Systems and aids of mathematical modeling of the alumina refinery methods: problems and solutions

V. O. Golubev, *Head of Department of Mathematical Modeling[1], e-mail: vladimir.golubev2@rusal.com*
D. G. Chistiakov, *Senior Engineer of Department of Mathematical Modeling[1], e-mail: Dmitriy.Chistyakov@rusal.com*
V. N. Brichkin, *Head of Department of Metallurgy[2], e-mail: Brichkin_VN@pers.spmi.ru*
T. E. Litvinova, *Professor of the Department of Physical Chemistry[2], e-mail: Litvinova_TE@pers.spmi.ru*

[1] *RUSAL Engineering & Technology Center, St. Petersburg, Russia.*
[2] *Saint-Petersburg Mining University, St. Petersburg, Russia.*

It is shown that the development of systems and aids of mathematical modeling of alumina production at the refinery of Russia has passed a long way of evolution and it is mainly connected with creating the specialized software products and domestic mainframe computers. At the present stage, the systems and aids of domesitic mathematical modeling of technological processes is an integral part of effective functioning of alumina refinery, the specifics of the engineering plan of which makes it difficult or even excludes the possibility of a unified approach to construction of their digital twins and necessitates flexible combining the individual and universal approaches. The functionality of the models is implemented in the Windows environment with the use of SysCAD software, which makes it possible to obtain information about properties of any material flow, parameters of each technological apparatus and to solve a complex of operational and system issues. Until the present time the relevance of profound understanding of the nature of the laws, phenomena and processes occurring in the alumina production systems, as well as building the special-purpose electronic databases. This would allow one to develop and apply relevant physical-chemical model of the plants at which alumina is manufactured not only from bauxites but also from the other types of aluminiferous raw materials. At the same time, further improvement of mathematical tool is associated with the need to improve the efficiency of multithreaded calculations in design of technological systems, which being combined with an access to powerful computing resources creates the conditions for transition to a new level of solving production technological problems, including multiparametric optimization of alumina plants and others.

Key words: mathematical modeling, alumina production, physicochemical equilibriums, calculation techniques.

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Introduction

In the domestic alumina industry, the mathematical modeling systems and aids has begun to develop since the end of 1960s, as computers have become more available. Intensive development of algorithms and domestic software complexes for modeling the technologies of alumina refineries started in 1968. By 1970, in the VAMI institute (ВАМИ, the All-Union research and planning institute of aluminum, magnesium and electrode industry) the first domestic program Bayer ("Байер") for modelling the technologies of alumina production for Minsk-22M ("Минск-22М") and Minsk-32 ("Минск-32") electronic computers has been elaborated. By 1975, SXEMA software package ("ПК СХЕМА") to calculate material balance of alumina production enterprises and TETPA software package ("ПК ТЕТРА") to calculate heat balance of digestion and evaporation trains have been written on FORTRAN 66 programming language. In the succeeding decade these programs have been modernized many times and translated into FORTRAN 77 and FORTRAN 80. In 1983, as a new ES-1045 (EC-1045) mainframe computer, tenfold more powerful than its predecessors, has become available in VAMI, the technological program complexes have begun to be used for optimizing the process flowsheets and cost per unit. In 1980s, the CAD-Aluminum system ("САПР-Алюминий") of designing the aluminum subindustry enterprises has

a

ПЕРЕДЕЛ N	ТИП	ВХОДЯЩИЕ ПОТОКИ				ВЫХОДЯЩИЕ ПОТОКИ	
11	12	111	6911	7311	0	1112	0
12	1	1112	0	0	0	1213	1214
13	6	1213	113	0	0	1314	0
14	4	1214	1314	0	0	1415	0
15	11	1415	0	0	0	1516	0
16	7	1516	0	0	0	1681	1601
81	4	1681	2081	0	0	8183	0
83	1	8183	0	0	0	8320	8384
20	26	8320	9320	0	0	2030	2081
30	26	2030	4030	0	0	3040	3091
93	4	9293	8793	0	0	9320	0
40	26	3040	5040	0	0	4095	4030
91	14	3091	7391	0	0	9192	0
92	1	9192	0	0	0	9294	9293
94	5	9294	0	0	0	9495	9401
95	4	4095	9495	0	0	9550	0
50	26	9550	6050	0	0	5060	5040
60	26	5060	7060	0	0	6070	6050

b

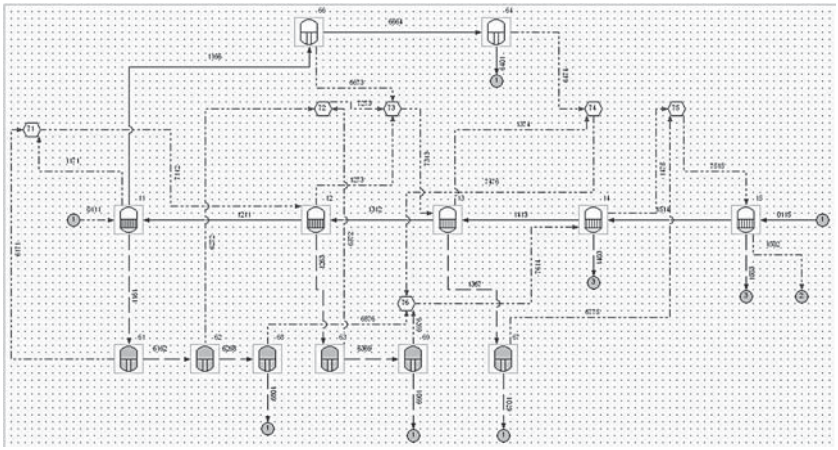

Fig. 1. Interface of domestic programs for design study of alumina enterprise technology:
a – SXEMA software for DOS; *b* – TETPA software for Windows

