Tuijin Jishu/Journal of Propulsion Technology
ISSN: 1001-4055
Vol. 45 No. 2 (2024)

Structural Identification of a Mathematical Model for the Processes of Blending and Melting of Copper Concentrates

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Abstract:- This article is aimed at constructing a mathematical formulation of the parametric identification problem for the process of electric melting of copper raw materials. A necessary condition for solving research problems with such a complex object as electric melting is the presence of its mathematical description in the form of a set of relations describing quantitative dependencies between the physical variables of the process (chemical compositions, costs, etc.), as well as generalized technical and economic indicators characterizing the quality of the process (productivity, cost, degree of extraction, specific the cost of materials and electricity, specific losses, etc.) and variables that are inaccessible to direct control and their indirect indicators (indirect control models), the values of extrapolated variables at discrete points in time (predictive models)

Keywords*: mathematical model, structural identification, copper concentrates, physico-chemical processes.*

1. Introduction

The development of a mathematical model (in the form of a set of relations describing quantitative dependencies between the physical variables of the process, chemical compositions, costs, temperatures, generalized technical and economic indicators characterizing the quality of the process, productivity, cost, degree of extraction, specific costs of materials and electricity, specific losses) is necessary during the process of mixing and electric melting, since the mathematical model It is an analogue of a real object, it is necessary when conducting experiments. Such a model can be used in the field of automation of technological processes, in metallurgy, in mechanical engineering, and in industry.

The purpose of this work is to create a structural identification of mathematical models of electric melting of copper concentrates in the technolic process. The structure of the created mathematical model for the technological process is determined based on the study of the hydrodynamic patterns of interaction of material flows in the unit, the conditions and nature of the processes of mass and heat transfer, the kinetics of physical and chemical transformations of substances and is implemented by a system of equations of the material (for substances and melting products) and thermal balances of the technological process with differential or finite relationships between variables [1].

In this case, the most rational is to build a mathematical description of the process in the class of analytical and statistical models. For all that relationships of the variables are described by the equations of material and heat balances taking into account a stoichiometry hydrodynamics and kinetics of process.

In the following works [2, 3] physical and chemical transformations and properties of mattes and slags the ore heat-treating furnaces are described, as well as an example of the distribution of electric and temperature fields of the electric furnace received by method of physical modeling is given.

The operation of an electric furnace is represented by a number of complex physical, physico-chemical and thermal processes occurring as a result of the passage of electric current, melting of the charge, separation of slag, matte in the furnace bath. An electric furnace can be schematically represented as a thermal bath with conductive electrodes dipped into molten slag, a layer of matte at the bottom of the bath. When an electric current is passed through solids or liquids, the latter heat up, i.e. as a result of their resistance, electric energy is converted into thermal energy. In accordance with the method chosen above, the following assumptions are made when determining the structure of the mathematical model, which do not distort the physical picture of the process.

1. The decomposition reactions of higher sulfides and limestone are represented by the following stoichiometric ratios equations (1-5):

$$2FeS_2 \rightarrow 2FeS + S_2 \tag{1}$$

$$2Cu_2FeS_4 \rightarrow 5Cu_2S + 2FeS + \frac{1}{2}S_2 \tag{2}$$

$$2CuFeS_2 \rightarrow Cu_2S + 2FeS + \frac{1}{2}S_2 \tag{3}$$

$$CaCO_3 \rightarrow CaO + CO_2 \tag{4}$$

$$S + 2O_2 = 2SO_2 \tag{5}$$

2. The decomposition reaction ends completely in the zone under consideration (zone I).

3. Heat fluxes at the boundaries of the zone are quasi-stationary.

4. The decomposition of sulfates and other compounds is neglected due to their small amount.

5. Ideal displacement in the solid and gas phases in opposite directions is assumed.

6. Heat transfer by radiation is neglected.

The rates of decomposition reactions of materials can be written as equations (6):

$$U_J = K_j G_j \tag{6}$$

here $K_j = K_{jo} e{-}^{\frac{E}{21}}$ - reaction rate constants determining the dependence of *Kj* on temperature;

Kjo - The pre-exponential multiplier;

E - reaction activation energy;

R - universal constant;

T - absolute temperature.

