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Mathematical Modeling of Chemical-Technological Processes During the Development of Various New Alloys

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Abstract. This article analyzes that the creation of mathematical models of chemical-technological processes during the development of various alloys is supported to obtain promising new alloys in the foundry industry. Mathematical models have been developed and analytically implemented using linear algebra methods. Numerical values were determined and graphs of changes in the required parameters were constructed. The development and analytical implementation of a mathematical model of the process makes it possible to simplify practical research, and it is possible to predict the results of subsequent experiments. This serves as the basis for the automation of chemical technological processes in the production of non-ferrous metals and alloys.

Keywords: mathematical modeling, chemical-technological process, synthesis and application, non-ferrous metals, new alloy.

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Математическое моделирование химико-технологических процессов в ходе разработки различных новых сплавов

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Аннотация. В статье проанализировано, что создание математических моделей химико-технологических процессов в ходе разработки различных сплавов поддерживается для получения перспективных новых сплавов в литейном производстве. Разработаны и аналитически реализованы математические модели методами линейной алгебры. Определены числовые значения и построены графики изменения искомых параметров. Разработка и аналитическая реализация математической модели процесса позволяют упростить практические исследования, можно спрогнозировать результаты последующих экспериментов. Это служит основой автоматизации химико-технологических процессов в производстве цветных металлов и сплавов.

Ключевые слова: математическое моделирование, химико-технологический процесс, синтез и применение, цветные металлы, новый сплав.

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Introduction

Globalization processes are accelerating at a rapid pace at the present time. As a result of these processes, the development of scientific foundations and mechanisms of modern innovative technologies as well as the introduction of these technologies into industrial production face new challenges. It is well known that significant scientific results cannot be obtained within one scientific engineering direction. The integration of fundamental and engineering disciplines is undeniable in obtaining new scientific results and substantiating scientific directions in this regard. In particular, the integration of theoretical mechanics, mathematics, and the theory of mechanisms and machines is a very urgent task for the development of general mechanical engineering and materials science.

A powerful lever for the development of theoretical foundations, designs, and innovative technologies in engineering materials science is the correct substantiation and formulation of the problem for the use of analytical studies, in particular, mathematical modeling. As you know, the basis of the method of mathematical modeling is algorithmization. Mathematical modeling is the study of phenomena, processes, systems, or objects by building and studying their models. These relationships are usually presented in the form of equations. Analytical, simulation, numerical, functional, and matrix mathematical models are known.

Based on an analytical review of world and domestic literature on engineering materials science, it was found that in many studies of the authors, insufficient attention is paid to the development of mathematical models of the process under study. Modeling of foundry production is carried out based on analytical and numerical methods. To compile a mathematical model, it seems necessary to be able to combine theory and practice to solve engineering problems; choose measuring instruments; use the basic concepts, laws, and models of thermodynamics, chemical kinetics, heat, and mass transfer. In addition, fundamental knowledge of differential and integral calculus; the theory of differential equations, and others.

Experimental

Scientists of Uzbekistan and Tajikistan have developed technologies for the high-temperature processing of industrial slags and wastes, separation processing in electric furnaces and a technology for extracting metals from liquid slag. Let's give some examples [1–5]. In addition, studies have been carried out on the anodic behavior and oxidation of the Zn22Al alloy doped with scandium, yttrium and erbium. At the same time, reliable protection against the corrosive effects of the agents in which they operate is necessary [6–11]. In the practice of protecting semi-finished steel products from corrosion, zinc-aluminum coatings such as “galfan” (Zn5Al, Zn55Al) and “galvalum” (Zn55Al-1.6Si) are currently used in various aggressive environments [12–24].

When developing a new generation of mechanisms in mechanical engineering materials science, the use of new and special alloys using foundry technology requires taking into account the primary mechanical, physical and chemical qualities of the object to build a mathematical model of the technological process. To develop a new stable nanostructured material based on an alloy, it seems necessary to select an appropriate method of mathematical modeling while taking into account the technological process. Below are the tasks for the development and analytical implementation of the mathematical model.

