reaction zone is supplied by means of convection from the melt to the skull layer surface, having the melt temperature:

$$\rho_1 L \frac{d\xi}{d\tau} + \alpha(T - T_L) = \lambda(T_L - T_0)/(\xi + \delta), \qquad (8)$$

where ξ — thickness of a skull layer; δ — thickness of a lining layer; λ — skull layer and lining thermal conductivity coefficient.

In case of steady-state conditions and smallness of a graphite lining thermal resistance let us write for thickness of a skull layer:

$$\xi = \lambda(T_L - T_0)/(\alpha T_L \theta)$$

A change of phase coordinate $r(y) = r_P - \xi$, where r_P — radius of a furnace bath.

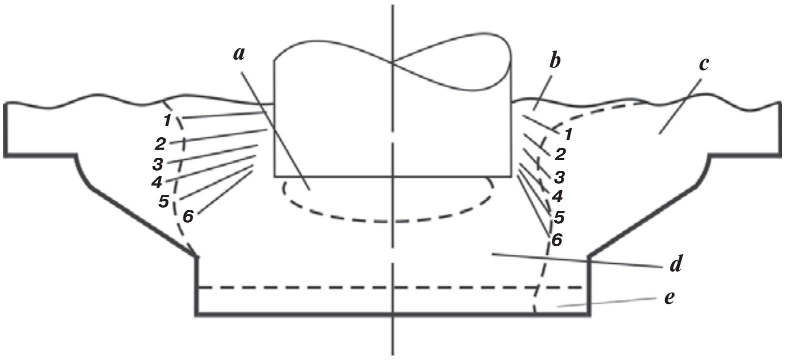

Fig. 5. Sounding results for a furnace of calcium carbide production [3]. Power 60 MW, electrode voltage 130–300 V, maximum current 120 kA, burden descent rate 0.3–0.33 m/h:
a — high-temperature zone; *b* — zone of an active burden materials descent; *c* — zone of a non-descent burden (skull); *d* – zone of a heavy slag (carbide); *e* — smelt of ferro-compounds;
1 — 750 °C; *2* — 1000 °C; *3* — 1250 °C; *4* — 1500 °C; *5* — 1750 °C; *6* — 2000 °C

From equation (7) it follows that temperature value is exponentially descending in depth, that is $\theta \sim \exp(-ky)$, where k — a proportionality coefficient. Then

$$r(y)/r_P = 1 - \xi/r_P \cong 1 - \lambda(T_L - T_0)/(\alpha r_P T_L \exp(-ky)). \quad (9)$$

Thus, the skull layer value is minimal in upper part of a reaction zone and becomes thicker in a hearth zone. This is strengthened by results of probing the furnaces (Fig. 5). The skull boundary in melting zone of carbide furnace in Fig. 5 is in a qualitative sense similar to that of the resulting from calculations. Estimation of an average skull layer thickness at $\lambda = 2.5$ W/mK, $(T_L - T_0) = 100$ K, $\alpha = 200$ W/mK, $T_L = 1100$ K produces a result of 0.28 m, which is close to the skull thickness values of 0.55m, detected during repair of a phosphorous furnace, operation of which has been stopped without slag tipping [15].

However, if skull layer thickness is not too large, then the skull layer failure and smelt direct contact with graphite lining is probable during slag tipping, when the heat emission coefficient is rising steeply on washing a tape drain. That may cause lining erosion and its death. That's why the skull layer thickness analysis at various operating modes of a reaction zone is of great importance for providing a reliable trouble-free resource-saving furnace operation.

Distribution of reagent concentration in a reaction zone

Mass transfer in smelt is also determined by turbulent mechanism in a reaction zone, in which connection the heterogeneousness of reagent concentration over zone volume should be forthcoming. Dissimilar response conditions are stipulated by temperature and concentration of reagent. An additional feature of mass exchange procedures during ore-smelting processes consists in a response surface (in other words, coke particles) vertical displacement. In a frame of reference bounded with the surface of coke particles this is equivalent the melt displacement with the same velocity v_m. Let us consider the mass exchange characteristics influence in a response zone at an average temperature under steady-state conditions. The response surface movement serves as a determining mechanism for vertical mass transfer and the diffusion transportation serve as that on a radius. This makes it possible to write an equation for distribution of concentration, in view of assumptions, in the following form:

$$v_m \frac{\partial c_\ell}{\partial y} = D_t \frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\partial c_\ell}{\partial r}\right) - \psi c_\ell. \quad (10)$$

Boundary conditions are as follows:

$$y = 0,\ c_\ell = c_{\ell 0}(r);\ r = 0,\ \frac{\partial c_\ell}{\partial r} = 0;$$

$$r = r_P,\quad \frac{\partial c_\ell}{\partial r} = 0, \quad (11)$$

where $\psi = S_k K_0 \exp(-E/RT_*)/m_\ell$, m_ℓ — mass of slag in a reaction zone.

That sort of boundary-value problems can be solved for example with the use of Hankel transform:

$$c_\ell(\mu_k, y) = \int_0^{r_P} r c_\ell(r, y) J_0(\mu_k r/r_P) dr. \quad (12)$$

The result is as follows:

$$c_\ell = \frac{2}{r_P^2} \sum_{k=0}^{\infty} \frac{J_0(\mu_k \bar{r}/\bar{r}_P)}{J_0^2(\mu_k)} e^{-q_k y} \times$$
$$\times \int_0^{r_P} c_{\ell 0}(r) r J_0(\mu_k r/r_P) dr, \quad (13)$$

where $q_k = (D_t \mu_k^2/r_P^2 + \psi)/v_m$, c_1, c_{l0} — reagent concentration in slag and furnace charge fed to a reaction zone after charge pieces smelting, correspondingly.