been constructed on their basis. With the advent of the Windows operation system, SXEMA and TETPA software have got a new visual interface, which made possible to draw the plant design models by means of lines and blocks (Fig. 1). Using these programs, the VAMI Institute has performed the balance process calculation of more than 40 plants.

The challenge of profound modernization and optimization of enterprises gave new impetus to development of the chemical production processes and apparatuses computer simulation. Alumina refineries are referred to the most complicated simulation objects, since:

– their functioning is based on several different technologies;

– several tens of returning flows may be present in their process flowsheets, as well as trains of apparatus with recycles;

– special models for describing the features of matters and solutions are required;

– it supposes calculation of the disperse particle population changeability during precipitation of aluminate solution, etc.

Statement of the research task

The obviousness of modern industrial production change to digital economy and the need to increase its efficiency allows formulating several questions concerning definition and perfection of mathematical models of metallurgical processes and industries. First of all, the inevitability of these questions is connected with the choice of progressive and promising tools of computer data handling and performing computations, providing solution of the process technology day-to-day management problems and manufacturing optimization as a whole. Among a series of peculiarities of metallurgical technologies, it is necessary to note their specificity, associated with diversity of the raw material base, originality of chemical properties of the metals and physical-chemical systems, available for their production, complexity and extension of the production cycle. This makes it difficult to use or even excludes a unified approach to construction of mathematical models for the most of metallurgical processes and necessitates flexible combining the individual and universal approaches. This in full measure relates to technologies of alumina production, which notwithstanding the common features of the chemical-metallurgical manufacturing process; possess a whole series of unique characteristics, connected with the use of alkaline physicochemical systems and special techniques, cyclic recurrence and considerable extent of work-in-progress, high quality requirements to the end products, etc. It is precisely these peculiarities that cause a lot of problem questions, revelation and solving of which determine the efficiency of further development of the mathematical modeling systems and aids.

Methods of calculation of process technologies and systems

Calculations of the complex production systems are fulfilled using the Lumped Systems modeling, in which an engineering procedure is represented as a usual process flow diagram (Fig. 2). The fundamentals of mathematical tool, employed for calculation of such systems of equations, have been originated in 1980–1990s but their development continues to the present day [1–2]. Complexity and labor-intensiveness of calculation of the real process flowsheets is stipulated by their multithreaded nature, including return of materials to the earlier stages, which makes the definable unknowns cyclically interdependent. To break cyclic recurrence, it is necessary to execute