In numerical programming problems with a wide range of applied problems, the extremum of a function (objective function) is determined which borders on a system of linear equations and inequalities. The mathematical model of the general linear programming problem has the form:

$$
\begin{aligned}
& f(x_1, x_2, \ldots, x_n) = \sum_{i=1}^{n} c_i x_i \to \min(\max), \\
& \sum_{j=1}^{n} a_{ij} x_j \le b_i, \; i = 1, 2, \ldots, k, \\
& \sum_{j=1}^{n} a_{ij} x_j = b_i, \; i = k, k+1, \ldots, l,
\end{aligned}
\tag{1}
$$

$$\sum_{j=1}^{n} a_{ij}x_j \geq b_i,\ i = l+1, l+2, ..., m,\ x_j \geq 0,\ j = 1, 2, ..., p,\ p \leq n.$$

In other words, this task is reduced to the task of qualitative assessment of economic, technical technological processes and determination of optimal solutions. If problem (1) has solutions, then the objective function reaches an extremum.

We explain this problem with the following problem. Suppose a metallurgical plant produces three types of alloys from raw materials A and B. The percentages of raw materials in the alloys are presented in the table below. In total, the plant has 7 tons of raw materials of type A and 17 tons of raw materials of type B. A ton of the first alloy costs 1.5 million conventional units, the second – 1.6 million conventional units, the third – 1.2 million conventional units. In this case, the need for the third alloy should not exceed 12 tons, and the need for the first alloy should not be less than 5 tons. The question is, how many tons of each alloy should be produced to achieve maximum economic efficiency?

№ Alloy / Alloy Type	1	2	3
А	8 %	17 %	20 %
Б	92 %	83 %	80 %

To solve the problem, it is necessary to develop a mathematical model. In accordance with the general model (1), we introduce the target function:

$$f(m_1, m_2, m_3) = 1,5m_1 + 1,6m_2 + 1,2m_3 \to \max. \tag{2}$$

The conditions set in the task require the implementation of the following inequalities:

$$\begin{aligned} &0,08m_1 + 0,17m_2 + 0,2m_3 \leq 7, \\ &0,92m_1 + 0,83m_2 + 0,8m_3 \leq 17, \\ &m_1 \geq 5,\ m_2 \geq 0,\ 0 \leq m_3 \leq 12. \end{aligned} \tag{3}$$

To solve problems (2) and (3), the MathCAD method will build the following sequence of operations:

$$\begin{aligned} &m_1 := 5 \quad m_2 := 9 \quad m_3 := 10 \\ &f(m_1, m_2, m_3) := 1,5m_1 + 1,6m_2 + 1,2m_3 \end{aligned} \tag{4}$$

Then we have

$$\begin{aligned} &m_1 \geq 5,\ m_2 \geq 0,\ 0 \leq m_3 \leq 12 \\ &0,08m_1 + 0,17m_2 + 0,2m_3 \leq 7 \\ &0,92m_1 + 0,83m_2 + 0,8m_3 \leq 17 \end{aligned} \tag{5}$$

$$\begin{aligned} &P := \max imize(f, m_1, m_2, m_3) = \begin{pmatrix} 5 \\ 6,15 \\ 12 \end{pmatrix} \\ &f(P_0, P_1, P_2) = 31892 \end{aligned} \tag{6}$$

Thus, we can conclude that when the first alloy is generated, 6.15 tons of the second and 12 tons of the third alloy will achieve the greatest economic effect (31,892 million conditional units). From synthesized new alloys, machine parts are made.

Now we consider the issue of assessing the change in the percentage of oxygen in the alloy by changing the amount of aluminum in the electrode using mathematical modeling.