The derived ratios allow to make an approximate estimation of temperature and concentration fields in a reaction zone and to obtain limiting dependences for verifying the computational task solution on determination of reagent concentration.

Calculations of a thermal state of a furnace bath have been carried out according to the suggested algorithm.

Concentration fields for a phosphorous furnace acquired by re-calculation of (13) for various values of coordinates with the use of (7) are presented in Fig. 6 as lines of constant concentration. It follows from the results

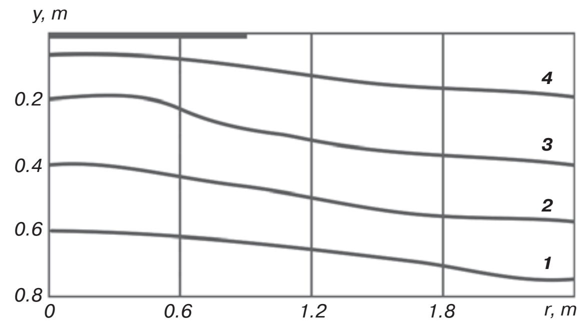

Fig. 6. Distribution of P_2O_5 concentration in a furnace reaction zone $C_{sl}^{P_2O_5}$ (*r*, *y*), kg/kg.
1 — 0.0001; *2* — 0.001; *3* — 0.05; *4* — 0.2

of calculation that the highest rates of the phosphorous reduction reactions take place in near-electrode areas. The coke layer height and specific surface of reducing agent have a pronounced effect on the phosphorous pentoxide concentration.

As temperature rises, an efficiency of a reaction zone increases not only due to acceleration of the chemical reaction, but owing to the response surface growth as well.

Calculations of temperature fields (Fig. 4) carried out for a phosphorous furnace reveal the melt temperature drop throughout the height at various capacities of a reactor. The smelt overheating in an under-electrode area may achieve essential values (Fig. 4). However, a high-temperature domain is also severe limited, in spite of intensive heat transmission.

Analysis of the furnace thermal state in a zone of proceeding of target processes

Analysis of thermal state of a furnace shows that heat exchange is generally localized close to the electrode. This suggests that electric and temperature fields of electrodes in a smelt bath of three-electrode furnaces are slightly interconnected. Total heat emission in a three-electrode ore-thermal furnace can be obtained using an additivity property.

Heat emission intensity is sharply decreasing in depth of a bath. Localization of thermal sources in the near-electrode zones and heterogeneity at different deepening of electrodes are distinctly traced.

Thus, the main part of reaction crucibles is separated in an under-electrode area, and a heat generating layer practically doesn't overstep the limits of a coke zone. Specific electrical resistance of slag differs from that of a coke layer. Analysis shows that heterogeneousness of such a type has slight influence upon the heat sources distribution. A two-dimensional type of the model has allowed us to investigate a spatial distribution of parameters affecting the furnace operation. Calculations of temperature fields in smelt show that the smelt overheating may achieve essential values in an under-electrode area (Fig. 4). The derived concentration fields in a reaction zone give limiting dependences for verifying the computational task solution, for determining the target product concentration in slag at the output of the reaction zone (Fig. 6).

If concentration at the point of entry into a reaction zone is radius-independent, the diffusion transfer losses its significance and the reaction zone becomes a reactor of ideal mixture. Temperature of waste gases determines both reliability of a unit operation and a product quality. Keeping it in the specified limits is one of important tasks for correct choice of an operational mode. Resulting from calculations, the reasons of waste gas temperature rising have been determined. Irregularity of heat emission in a reaction zone stipulates unevenness of temperature distribution in a reaction zone over furnace section, which influences on a gas generation chemical reaction rate and a burden melting rate. As a consequence of that, the primary gas output with the highest temperature is observed in near-electrode zones, where also the principal burden descent takes place, despite the fact that in peripheral zones the burden practically doesn't descend. Such an irregularity results in a high temperature of the waste gases in the near-electrode areas and at the furnace periphery.

A nonuniform slip of electrodes leads to heat emission redistribution over the furnace space along with decrease of its value under the electrode mostly submerged into working zone. This results in augmentation of smelt temperature, which defines the gas temperature. Such local temperature augmentation requires lowering the capacity of the unit which may decrease temperature in other areas lower than condensation point of phosphorous. The temperature field smoothing may be achieved be means of distribution control of the gas flow in a charge zone by changing penetrability of the near-electrode and peripheral zones using their feeding by more fine graded fractions of burden material. This significantly affects the heat exchange and gases temperature distribution [16].

Within the areas peripheral to electrodes the burden is slowly moving and well warming-up. Gases in such areas are not cooling, which increase an average temperature in an under-roof space up to 400–600 ^{o}C. As a whole, temperature of gases under a furnace roof is determined by the furnace parameters, burden properties and granulometric burden composition.

It should be mentioned that irregularities of furnace parameters are prone to self-regulation. In particular, skull formation in peripheral zones removes zones with high temperature out of operation, which makes an inoperative space but forms the reaction crucibles.

Conclusion

Considered is a two-dimensional analytical approach to the thermal state analysis of a reaction zone of electrothermal reduction reactor.

The proposed simplified mathematical model for describing heat exchange in a furnace volume allows to reveal the primary rules of energy metabolism and to bind them with the output mode parameters. So, calculations of an average temperature of gases in an under-roof space of furnaces designed for different power show that rise of the ore-thermal unit power rating leads to lessening the temperature of the gases in an under-roof space. The furnace constructive parameters have an essential influence on thermal conditions by changing gas dynamics and intensity of heat-mass exchange processes.

Examined approach to analysis of electrothermal reactors can be applied to forecasting of operating modes of reactors in the process of designing new high-performance equipment.

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