Let's write down the equations of material and thermal balances for e-sv substances for each of the sections equations (7):

$$(e - FeS_2, Cu_5FeS_4, CuFeS_4, CaCO_3, FeS, Cu_2S, CaO, S_2) \tag{7}$$

The heat balance equation equations (8):

$$(G^1C_s)\frac{dT^1}{d\tau} = G_s\mathrm{C}_sT_s - \sum_{j=1}^{k} bq_j^1\, \nu_j^1 - \varphi^1 C_s T^1 + \lambda_s F(T^2 - T^4) - \alpha_r F(T^4 - T_r) \tag{8}$$

For (the area adjacent to the melting zone) we write:

Equations of material balance for solid matter equations (9):

$$\frac{dG_e^i}{d\tau} = \varphi_e^{i-1} - \sum_{j=1}^{k} \alpha_j \nu_j^i - \varphi_e^i \tag{9}$$

The equation of the material balance of a gaseous substance equations (10):

$$\frac{dQ_r^i}{d\tau} = \varphi_e^{i-1} - \sum_{j=1}^{k} a_j\, \nu_j^i - \varphi_r^i \tag{10}$$

The heat balance equation (11):

$$(G^i C_s)\frac{dT^i}{d\tau} = \varphi^{i-1} C_s T^{i-1} - \sum_{j=1}^{k} bq_j^i\, \nu_j^i - \varphi^i C_s T^i - \lambda_s F^{i-1}(T^i - T^{i-1}) + \lambda_s F^i (T^{i+1} - T^i) + \varphi_r^{i+1} + C_r T^{i+1} - \varphi_r^i C_r T^i \tag{11}$$

Thus, the structure of the mathematical model of zone I, reflecting in the relationship the chemistry of the process (12-21), the equation of kinetics (14), the equation of material (15-16) and thermal (17) balances for the i-th section is represented by the following system of equations:

$$\frac{dG_{FeS_2}^i}{d\tau} = G_{FeS_2}^{i-1} - 2K_1 G_{FeS_2}^i - G_{FeS_2}^{i+1} \tag{12}$$

$$\frac{dG_{CuSFeS_4}^i}{d\tau} = G_{CuSFeS_4}^{i-1} - 2K_2 G_{Cu_5FeS_4}^i - G_{Cu_5FeS_4}^{i+1} \tag{13}$$

$$\frac{dG_{CuSFeS_2}^i}{d\tau} = G_{CuSFeS_2}^{i-1} - 2K_3 G_{CuFeS_2}^i - G_{CuFeS_2}^{i+1} \tag{14}$$

$$\frac{dG^i CaCO_3}{d\tau} = G_{CaCO_3}^{i-1} - 2K_4 G_{CaCO_3}^i - G_{CaCO_3}^{i+1} \tag{15}$$

$$\frac{dG_{FeS}^i}{d\tau} = \frac{\mu FeS}{\mu FeS_2} K_1 G_{Cu_5FeS_4}^i + \frac{\mu FeS}{\mu Cu_5FeS_2} - K_2 G_{Cu_5FeS_4}^i + \frac{\mu FeS}{\mu CuFeS_2} K_3 G_{CuFeS_2}^i - G_{FeS}^{i+1} \tag{16}$$

$$\frac{dG^i Cu_2S}{d\tau} = \frac{5}{2}\frac{\mu Cu_2S}{\mu Cu_5FeS_4} K_2 G_{Cu_5FeS_4}^i + \frac{1}{2}\frac{\mu Cu_2S}{\mu CuFeS_2} K_3 G_{CuFeS_2}^i - G_{Cu_2S}^{i+1} \tag{17}$$

$$\frac{dG_{S_2}^i}{d\tau} = \frac{1}{2}\frac{\mu S_2}{\mu FeS_2} K_1 G_{FeS_2}^i + \frac{1}{4}\frac{\mu S_2}{\mu Cu_5FeS_4} K_2 G_{Cu_5FeS_4}^i + \frac{1}{4}\frac{\mu S_2}{\mu CuFeS_2} - K_{S_2} G_{S_2}^{i+1} \tag{18}$$