We determine the percentage of oxygen in the alloy corresponding to a change in the amount of aluminum in the electrode depending on the diameter of the crystallizer. According to general mathematical theories, this problem is solved using the regression model. From the point of view of linear algebra, the functional connection is determined by the solution of the system of linear algebraic equations. If we denote the interpolation in the form of a function, then it is necessary to solve the system of equations:

$$P(x_0) = y_0, P(x_1) = y_1, ..., P(x_n) = y_n$$

$$\begin{cases} a_0 + a_1x_0 + a_2x_0^2 + ... + a_nx_0^n = y_0, \\ a_0 + a_1x_1 + a_2x_1^2 + ... + a_nx_1^n = y_1, \\ ...., \\ a_0 + a_1x_n + a_2x_n^2 + ... + a_nx_n^n = y_n. \end{cases} \tag{7}$$

One of the results of the experiment conducted in the foundry shows a decrease in oxygen content in the alloy as the amount of aluminum in the electrode is given in the tabular form in the work [2]. Of the four numerical values in this table, the target function based on regression analysis is compiled:

1. If the diameter of the crystallizer is 400 mm:

$$n = 3,\ x_0 = 4,\ x_1 = 8,\ x_2 = 12,\ x_3 = 16;$$
$$y_0 = 0{,}035,\ y_1 = 0{,}011,\ y_2 = 0{,}006,\ y_3 = 0{,}002.$$

In accordance with these numerical values, the system of equations (7) is led to the following type:

$$\begin{cases} a_0 + 4a_1 + 16a_2 + 64a_3 = 0{,}035 \\ a_0 + 8a_1 + 64a_2 + 512a_3 = 0{,}011 \\ a_0 + 12a_1 + 144a_2 + 1728a_3 = 0{,}006 \\ a_0 + 16a_1 + 256a_2 + 4096a_3 = 0{,}002 \end{cases} \tag{8}$$

In accordance with the equation (8), it was established that a_0 = –0,073824, a_1 = –0,011673, a_2 = –0,000506, a_3 = –0,000004. In turn, the target function characterizing the change in the amount of aluminum in the electrode corresponding to the diameter of the crystallizer is led to the following type:

$$P(x) = 0{,}073824 - 0{,}011673x + 0{,}000506x^2 - 0{,}000004x^3. \tag{9}$$

Functional bond (9) completely determines the amount of oxygen in the alloy obtained with arbitrary values of the amount of aluminum in the electrode corresponding to a particular diameter of the crystallizer (400 mm).

2. If the diameter of the crystallizer is 300 mm:

$$n = 3,\ \lambda_0 = 4,\ \lambda_1 = 8,\ \lambda_2 = 12,\ \lambda_3 = 16;$$
$$\mu_0 = 0{,}035,\ \mu_1 = 0{,}021,\ \mu_2 = 0{,}013,\ \mu_3 = 0{,}011.$$

The system of equations (7), taking into account the above numerical values, will have the form:

$$\begin{cases} a_0 + 4a_1 + 16a_2 + 64a_3 = 0{,}035 \\ a_0 + 8a_1 + 64a_2 + 512a_3 = 0{,}021 \\ a_0 + 12a_1 + 144a_2 + 1728a_3 = 0{,}013 \\ a_0 + 16a_1 + 256a_2 + 4096a_3 = 0{,}011 \end{cases} \tag{10}$$

Based on the system of equations (10), it becomes known that a_0 = 0,055, a_1 = 0,00575, a_2 = 0,000188, a_3 = 0,00002. At the same time, the percentage of oxygen in the alloy corresponding to a change in the amount of aluminum in the electrode according to the known diameter of the crystallizer will have the following target function:

$$\mu(\lambda) = 0{,}055 - 0{,}00575\lambda + 0{,}000188\lambda^2 - 0{,}000003\lambda^3. \tag{11}$$

The free variable in expression (11) characterizes the amount of AL in the electrode, and the amount of oxygen in the resulting alloy corresponds to the amount of AL. 3. The case when the diameter of the crystallizer is 200 mm:

$$n = 4,\ \lambda_0 = 4,\ \lambda_1 = 8,\ \lambda_2 = 12,\ \lambda_3 = 16;$$
$$\mu_0 = 0{,}035,\ \mu_1 = 0{,}025,\ \mu_2 = 0{,}019,\ \mu_3 = 0{,}013.$$

The algebraic system of equations (7), accordingly, will take the form

$$\begin{cases} a_0 + 4a_1 + 16a_2 + 64a_3 = 0{,}035 \\ a_0 + 8a_1 + 64a_2 + 512a_3 = 0{,}025 \\ a_0 + 12a_1 + 144a_2 + 1728a_3 = 0{,}019 \\ a_0 + 16a_1 + 256a_2 + 4096a_3 = 0{,}013 \end{cases} \tag{12}$$

