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The Application of Mechanistic Mathematical and Connectionist Models in the Control of Biotechnological Processes in the Context of Refractory Gold-Arsenic Sulphide Ores Concentrates Oxidation

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Problems related to the control of complex biotechnological processes were considered on the example of biooxidation of refractory gold-arsenic sulphide concentrates for the subsequent gold recovery. Two possible approaches to the problem were considered: a) building "mechanistic" mathematical model and b) applying neural network model. An attempt to construct a mixed mechanistic-phenomenological model using various combinations of formulas given in literature and general description of bioleaching processes has given not satisfactory result. The models were able to describe only the general properties and trends of the process. Neural network analysis of time series of the bioleaching process has revealed dependences between the process, control parameters, and feed composition. Obtained 10% level of the forecast error (MAPE) is quite satisfactory if compare with the forecasts of any natural ecosystem. It can be argued that the relatively low complexity of neural network indicates the possibility of developing a fairly simple mechanistic model of the bioleaching process.

Keywords: bioleaching prediction, neural network analyses of biotechnological processes.

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Применение механизменных математических и нейросетевых моделей для управления биотехнологическими процессами на примере окисления концентратов тугоплавких золото-мышьяковых сульфидных руд

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Проблемы, связанные с контролем сложных биотехнологических процессов, были рассмотрены на примере биоокисления тугоплавких золото-мышьяковых сульфидных концентратов для последующего извлечения золота. Проанализированы два возможных подхода к проблеме: а) построение «механистической» математической модели и б) применение нейросетевой модели. Попытка построить смешанную механистическо-феноменологическую модель с использованием различных комбинаций формул, приведенных в литературе, и общего описания процессов биовыщелачивания дала неудовлетворительный результат. Модели смогли описать только общие свойства и тенденции процесса. Анализ временных рядов процесса биовыщелачивания с помощью нейронной сети выявил зависимости между протеканием процесса, параметрами управления и составом минерального субстрата. Полученный 10%-ный уровень ошибки прогноза (MAPE) является вполне удовлетворительным, если сравнивать его с прогнозами любой природной экосистемы. Можно утверждать, что относительно низкая сложность нейронной сети указывает на возможность разработки довольно простой механистической модели процесса биовыщелачивания.

Ключевые слова: прогнозирование биовыщелачивания, нейросетевой анализ биотехнологических процессов.

Introduction

Traditional biotechnology is intended for the production of various valuable substances and products using natural biological objects (microorganisms, plant and animal cells), parts of cells (cell membranes, ribosomes, mitochondria, chloroplasts) and processes. Since these biological objects are very complex, their behavior depends on many factors, and the response, as a rule, is nonlinear, then the management of biotechnological processes is a challenging objective. Effective control is impossible without a high-quality forecast of the response of the controlled system to external impact.

Forecasting the behavior of the system can be carried out using two approaches:

a) building "mechanistic" mathematical model, which potentially able to forecast system response to impacts, which have not been faced during its exploitation;

b) applying regression model, which reproduces the regularities of the biotechnological process identified through statistical analysis of technological data.

We consider problems related to the control of biotechnological processes on the example of biooxidation of refractory gold-arsenic sulphide concentrates for the subsequent gold recovery.

Bioleaching process description

The process of bioleaching is the gradual oxidation of sulfur-containing minerals, carried out by the chemolithotrophic bacterial community, during which microscopic gold particles are released. Bioleaching at Olimpiada Mining Processing Complex is being carried out at special tanks arranged in lines of sequential oxidation.

The main members of the association of chemolithotrophic microorganisms in the pulp are: *Sufobacillus olympiadicus*, *Ferroplasma acidiphilum*, and *Leptospirillum ferrooxidans*. The first microorganism is a mixotroph; it needs small amounts of organic substances for the oxidation of inorganic substrates. Without organic substances, this major part of the microorganisms association dies and lysed. Archea *F. acidiphilum* is autotrophic, but it needs vitamins and small amounts of some organic substances. *L. ferrooxidans* does not need organic substances and can supply organic substances (exometabolites) to the first two members of the association.