$$\frac{dG_{CaO}}{d\tau} = \frac{\mu_{CaO}}{\mu_{CaCO_3}} K_4 G_{CaCO_3}^i - G_{CaO}^{i+1} \tag{19}$$

$$\frac{dG_{CO_2}^i}{d\tau} = G_{CO_2}^{i+1} + \frac{\mu_{CO_2}}{\mu_{CaCO_3}} K_4 G_{CaCO_3}^i - G_{CO_2}^S \tag{20}$$

$$(G^i G_s^i)\frac{dT^i}{d\tau} = \varphi^{i-1} C_s T^{i-1} - \sum_{j=1}^{k} bq_j^i\, \nu_j^i - \varphi^i C_s T^i - \lambda_s F^{i-1}(T^i - T^{i-1}) + \lambda_s F^i (T^{i+1} - T^i) + \varphi_r^{i+1} C_r T^{i+1} - \varphi_r^i C_r T^i \tag{21}$$

The designations are accepted here:

G^i, Q_r^i– the amount of solid and gaseous matter in the i-th section of the zone ($i = 1, \dots, n$);

φ^i, φ_r^i- the amount of solid and gaseous matter passing from the i-th section to the i+1 section;

ν_j^i - the rate of formation of a substance at the i-th site as a result of the j-th reaction;

Q_i - stoichiometric coefficient;

T^i- the temperature in the i-th section of the zone;

C_s- heat capacity of the charge;

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q_j^i - the thermal effect of the formation of a substance at the i-th site as a result of the j-th reaction;

λ_s- the heat transfer coefficient of the charge;

F_i- the surface of the I-th section of the mine;

α_r- coefficient of heat entrainment with gases;

β, σ - constant coefficients;

ν_b - the melting rate of the substance;

μ_e- the molecular weight of the eth substance.

2. Results

Under the action of the heat flow coming from the slag bath zone, the lower surface layer of the charge is heated to the melting point, melts and passes into the furnace bath. At the same time, physico-chemical transformations also occur in the charge layer, slag formation and matte formation reactions occur.

From the above substantial description of the processes of the melting zone and physico-chemical transformations of the charge, it can be seen that the elementary acts of the zone are: melting of the charge, under the influence of convective heat flow from the zone, physico-chemical transformations of the molten charge, slag and matte formation.

When determining the structure of the mathematical model of the zone, we will make the following assumptions about the nature of the flow of elementary acts:

The reactants and temperature in the volume of the zone are evenly distributed.

Chemical reactions of decomposition of higher sulfides, sulfates, carbonates end in the heating zone of the charge.

Chemical transformations in the melting zone are described quite fully by the following basic stoichiometric ratios (22-29):

$$Cu_2S + 6CuO = 4Cu_2O + SO_2; \quad (22)$$

$$4FeS + 6CuO = 3Cu_2S + 4FeO + SO_2; \quad (23)$$

$$FeS + CuO = Cu_2S + FeO; \quad (24)$$

$$Cu_2S + 2Cu_2O = 6Cu + SO_2; \quad (25)$$

$$FeS + 10Fe_2O_3 = 7Fe_3O_4 + SO_2; \quad (26)$$

$$FeS + 3Fe_3O_4 = 10FeO + SO_2; \quad (27)$$

$$2FeO + SiO_2 = 2FeO * SiO_2; \quad (28)$$

$$CaO + SiO_2 = CaO * SiO_2; \quad (29)$$

Chemical reactions (37-44) occur in the molten state and are described by the equations of the homogeneous theory.

The removal of substances from the zone is proportional to their quantity in the zone.

Taking into account assumptions 1-4, the chemical transformations of substances in the N zone can be described by the following kinetic equations.

