Neuro-Fuzzy Analysis of Carbonate Dissociation Processes During High-Temperature Roasting of Ore Phosphate Raw Materials

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Abstract: A neuro-fuzzy model is proposed for analyzing the processes of carbonate dissociation during high-temperature roasting of ore phosphate raw materials, considering the complexity and nonlinearity of dependent parameters, the uncertainty of dynamic processes behavior, the features of power-intensive systems for the production of pellets and sinter, the influence of environmental parameters and the variation of ore phosphate raw materials. The conducted studies show the influence of the carbonates content on the intensity of the endothermic reaction of their dissociation in phosphorite pellets. The temperature and heating rate at a known content of carbonates determine the control parameters of the energy-technological process for calcination. The use of the proposed neuro-fuzzy model provides adaptive fuzzy granulation of input parameters, the necessary level of interpretation for the regularity of physical and chemical transformations, as well as an increase in the learning rate of the model and a decrease in the modeling error.

1 INTRODUCTION

Taking into account modern trends in the field of rational environmental management, there is an acute problem of ensuring the required quality of thermal preparation of pelletized ore phosphate raw materials using conveyor roasting and sintering machines, which largely depends on the implementation features of carbonate dissociation processes (Bobkov, Dli & Rubin, 2022).

At the same time, the substantiation of the parameters for the carbonates dissociation processes during high-temperature roasting of ore raw materials is complicated by the following things: a large number of considering factors; the complexity and cost of conducting experimental studies; the need to take into account data of different quality (Meshalkin, Bobkov, Dli, Orekhov & Garabadzhiu, 2022); the need to identify and interpret the regularities of physical and chemical transformations that directly affect the quality of decarbonization and sintering of phosphorite (Puchkov, Dli, Prokimnov & Shutova, 2022).

The choice of rational schemes and optimization of the modes for thermal preparation of ore phosphate raw materials should be based on reliable results using adequate models that reliably reflect the kinetics of the main physicochemical and structural transformations and ensure the interpretability of the processes and research results.

That is why the use (which has already become traditional for solving such problems) of a typical neural network approach in this case is problematic due to the complexity of forming a representative and consistent training sample, a large number of cycles and duration of training; the impossibility to provide the required level of interpretation for the revealed regularities. Moreover, some input variables are determined on the basis of experimental studies, while others are determined by expert means, which significantly complicates the process of building and

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configuration of neural network models (Puchkov, Lobaneva & Kultygin, 2022).

The approach to the hybridization of neural network and fuzzy models is advisable to be used for these features (Elgharbi, Horchani-Naifer & Férid, 2015).

To analyze the processes of carbonate dissociation during high-temperature roasting of ore phosphate raw materials the article proposes to use a CANFIS-type neuro-fuzzy model (CoActive Neuro-Fuzzy Inference System) (Jang, 1993), in which a fuzzy production model is used for parametric configuration (for synaptic weights between neurons and threshold values for neuron activation functions) of the neural network model (Takagi & Sugeno, 1985).

The use of this hybrid neuro-fuzzy model provides, on the one hand, adaptive fuzzy granulation of input parameters and the necessary level of interpretation for the regularities of physical and chemical transformations, and on the other hand, an increase in the learning rate of the model and a decrease in modeling error.

2 CARBONATE DISSOCIATION FEATURES DURING HIGH-TEMPERATURE ROASTING OF ORE RAW MATERIAL

High-temperature roasting of ore phosphate raw materials is accompanied by physicochemical and structural transformations, which primarily include the decomposition of free carbonates, decarbonization of the main phosphate substance and sintering. The completion of these transformations at the stage of thermal preparation of ore raw materials has a significant impact on the technical and economic indicators for the production of phosphorite pellets in conveyor roasting and sintering machines (Meshalkin, Bobkov, Dli & Khodchenko, 2017).

A feature of the carbonates dissociation reactions is considered to be their usual localization in the area of the separation surface between the solid phases of the initial ore raw material and the reaction products. The formation and change of this surface determines the dependence of the reaction rate on time (Puchkov, Sokolov & Fedotov, 2022).