The main processes occurring in the reactors are described by the following chemical equations (Sovmen et al., 2007).

Pyrrhotite:

$$FeS + 2Fe^{3+} = 3Fe^{2+} + S^0.$$

Pyrite:

$$FeS_2 + 14Fe^{3+} = 15Fe^{2+} + 0{,}34S^0 + 1{,}66H_2SO_4.$$

Arsenopyrite:

$$FeAsS + 5Fe^{3+} = 6Fe^{2+} + S^0 + As^{3+}.$$

Antimonite:

$$Sb_2S_3 + 21Fe^{3+} = 21Fe^{2+} + 0{,}5S^0 + 2{,}5H_2SO_4 + Sb^{3+}.$$

The reactions catalyzed by bacteria are summed up in the following form:

$$4Fe^{2+} + O_2 + 4H^+ = 4Fe^{3+} + 2H_2O. \quad (1)$$

$$2S^0 + 3O_2 + 2H_2O = 4H^+ + 2SO_4^2. \quad (2)$$

It is important to note that the oxidation of sulfur, unlike the oxidation of Fe^{2+}, is carried out by bacteria attached to the surface of the pulp particles. The distribution of ferrobacteria between the free and attached states is unknown, and only the biomass of free bacteria is measured. Which of the forms contribute to the main increase in biomass is also still unknown.

In addition, there is an electrode interaction between minerals in the system, which can block the oxidation of minerals standing to the right of the potential scale: pyrrhotite → arsenopyrite → pyrite, which leads to a certain order of oxidation of sulphides in the flotation concentrate.

An attempt of mechanistic mathematical model building

Presented above far from complete list of processes equations demonstrates the

complexity of processes occurring in the bioreactors' pulp. In addition the situation is complicated by the fact that up to the present time an adequate description of the dependence of the specific growth rate of bacteria on cultivation conditions has not been obtained (Ojumu et al., 2005). Different formulas are proposed for different conditions, and even if we assume that these formulas describe the system adequately, a problem of determining the limits of applicability of these conditions and the way of transition to a model from one formula to another still remains.

Nevertheless, the mechanistic model gives a huge advantage over the regression model – this model allows to predict the behavior of the system even under conditions that were not previously observed. Therefore, an attempt was made to construct a mixed mechanistic-phenomenological model using various combinations of formulas given in literature (Bentel et al., 1999; Beolchini, Veglio, 1999; Bircumshaw et al., 2006; Breed et al., 1997; Breed et al., 2000; Kulebakin et al., 1974; Kuzmanovska et al., 1999; Liu et al., 2004; May et al., 1997; Ojumu et al., 2005; Sovmen et al., 2007; Sylvie et al., 2006; Wang, 2007; Zheng et al., 1986).

This great variety of description of both the chemical and biological stages of leaching indicates both high lability and multivariate implementation of these processes under different conditions and insufficient knowledge of these mechanisms. The models shown in the above-mentioned literature satisfactorily describe either individual stages of the leaching process, or the oxidation kinetics of the monomineral substrate, or the stationary state of the process. At the same time, technological processes almost always are in a transitional state, since the mineral composition of the pulp fed to the manufactoring lines is constantly changing.

An attempt of mathematical model building was made for testing the applicability of bioleaching models known from the literature to the description of experimental data obtained by biooxidation of the Olimpiada deposit flotation concentrates. The community of bacteria with different growth rate dependences on Eh and pH is considered (Hansford, 2005). The electrode interaction between the minerals described above was also taken into account.