The reaction rates in the melt will be expressed in general terms (30):

$$v_j^s = K_j \prod_{j=1}^{8} G_{ij} \quad (30)$$

где v_j^s - the speed of the j-th reaction $(j = 1,2, \dots,)$;

Kj - The rate constant j is the reaction whose dependence on temperature is described by the well-known Arrhenius equation.

Then the equations of the material balance for the i-th substance for the melting zone and the main chemical transformations will be written as follows (31):

$$\frac{dG_i}{d\tau} = \gamma_i^s \nu_{\text{пл}} + \sum_{j=1}^{K} a_{ij}\, \nu_j - \alpha_i G_i; \qquad (31)$$

here G_i– the weight amount of the i-th substance in the zone;

γ_i^s- the content of the i-th substance in the charge, taking into account the decomposition reactions of higher sulfides, sulfates and carbonates in zone I;

$\nu_{\text{пл}} = \frac{dG_b^s}{d\tau}$ - melting rate of the charge;

α_i - the proportionality coefficient of the removal of the i-th substance from the zone.

When composing the heat balance equation of the zone, it was taken into account that the charge is melting in the zone with heated slag coming from zone III as a result of free convection, and the following assumptions were made:

1. Melting occurs in a charge layer lowered into the melt.
2. Charge melting is considered as the process of melting a semi-infinite body with continuous removal of the melt from the surface.
3. The area of the furnace walls in the zone is assumed to be constant.
4. Heat sources in the zone are the molten mass coming from the zone and cooling down to the melting point of the charge, exothermic reactions, as well as the physical heat of the incoming charge.
5. Heat is spent on heating the charge, on endothermic reactions, is carried away with substances into the zone, is discharged by the walls of the furnace.
6. Heat losses with gases are considered proportional to the melt.

Thus, taking into account the above assumptions, the equation of the thermal balance of the zone will be written as:

$$G_i C_i^p \frac{dT}{d\tau} = \varphi_s \mathrm{C}_s (t_s - t_s) + \sum_{j=1}^{k} (G_i q_i) - \sum_{j=1}^{K} (G_i q_i) -$$

$$-\frac{\lambda_{\text{ших}}}{\sigma} F_s (t_b - t_s) - \nu_b q_b - \sum_{j=1}^{K} \alpha_r G_r\, C_r t_b; \qquad (32)$$

The temperature in the zone is assumed to be constant and equal (stationary mode), i.e. all excess heat is spent on melting the charge.

Then we get the following expression for the melting rate of the charge (32):

$$\nu_b = \frac{dG_s}{d\tau} = \frac{1}{q_b} \left[\begin{matrix} \varphi_s C_s (t_s - t_b) - \sum_{j=1}^{K} (G_i q_i) - \\ - \sum_{j=1}^{K} (G_i * q_i) - F_s \frac{\lambda_s}{\sigma} (t_b - t_s) - \sum_{j=1}^{K} \alpha_r G_r C_r t_b \end{matrix} \right] \qquad (33)$$

here ν_b – melting rate of the charge, (kg/sec);

G_s - the amount of charge to be melted, (kg);

q_b - specific heat of melting, (Kcal/kg);

φ_s - convective flow from zone III to zone II;

C_s, C_r - the heat capacity of slag and gases, respectively, (kcal/kg*deg);

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t_s, t_b, t - charge, slag and melting temperature, (0^C);

G_i, G_i– the number of i-th substances involved in exothermic and endothermic reactions, (kg);

q_i, q_i- thermal effects of exothermic and endothermic reactions, (kcal);

α_r- coefficient of heat entrainment with gases;

F_s- the surface of the fused slopes (m^2);

Λ – heat transfer coefficient;

σ - the thickness of the charge layer, (m).

The melting point of the charge depends on its composition and can be expressed by the equation (34):

$$t_b = t_b^0 + K_{SiO_2} + K_{CaO}a_{CaO} + K_{FeO}a_{FeO}; \qquad (34)$$

where

$K_{SiO_2}, K_{CaO}, K_{FeO}$- are the coefficients of the equation;

$a_{SiO_2}, a_{CaO}, a_{FeO}$- - accordingly , the content in the charge.