Solving this system of equations determines the following roots a_0 = 0,053, a_1 = –0,005833, a_2 = 0,000375, a_3 = –0,00001. For this case, as in previous cases, the target will look like:

$$\mu(\lambda) = 0{,}053 - 0{,}005833\lambda + 0{,}000375\lambda^2 - 0{,}00001\lambda^3. \tag{13}$$

4. The case when the crystallizer diameter is 100 mm:

$$n = 4,\ \lambda_0 = 4,\ \lambda_1 = 8,\ \lambda_2 = 12,\ \lambda_3 = 16;$$
$$\mu_0 = 0{,}035,\ \mu_1 = 0{,}027,\ \mu_2 = 0{,}023,\ \mu_3 = 0{,}019.$$

Ad hoc a_0 = 0,053, a_1 = –0,005833, a_2 = 0,000375, a_3 = –0,00001 and the corresponding objective function will be in the form:

$$\mu(\lambda) = 0{,}053 - 0{,}005833\lambda + 0{,}000375\lambda^2 - 0{,}00001\lambda^3. \tag{14}$$

By constructing a graph of functional dependence (14), we determine the amount of Al in the electrode required for the minimum amount of oxygen in the alloy.

Under production conditions, based on complex experiments, the degree of dependence of the amount of hydrogen and oxides, gas additives in the alloy formed during the liquefaction of slag on the average diameter of the slag was determined, given in [3, 5]. Using these experimental data, we will consider the problem of mathematical modeling of quantitative changes in the additions of hydrogen and oxides in the alloy, that is, by determining the functional dependence, we will determine the results of the experiment from an analytical and mathematical point of view. In the future, they can be assessed without conducting further experiments. First, we will build a model that estimates the change in hydrogen content in the alloy with a change in the average diameter of the charge. From the data determined experimentally, the following data can be cited in [5]:

$$\begin{aligned} &d_1 = 6мм,\ d_2 = 10мм,\ d_3 = 14мм,\quad d_4 = 20мм,\quad d_5 = 30мм; \\ &\lambda_1 = 0,52,\ \lambda_2 = 0,48,\ \lambda_3 = 0,44,\quad \lambda_4 = 0,38,\quad \lambda_5 = 0,34,\ \left[см/_{100г} \right]. \end{aligned} \tag{15}$$

Then the system of equations generated to determine the objective function in the regression model will be as follows:

$$\begin{cases} a_1 + 6a_2 + 36a_3 + 216a_4 + 1296a_5 = 0,52 \\ a_1 + 10a_2 + 100a_3 + 1000a_4 + 10000a_5 = 0,48 \\ a_1 + 14a_2 + 196a_3 + 2744a_4 + 38416a_5 = 0,44 \\ a_1 + 20a_2 + 400a_3 + 8000a_4 + 160000a_5 = 0,38 \\ a_1 + 30a_2 + 900a_3 + 27000a_4 + 810000a_5 = 0,34 \end{cases} \tag{16}$$

Solving this system of equations using the *Maple 13* software package method we obtain the following numerical values $a_1 = \frac{949}{1600}, a_2 = \frac{-483}{32000}, a_3 = \frac{221}{320000}, a_4 = \frac{-1}{25600}, a_5 = \frac{1}{1280000}$. As a result, we obtain the target function for changing the amount of hydrogen in the alloy with a change in the average diameter in the form:

$$\lambda(d) = 0,593125 - 0,01509375d + 0,000690625d^2 - 0.000078125d^3. \tag{17}$$