To illustrate the complexity of the system, one of the investigated models is shown (Eq. 3).

$$
\begin{cases}
\dfrac{dS_i}{dt} = -kf_i(F_3,F_2,A)S_i - \dfrac{1}{Y_1}\nu_i(S_i,X_i,A,As)X_i \\
\dfrac{dF_3}{dt} = \dfrac{1}{Y_0}\mu(F_2,F_3,A,As)X_0 - \sum_i C_i kf_i(F_3,F_2,A)S_i \\
\dfrac{dF_2}{dt} = \sum_i \left(\dfrac{1}{Y_1}\nu_i(S_i,X_i,A,As) + D_i kf_i(F_3,F_2,A) \right) S_i - \dfrac{2}{Y_0}\mu(F_2,F_3,A)X_0 \\
\dfrac{dS}{dt} = kf_1(F_3,F_2,A)S_1 - \dfrac{1}{Y_s}v(S,X_S,A)X_S \\
\dfrac{dA}{dt} = \sum_i B_i kf_i(F_3,F_2,A)S_i + \dfrac{1}{Y_s}v(S,X_S,A)X_S - \dfrac{0.5}{Y_0}\mu(F_2,F_3,A)X_0 - k_s F_3 A \\
\dfrac{dX_0}{dt} = \mu(F_2,F_3,A)X_0 - k_{on}X_0\sum_i S_i + k_{out}\sum_i X_i - k_d X_0 \\
\dfrac{dX_i}{dt} = v(S_i,X_i,A)X_i + k_{on}S_i X_0 - k_{out}X_i - k_d X_i
\end{cases}
, \quad (3)
$$

where

$$\mu(F_2,F_3,A,As)=\frac{\mu_0 F_2}{F_2+K_M F_3}\cdot\frac{A}{K_1+A+K_i A^2}\cdot\frac{1}{1+(K_i As)^2}$$

is specific growth rate of free bacteria;

$$\nu(S,X,A,As)=\mu_2(K_S S^{\frac{2}{3}}-X)\cdot\frac{A}{K_2+A+K_i A^2}\cdot\frac{1}{1+(K_i As)^2}$$

is specific growth rate of the attached bacteria;

$kf(F_3,F_2,A)=\frac{VF_3}{(a+bF_3+F_2+cF_3A)^{\frac{3}{2}}}$ is leaching rate constant depending on Eh and pH; S_1 – FeS; S_2 – FeAsS; S_3 – FeS_2; F_3 – Fe^3; F_2 – Fe^{2+}; S – S^0; A – H_2SO_4; X_0 is nonsymbiotic bacteria; X_i are attached to the corresponding substrate forms of microorganisms. The meaning of other notations is clear from the context.

The parameters of the model were chosen in accordance with published data or the best match to experimental kinetic curves obtained for simplified composition of the pulp.

It turned out that the models constructed in this way describe only the general properties and trends of the process. In particular, they can reproduce indicative duration of transition processes, course of changes in electro-chemical potential and pH for the considered flotation concentrate types, and the response to full reactor loading.

The model is failed. Long live the model!

We have to admit that the building of a mechanistic model for describing the real technological process is a longshot. It is naturally to ask: "Is everything really so bad?", "Is it possible to find another way to solve the problem of effective control?"

At this situation we have to make sure that the set of measured and control parameters is sufficient to predict the behavior of the system. If there are any consistent patterns between the inputs and outputs, then one can speak of a cause-effect relationship and the possibility of modeling the system. As an example, typical dependences of biomass amount in a reactor on two process parameters is shown on Fig. 1. As can be seen from the figure, a wide range of values of the output corresponds to the same value of the input parameter. This difference naturally is not a consequence of a measurement error, but is the manifestation of other parameters influence. Obviously this problem cannot be solved by simple pair wise comparisons and two-dimensional regression equations. It is necessary to use multidimensional nonlinear regression models.