Thus, the mathematical model of the dynamics of physico-chemical processes occurring in the II zone of the electric furnace, reflecting the chemistry of the process, the equations of kinetics, the equations of material and thermal balances in the relationship, is represented by the following system of equations (35-47):

$$\frac{dG_{FeS}^2}{d\tau} = \gamma_{FeS}\nu_b - \frac{4}{6}\frac{\mu_{FeS}}{\mu_{CuO}}K_6 G_{FeS}G_{CuO} - \frac{\mu_{FeS}}{\mu_{Cu_2O}}K_7 G_{FeS}G_{Cu_2O} -$$

$$-\frac{1}{10}\frac{\mu_{FeS}}{\mu_{Fe_2O_3}}K_9 G_{FeS} - \frac{1}{3}\frac{\mu_{FeS}}{\mu_{Fe_2O_3}}K_{10}G_{FeS}G_{Fe_3O_4} - \alpha_{FeS}G_{FeS} \qquad (35)$$

$$\frac{dG_{CuS}^2}{d\tau} = \gamma_{Cu_2S\nu_b} + \frac{3}{4}\frac{\mu_{Cu_2S}}{\mu_{FeS}}K_6 G_{Fes}G_{CuO} + \frac{\mu_{Cu_2S}}{\mu_{FeS}}K_7 G_{FeS}G_{Cu_2O} -$$

$$-\frac{1}{6}\frac{\mu_{Cu_2S}}{\mu_{CuO}}K_5 G_{Cu_2S}G_{CuO} - \frac{1}{2}\frac{\mu_{Cu_2S}}{\mu_{Cu_2O}}K_8 G_{Cu_2S}G_{Cu_2O} - \alpha_{Cu_2S}G_{Cu_2S} \qquad (36)$$

$$\frac{dG_{CuO}}{d\tau} = \gamma_{CuO}\nu_b - 6\frac{\mu_{CuO}}{\mu_{Cu_2S}}K_5 G_{Cu_2S} - \frac{6}{4}\frac{\mu_{CuO}}{\mu_{FeS}}K_6 G_{CuO}G_{FeS} - \alpha_{CuO}G_{CuO}; \qquad (37)$$

$$\frac{dG_{Cu_2O}}{d\tau} = \gamma_{Cu_2O}\nu_b + 4\frac{\mu_{Cu_2O}}{\mu_{Cu_2S}} - K_5 G_{Cu_2S}G_{CuO} - \frac{\mu_{Cu_2O_2}}{\mu_{FeS}} *$$

$$* K_1 G_{FeS}G_{Cu_2O} - 2\frac{\mu_{CuO}}{\mu_{Cu_2S}}K_8 G_{Cu_2O}G_{Cu_2S} - \alpha_{Cu_2O}G_{Cu_2O} \qquad (38)$$

$$\frac{dG_{FeO}}{d\tau} = \gamma_{Feo}\nu_b + \frac{\mu_{FeO}}{\mu_{FeS}}K_6 G_{FeS}G_{CuO} + \frac{\mu_{FeO}}{\mu_{FeS}} *$$

$$K_7 G_{FeS}G_{Cu_2O} - 2\frac{\mu_{FeO}}{d\tau}K_{11}G_{FeO}G_{SiO_2} - \alpha_{FeO}G_{Feo} \qquad (39)$$

$$\frac{dG_{Fe_2O_3}^{II}}{d\tau} = \gamma_{Fe_2O_3}\nu_b - 10\frac{\mu_{Fe_2O_3}}{\mu_{FeS}}K_9 G_{FeS}G_{Fe_2O_3} - \alpha_{Fe_2O_3}G_{Fe_2O_3}; \qquad (40)$$

$$\frac{dG_{Fe_3O_4}^{II}}{d\tau} = \gamma_{Fe_3O_4\nu_b} - 7\frac{\mu_{Fe_3O_4}}{\mu_{FeS}}K_9 G_{Fes}G_{Fe_2O_2} - 3\frac{\mu_{Fe_3O_4}}{\mu_{FeS}}K_{10}G_{FeS}G_{Fe_3O_4} - \alpha_{Fe_3O_4} \qquad (41)$$