Expression (17) clearly allows one to calculate the amount of hydrogen in the alloy with an accuracy of 97 percent when the average diameter of the charge changes. Subsequent studies will present the quantitative change in oxide inclusions in the alloy with a change in the average diameter of the charge. Based on the data of complex experimental studies, we present the following numerical values of the sought parameters and the resulting inhomogeneous system of algebraic equations

$$\begin{aligned} &d_1 = 6мм,\ d_2 = 10мм,\ d_3 = 14мм,\quad d_4 = 20мм,\quad d_5 = 30мм; \\ &\alpha_1 = 7\%,\ \alpha_2 = 8\%,\ \alpha_3 = 7\%,\quad \alpha_4 = 6\%,\quad \alpha_5 = 5\%. \end{aligned} \tag{18}$$

$$\begin{cases} a_1 + 6a_2 + 36a_3 + 216a_4 + 1296a_5 = 7 \\ a_1 + 10a_2 + 100a_3 + 1000a_4 + 10000a_5 = 8 \\ a_1 + 14a_2 + 196a_3 + 2744a_4 + 38416a_5 = 7 \\ a_1 + 20a_2 + 400a_3 + 8000a_4 + 160000a_5 = 6 \\ a_1 + 30a_2 + 900a_3 + 27000a_4 + 810000a_5 = 5 \end{cases} \tag{19}$$

Solving this system of equations using the Maple 13 software package method, we obtain the following numerical values of the roots of the equation

$$a_1 = -\frac{99}{16},\ a_2 = \frac{27673}{6720},\ a_3 = -\frac{27439}{67200},\ a_4 = \frac{431}{26880},\ a_5 = -\frac{59}{268800}.$$

As a result, we obtain the following target function for the quantitative change in oxide inclusions in the alloy with a change in the average diameter of the charge:

$$\alpha(d) = -\frac{99}{16} + \frac{27673}{6720}d - \frac{27439}{67200}d^2 + \frac{431}{26880}d^3 - \frac{59}{268800}d^4. \quad (20)$$

This expression characterizes the quantitative change in oxide inclusions in the alloy with a change in the average diameter d of the charge.

Results and discussion

If the variable in expression (9) represents the amount of AL in the electrode $P(x)$, it represents the corresponding amount of oxygen in the resulting alloy. In the following table, we present the results obtained on the basis of the mathematical model, and compare their reliability with the above experimental results.

We evaluate the error of the mathematical model,

$$\Delta_4 = \frac{0.035 - 0.03497}{0.035} \cdot 100\% = 0.09\%,\ \Delta_8 = \frac{0.11 - 0.1078}{0.11} \cdot 100\% = 2\%,\ \ldots$$

From the results of mathematical modeling, it can be seen that the O_2 content in the alloy reaches the minimum value (close to 0) with the content of Al 11.776 %.

From Fig. 1, it can be seen that the oxygen content in the alloy reaches the minimum value (close to zero) with the Al 21.89 % content. As above, a function is generated that determines the amount of oxygen in an alloy obtained with arbitrary values of aluminum content in an electrode suitable for a crystallizer of any diameter.

Expressions (9), (11), (13), (14) have another advantage, that is, using these expressions, the required amount of aluminum in the electrode corresponding to the necessary percentage of oxygen in the alloy is determined. The obtained mathematical expressions based on the results of the first experiment allow you to determine the results of the next experiment without these experimental studies. Comparison of the target function built to assess the change in hydrogen content in the alloy when the average diameter of the screen is changed, and the experimental results are presented in Table 2.

Table 1. The results obtained on the basis of a mathematical model

The amount of aluminum in the electrode, Al, [%]		4	5	6	7	8	9	10	11	11.776
The amount of oxygen in the alloy, O^2, [%]	Experiment	0.035	0.028	0.021	0.0153	0.011	0.0067	0.0037	0.0013	0
	Model	0.03497	0.0276	0.02114	0.0155	0.01078	0.0068	0.00369	0.00132	0.00001
Error, %		0.09	1.43	1.44	1.3	2	1.5	0.27	1.54	1.5

As a result, it turns out that the maximum deviation does not get used to 2 %.