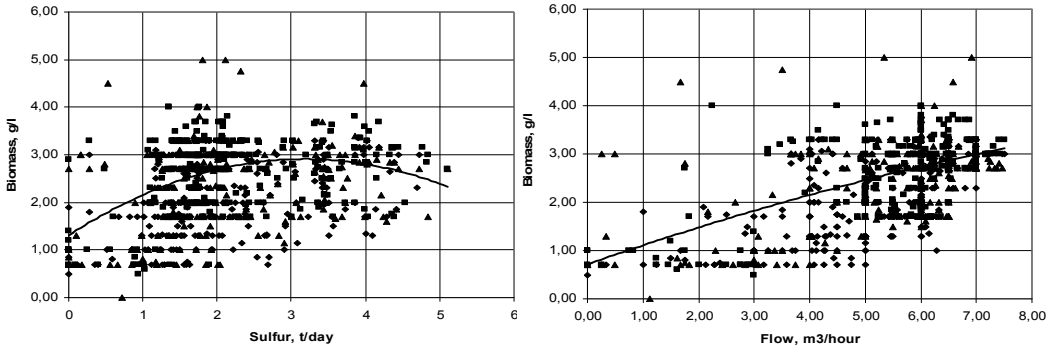

Fig. 1. Typical dependences between bioleaching process parameters. Cube, rhombus, and triangle represent data from 1st, 2nd and 3rd reactors of the technological line, respectively. Curves represent quadratic approximation of the 1st reactor data

One of the effective approaches to detection of hidden dependencies is neural network analysis. Neural networks (for example, Khaikin, 2006) are capable of carrying out multidimensional nonlinear regression, and, unlike most regression approaches, there is no need to specify a prospective pattern of functional dependence, which will be adjusted to the available experimental data.

A possible methodologically promising approach is: 1) description of the bioleaching processes dynamics by means neural networks; 2) carrying out the reduction of the neural network complexity maintaining the quality of the system description; 3) evaluating by this the order of complexity of the system. Having information about the system's complexity level, it is possible to start building mechanistic mathematical model.

A similar methodology was used to construct a model of soil formation. Attempts to build a compartmental soil model (Bartsev et al., 2012b) led to a very complicated model with a large number of adjustable parameters. The neural network analysis of the dependences of soil parameters showed that the pedotransfer function can contain not 16, as it was initially, but only two or three input parameters (Bartsev et al., 2012a). It was an obvious indication of the low dimensionality of the required mathematical model. This result allowed to substantiate and formulate the goal of constructing an extremely simple mathematical model of soil formation, adequately describing the experimental data (Bartsev, Pochekutov, 2015, 2017).

Neural network model of bioleaching process

In this paper a neural network add-on to MS Excel developed at the Institute of Biophysics SB RAS (Simonov et al., 2002) was used. The functioning of the network is described by the following formula:

$$y_k = a_k\left[\sum_i \sin\left(\sum_j x_{ij} A_j + b_{ik}\right)\right] + c_k$$

where $\{y_k\}$ – multiple outputs of neural network; $\{A_j\}$ – multiple inputs; $\{x_{ij}\}$, $\{b_{ik}\}$, $\{a_k\}$, $\{c_k\}$ set of adjustable neural network parameters; k – neural network output number; i – neuron number; j – neural network input number. In fact, the structure of this neural network produces the decomposition of an arbitrary function into a finite trigonometric series with adjustable frequencies.

The use of neural network methods makes it possible to reveal the various dependencies present in the initial data. The accuracy of the neural network forecast can be limited by the following reasons: 1) the impact of factors which are not taken into account in working journals; 2) the sensitivity (instability) of the biological system itself to small perturbations; 3) unregistered or unaccounted actions of personnel, as well as log errors.

The neural network model was trained to predict the amount of free biomass as a parameter affecting the total process. As a quantitative measure of the quality of the forecast well known mean absolute percentage error (MAPE) was used. Since the duration of the biooxidation process is approximately 120 hours (Sovmen et al., 2007), then no sense is to use data older than four days.

Processes of different complexity require different numbers of adaptive elements of the neural network – neurons for description. Experiments showed that with the increase in the number of neurons up to 10 neurons the quality of the forecast increases, although not very significantly.

Neural networks were trained to predict biomass for 12 hours ahead based on current process state, then the same plus the state of 12 hours before the current state. The 12-hour interval is chosen because biomass, which is

predicted by a neural network, is measured once per shift. Experiments showed that increasing the tracking time from 12 to 24 hours increases the accuracy of the forecast, but a further increase of tracking time gives a significantly smaller increase in accuracy (Fig. 2). It can take place due to the growth of population has no inertia, no memory and current state mostly determines further dynamics.