$$\frac{dG_{Cu}^{II}}{d\tau} = \gamma_{Cu}\nu_b + 6\frac{\mu_{\mathrm{Cu}}}{\mu_{Cu_2S}}K_8 G_{Cu_2S}G_{Cu_2O} - \alpha_{Cu}G_{Cu}; \qquad (42)$$

$$\frac{dG_{SO_2}^{II}}{d\tau} = \frac{\mu_{so_2}}{\mu_{Cu_2S}} K_5 G_{Cu_2S} G_{Cu_2O} + \frac{\mu_{SO_2}}{\mu_{FeS}} K_9 G_{FeS}$$

$$G_{Fe_2O_3} + \frac{\mu_{SO_2}}{\mu_{FeS}} K_{10} G_{FeS} G_{Fe_3O_4} - \alpha_{SO_2} G_{SO_2} \tag{43}$$

$$\frac{dG_{2FeO*SiO_2}}{d\tau} = \frac{\mu_{2FeO*SiO_2}}{\mu_{SiO_2}} K_{11} G_{Feo} G_{SiO_2} - \alpha_{2FeO*SiO_2} G_{2FeO*SiO_2} \tag{44}$$

$$\frac{dG_{CaO*SiO_2}}{d\tau} = \frac{\mu_{CaO*SiO_2}}{\mu_{CaO}} K_{12} G_{CaO} G_{SiO_2} - \alpha_{CaOSiO_2} G_{CaO*SiO_2} \tag{45}$$

$$\nu_b = \frac{dG_S}{d\tau} - \frac{1}{q_b} \begin{vmatrix} \varphi_s C_s(\tau_s - \tau_b) \\ -\sum_{j=1}^{K}\left(G_i^i q_i^i\right) \end{vmatrix} \tag{46}$$

$$t_b = t_b^0 + K_{SiO_2} + a_{SiO_2} + K_{CaO} a_{CaO} + K_{FeO} a_{FeO} \tag{47}$$

3. Discussion

We assume that this structural identification of the mathematical model developed by us can be used in studying the process, identifying patterns and the influence of various input factors on the output parameters of mixing and melting of copper concentrates, as evidenced by the results obtained. The results obtained allow us to substantiate the possibility of using this model for automated production and technological process control systems.

In addition, due to the complexity of studying the process of charging and electric melting of copper concentrates in industrial conditions, the structural identification of the mathematical model developed by us belongs to the class of epistemological models

4. Conclusions

The resulting system of equations represents the structure of a mathematical model of the melting zone of the charge and physico-chemical transformations.

The melting products formed as a result of melting and physico-chemical transformations of the charge fall into the zone of the slag bath, where heat release and separation of slag and matte occur (zone III), and then, as a result of precipitation, sulfide materials fall into the zone of the matte bath (zone IV).

The structure of the mathematical model of zones III and IV has been restored taking into account the physico-chemical, hydrodynamic and thermal patterns of the process. The physical picture of the process occurring in the considered zones can be presented as follows. The main melting products-matte and slag formed in the melting zone and physico-chemical transformations of the charge enter the slag bath zone, in addition, liquid converter slag poured into the furnace enters the same zone. The process of separating matte and slag is associated with the deposition of molten matte particles in the slag layer of the bath. The successful course of this process depends on the difference in the specific weights of the materials, the viscosity of the slag, the temperature of the melt, etc. These factors largely determine the loss of valuable metals with slags. The loss of copper with waste slag is also influenced by the processes of dissolution and oxidation of sulfides.

The thermal energy required to carry out the process of ore-thermal electric melting is released in the slag bath (zone III) of the furnace as a result of its active resistance to electric current.

When constructing the mathematical model of zone III, the following assumptions were made that do not distort the overall picture of the process.

Research were carried out within the framework of the Grant Financing Project No. AP19679153 “Research and development of a method and technology for creating composite structures with built-in photonic sensors PSBC (Photonic Smart Bragg Composites)” Institute of Information and Computing Technologies of the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan.

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