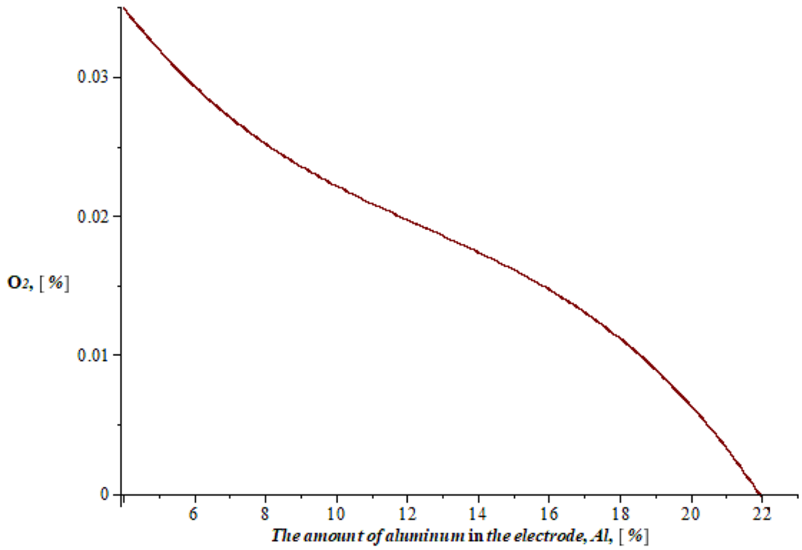

Fig. 1 change in the amount of oxygen in the resulting alloy with an increase in the content of Al (crystallizer diameter 100 mm)

Table 2. Compare the mathematical model and experimental research

The average diameter of the screen, d [mm]		6	10	14	20	30
The amount of hydrogen, [sm/100 gr]	Experment	0.52	0.48	0.44	0.38	0.34
	Model	0.51055	0.4731	0.4364	0.0375	0.3451
Error, %		1.8	1.44	0.82	1.3	1.5

As a result, even in this case, the error does not reach 2 %.

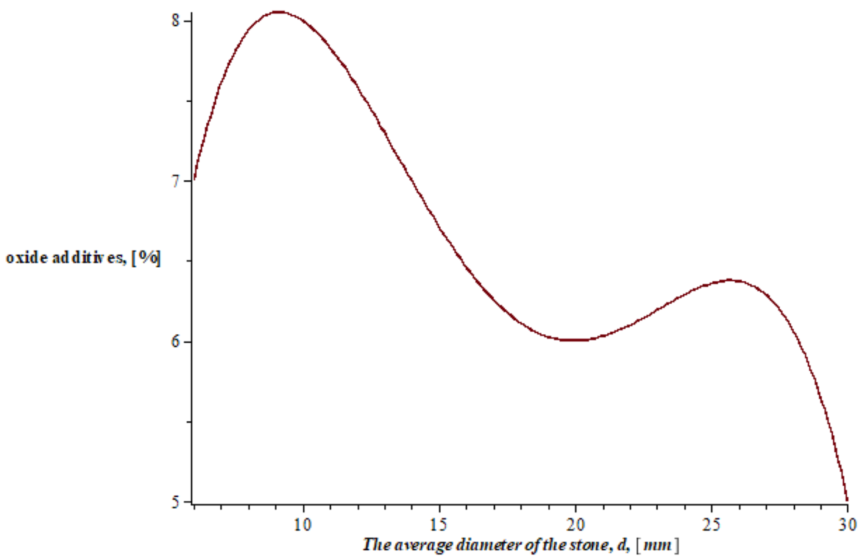

Fig. 2. Graph of quantitative changes in oxide inclusions in the alloy when the average forking diameter changes

Conclusions

It has been determined, based on an analysis of literary sources, that the building of mathematical models receives minimal consideration in scientific research on engineering materials science. In this regard, the issues and potential for the creation of mathematical models of heat and mass transfer processes are supported in order to get promising alloys in the foundry business.

When mathematical modeling of the results of a complex experiment, it is important that the information determined as a result of the experiment is integral and unambiguous. The condition of unambiguous function is important for determining the laws of changing another parameter corresponding to the natural variable parameter. The definition of the function of one variable is considered as the main issue of the formation of analytical expressions. It is necessary to create an unambiguous function of communication. The advantage of the formed mathematical function is that it not only reflects the results of the experiment, but also makes it possible to determine the results of the next experiment without conducting these experiments.

Declaration of interest

The authors declare no conflict of interest.

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