The next step of investigation was aimed to check the sameness of the input-output dependences of different reactors. It was shown that the neural network model trained to predict dynamics of one reactor can be used to predict the dynamics of another reactor. The quality of "unfamiliar" reactor forecast is only slightly worse than quality of "familiar" reactor forecast. A similar result was obtained in predicting the dynamics of a number of other reactors. Generally, quality of forecasting the most important process parameters is presented on Fig. 3.

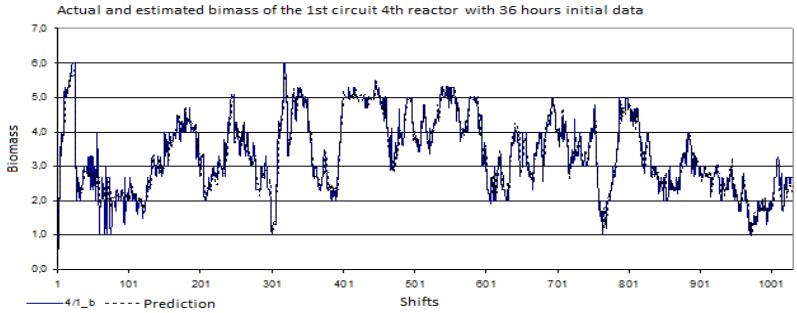

Fig. 2. Biomass prediction quality assessment in the 1st circuit 4th reactor for the next 12 hours (shift) using additional 12 and 24 hours data. The average relative deviation is 8.2%

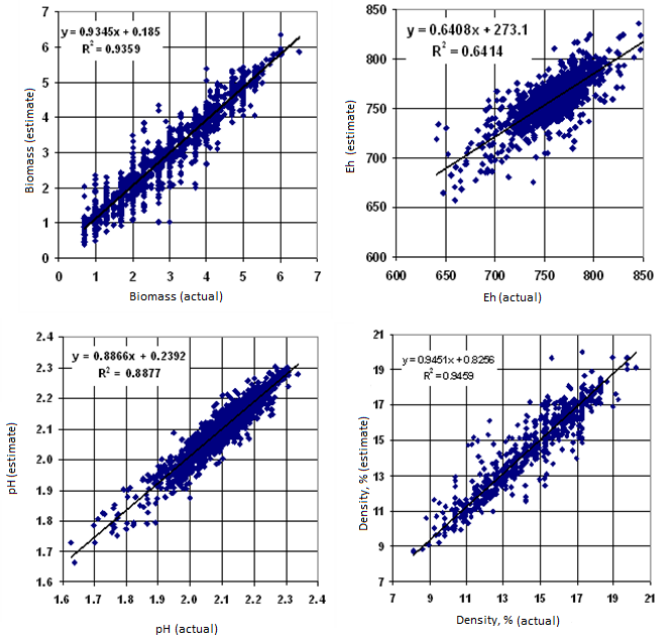

Fig. 3. Diagrams of correspondence between actual data and neural network forecast

It can be seen that the quality of parameters forecasting can be estimated as quite satisfactory.

This result gives serious reasons to assert that the key mechanisms which determine the process dynamics are, firstly, rather simple, and secondly, fairly stable for building mathematical models. Moreover the neural network software allows to evaluate which factors affect the technological process more, and which to a lesser extent. In the given case neural network selected amount of sulfur and iron in pulp as the most affecting factors among 16 others.

Conclusions

Neural network analysis of time series of the biotechnological process made it possible to reveal regularities that reflect the dependence of flow of the process on control parameters and feed composition. Obtained 10% level of the forecast error (MAPE) is high enough if compare with the forecasts of any natural ecosystem. Even at this stage of the study it can be argued that the relatively low complexity of the neural network (10 neurons) and small number of significant input factors indicates the possibility of developing a fairly simple mechanistic model of the bioleaching process.

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