Modeling the processes of dissociation for carbonates during the phosphorite pellets roasting is based on identifying the mechanism of chemical reactions and determining the kinetic parameters for individual stages of these processes by means of a kinetic analysis of homogeneous reactions. This approach is used in works (Bobkov et al., 2022; Meshalkin et al., 2022).

Internal heat transfer in phosphorite pellets is described by a non-stationary heat equation for a ball, considering the endothermic effect of carbonate dissociation reactions: $MgCO_3 \rightarrow MgO+CO_2 - Q_1$ and $CaCO_3 \rightarrow CaO+CO_2 - Q_2$, where $Q_1 = 1{,}21 \cdot 10^5$J/mol – the thermal effect of the decomposition reaction $MgCO_3$, $Q_2 = 1{,}78 \cdot 10^5$J/mol – the thermal effect of the decomposition reaction of $CaCO_3$, which is given by a non-homogeneous equation, closed by the corresponding initial and boundary conditions. The relative degree of the carbonate dissociation reaction is determined by the kinetic ordinary differential equation (Bobkov et al., 2022; Meshalkin et al., 2022). An implicit finite difference scheme was used to solve the system of these differential equations. As a result, a system of linear algebraic equations was obtained, which has an ordered band-diagonal structure (Khaikin, 1996).

Since the process of carbonates dissociation in phosphorite pellets occurs on the conveyor of the roasting machine in a moving dense multilayer mass, the calculation of the calcination kinetics for each pellet is a very time-consuming procedure (considering the significant variation of all kinetic and thermophysical coefficients). Therefore, it is not possible to control this process in a real time mode.

The thermal conductivity of a phosphorite pellet is described by an inhomogeneous differential equation in partial derivatives for a sphere with thermophysical characteristics ρ_m – density, c_m – thermal capacity, λ – thermal conductivity, T_m – pellet material temperature, x – pellet radius coordinate, τ – time, Q – thermal effect, ω – rate of carbonate dissociation (for $MgCO_3$ or $CaCO_3$), $q(\omega, Q)$ – thermal effect of carbonate dissociation reaction:

$$\rho_m c_m \frac{\partial T_m}{\partial \tau} = \frac{1}{x^2} \frac{\partial}{\partial x}\left(\lambda x^2 \frac{\partial T_m}{\partial x} \right) - q(\omega, Q).$$

The degree of conversion η in the reaction of carbonates dissociation (for $MgCO_3$ or $CaCO_3$) is determined by kinetic ordinary differential equations with the corresponding kinetic characteristics: k_0 – permeability coefficient of the corresponding reaction, E – energy of reaction activation, R – universal gas constant:

$$\omega = \frac{\partial \eta}{\partial \tau} = k_0 (1-\eta)^{1.5} \exp\left(-E/RT_m\right)$$

with initial and boundary conditions:

$$\tau = 0,\ T_m = T_{m0},\ \eta = 0,$$

$$x = 0,\ \frac{\partial T_m}{\partial x} = 0,$$

$$x = r,\ -\lambda \frac{\partial T_m}{\partial x} = \alpha \left(T_g - T_m \right)_{x=r},$$

where r – pellet radius; T_g – heating gas temperature; T_{m0} – initial pellet temperature; α – coefficient of the heat transfer from the pellet surface.

3 NEURO-FUZZY MODEL FOR ANALYSIS OF CARBONATE DISSOCIATION PROCESSES

The most consuming (from a computational point of view) is the procedure for calculating the values of η, consequently to set the dependencies $\eta = F\left(k_0, E, T_g, T_{m0}, \alpha, r, \lambda, \rho_m, c_m, \tau\right)$ and build the corresponding model, a CANFIS-type neuro-fuzzy model is proposed to be used, which includes:

- firstly, a neural network model trained, for example, using the back propagation algorithm (Borisov, 2014);
- secondly, a fuzzy model like ANFIS (Adaptive Network-based Fuzzy Inference System) (Mizutani & Jang, 1996; Borisov, Kurilin & Luferov, 2022), implementing Takagi-Sugeno fuzzy inference algorithm (Takagi & Sugeno, 1985).

Note. For clarity, let the input variables of the model be executed:

$$p_1 - k_0,\ p_2 - E,\ p_3 - T_g,\ p_4 - T_{m0},\ p_5 - \alpha,$$

$$p_6 - r,\ p_7 - \lambda,\ p_8 - \rho_m,\ p_9 - c_m,\ p_{10} - \tau.$$

In the neural network model, the neurons of the hidden and output layers perform transformations in accordance with the expressions:

$$y_j = f_j(w_{0j} + \sum_{i=1}^{10} w_{ij} p_i),\ \ j = 1,...,n,$$

$$\eta = f(\beta_0 + \sum_{j=1}^{n} \beta_j y_j),$$

where f_j, f – sigmoidal functions.

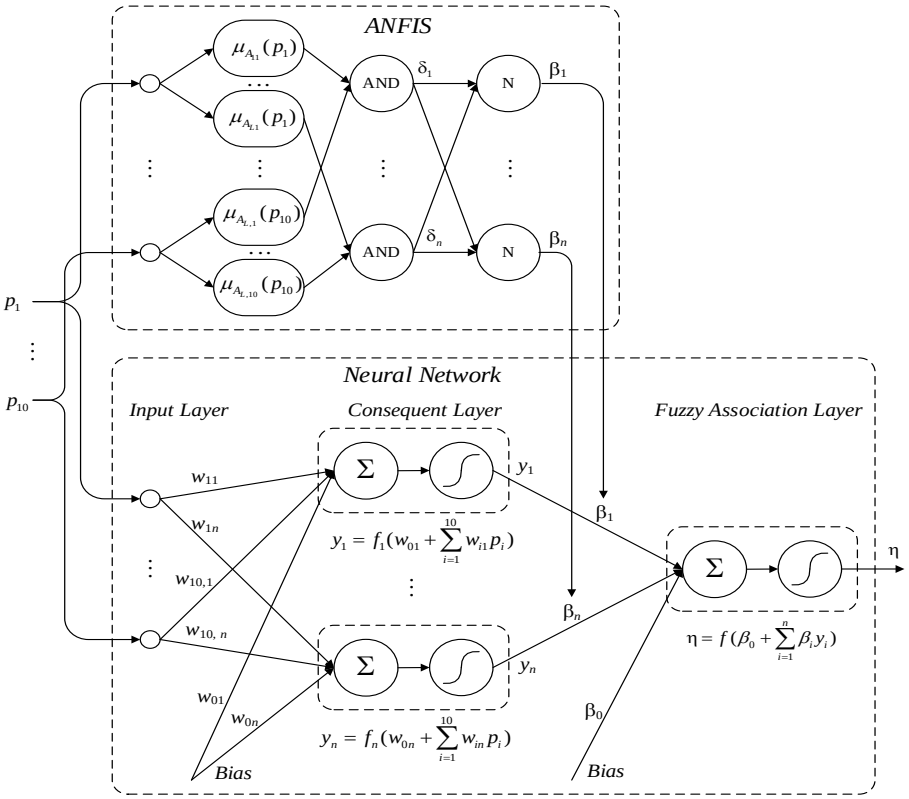

Figure 1: The structure of the neuro-fuzzy model for the characteristics analysis of the thermally activated carbonate dissociation processes.

The weight coefficients β_j ($j = 1, \ldots, n$) for the neuron of the output layer in the neural network model, called *Fuzzy Association Layer*, are formed by the ANFIS model implementing the Takagi-Sugeno fuzzy inference algorithm in accordance with the rules of the form:

Π_i: **IF** p_1 is A_{i1} **AND** … **AND** p_{10} is $A_{i,\,10}$,
THEN $y_i = w_{i0} + w_{i1}p_1 + \ldots + w_{i,\,10}p_{10}$, $i = 1, \ldots, n$.

The fuzzy ANFIS model consists of:

- *firstly*, a layer of elements, whose outputs are the values of membership functions for the set values of input variables, for example:

$$\mu_{A_{ij}}(p_j) = \exp\left(-\frac{1}{2}\left(\frac{x_j - a_{ij}}{b_{ij}}\right)^2\right),$$

where a_{ij}, b_{ij} – adjustable parameters of the corresponding fuzzy set membership function A_{ij};

- *secondly*, a layer of elements that perform the aggregation of the truth degrees for each rule prerequisite according to the *t*-norm operation (for example, the minimum operation):

$$\delta_j = \min\left(A_{j1}(p_1), \ldots, A_{j10}(p_{10})\right), \; j = 1, \ldots, n.$$

- *thirdly*, a layer whose purpose is to form weight coefficients β_j for the neuron of the output layer of the multilayer perceptron:

$$\beta_j = \frac{\delta_j}{\delta_1 + \ldots + \delta_n}.$$

At the same time, the neurons weight coefficients in the hidden layer of the neural network model are parameters for the ANFIS model (Silva-Ramírez & Cabrera-Sánchez, 2021).

Such a "cross" interaction between the neural network model and the ANFIS model can significantly increase the learning rate (Jang, 1993).

The procedure for determining η values using a trained neural network model can be parallelized. The maximum efficiency of the calculation is achieved by parallelizing the calculations into *n* independent processes, the number of which corresponds to the number of neurons in the hidden layer (Tian, Qin, Zhang, Zhao & Yang, 2020).

3 RESULTS OF THE ANALYSIS FOR CARBONATE DISSOCIATION PROCESS

Computational experiments were carried out at various values of the heating gas temperature, the initial content of magnesium and calcium carbonates, the initial temperature, the radius of the phosphorite pellet, and other parameters.

Figures 2 and 3 show examples of the dependences for the values of the degree of conversion η for the dissociation of magnesium and calcium carbonates on the pellet temperature during high-temperature roasting at various heating rates, obtained using the developed model.

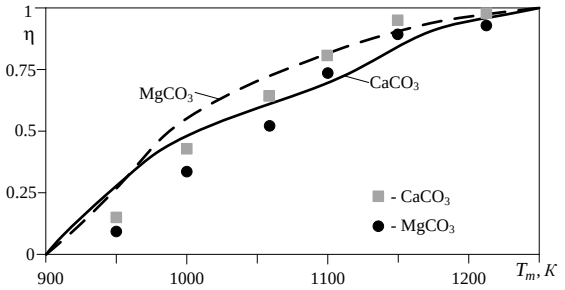

Figure 2: Comparison of the results for natural and computational experiments of the transformation degree in the carbonates dissociation reactions at a heating rate of 0.1(K·s^{-1}).

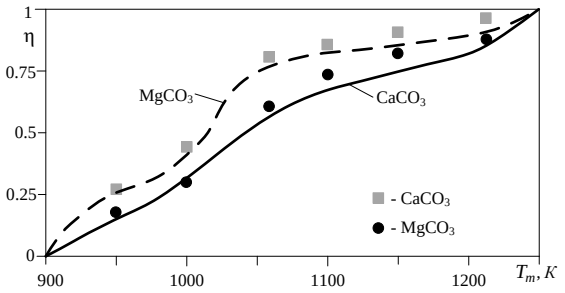

Figure 3: Comparison of the results for natural and computational experiments of the transformation degree in the carbonates dissociation reactions at a heating rate of 0.4(K·s^{-1}).

The data analysis on the characteristics for thermally activated processes of carbonate dissociation during high-temperature roasting of phosphorite pellets, obtained from the calculated results of hybrid fuzzy neural network modeling, correspond to experimental data, which confirms the adequacy of the proposed model.

4 CONCLUSIONS

Comparative evaluation of the built dependences with dependences based on experimental data allows concluding that the developed neuro-fuzzy model is adequate and the modeling results of carbonate dissociation processes during high-temperature roasting of ore phosphate raw materials are reliable.

The use of the proposed neuro-fuzzy model provides adaptive fuzzy granulation of input parameters, the necessary level of interpretation for the regularities of physical and chemical transformations, as well as an increase in the speed of model learning and a decrease in modeling error.

The results obtained will be used to exclude the negative phenomena of softening and destruction of pellets due to the reactions of carbonate dissociation and the formation of new phases. The considered neuro-fuzzy model will also allow taking into account the arising temperature gradient in the pellets caused by the occurrence of endothermic reactions of carbonate dissociation.

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