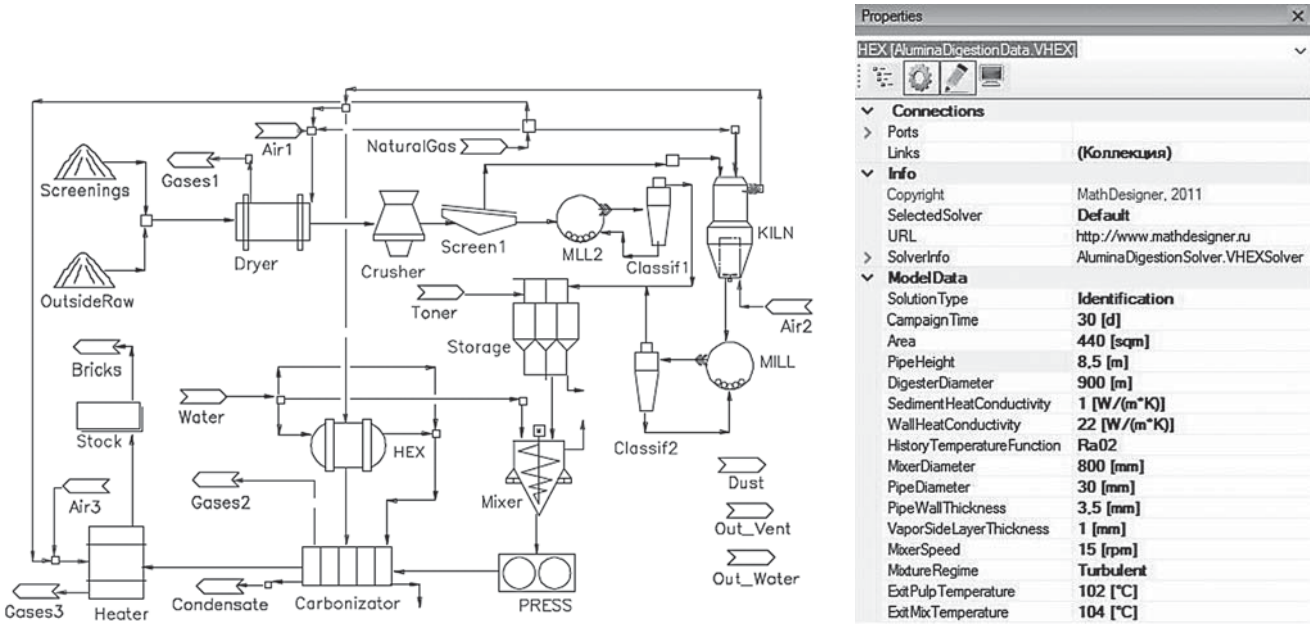

Fig. 2. An example of the design-process flowsheet and the device input data specification in a software for process flow simulation

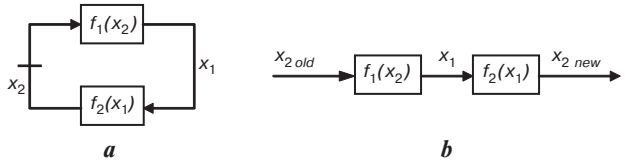

Fig. 3. Principle of tearing systems with recirculation [4]: *a* — an original scheme; *b* — an open scheme

a loop break (or to use a so called tearing technique), which will make calculation the successive one [3]. For example, the diagram exhibited in Fig. 3, *a*, is described by the system of two interdependent equations as follows: $x_1 = f_1(x_2)$ and $x_2 = f_2(x_1)$. After tearing, as it is shown in Fig. 3, *b*, this problem may be reduced to solution of one equation, since x_2 remains the only unknown variable and $x_2 - f_2[f_1(x_2)] = 0$. Structural decomposition is also used in case of large sets of equations to gain simplification, to detach smaller subsystems, to depress equations; the equations are classified in two types as differential and algebraic, the systems are classed as stiff or sparse. In the example cited above, selection of x_2 may be implemented by method of simple iterations, but modeling the complicated technological processes results in formation of a sparse system of nonlinear equations, solving of which by forward substitution requires heavy computer facilities. At that, the dynamic relaxation methods are used for accelerated variables fitting at the points of tearing [4–6].

Functional dependences incorporated into the structural blocks of the model similar to $f_1(x_2)$ and $f_2(x_1)$, may contain non-linear, differential, transcendental equations and their systems. In most cases such functions are being arranged as submodels and are calculated each by itself because of their intrinsic computational complexity. For lack of a unified matrix of the process system coefficients, the array computation parallelizing methods are of limited application in solving such problems, and their use gains no essential additions to capacity on multi-core and multiprocessor computers. In this connection, the efficiency challenge of the multithreaded computation in the problems of the process system calculations has been keeping its urgency yet [7–9].

Special algorithms for the models of alumina refineries

Several tens of different software products for producing models based on the lumped systems modeling method are represented in the market the present day. They are adapted for the needs of oil and gas processing, pulp and paper industry, or simulate isolated processes, for example, crushing, separation and classification; heap leaching; flotation, etc. At the same time, critical shortage of the programs suitable for developing the models of alumina refineries takes place. In essence, an assortment is limited by a single software package — SysCAD, produced by KWA Kenwalt Pty Ltd (Australia). The difficulties are caused by specific character of subjects to simulate. The software for modeling alumina refineries should comprise specific libraries of properties and calculation algorithms, which are absent in the programs designed for application in petroleum organic synthesis and production of nonorganic substances, such as AspenPlus software, for example. Amongst the main distinctions there is the need to use the data on equilibrium solution compositions for a wide range of state parameters, system usage of the data on physical properties of technological solutions (density, viscous, heat capacity, etc.), methods of computing a completeness degree of physical-chemi-

Table 1
The Rosenberg-Healy equation coefficients for two RUSAL's refineries: RUSAL Kamensk-Uralsky (UAZ) and RUSAL Krasnoturyinsk (BAZ)

Empirical coefficients	The Worsley Plant solutions [12]	UAZ	BAZ
a_0	–9.2082	–8.4268	–8.4983
a_3	–0.8743	–0.6812	–0.6629
a_4	0.2149	0.1710	0.1688
k_1	0.9346	0.8555	0.6910
k_2	2.0526	0.9861	0.8288
k_3	2.1714	1.8024	1.3897
k_4	1.6734	1.5263	1.0425

cal transformations, methods of accelerated convergence of solutions for the trains of apparatus with recycles and some others.

At that, one of the principal aspects in developing modern models of alumina refineries concerns a question of adequate description of equilibriums in the corresponding technological systems, satiety of which is of governing impact on their metastable steadiness; rate and indices of the processes. This makes it possible to choose the well-studied physical-chemical system Na_2O–Al_2O_3–H_2O as the basic one. In conditions of a real refinery process, it becomes more complicated at least to the level of $K_2O - Na_2O - Al_2O_3 - H_2O - An^{n-}$, where An^{n-} – SO_4^{2-}; Cl^-; CO_3^{2-}; $C_2O_4^{2-}$ and others. Thereupon it is necessary to mark a vital importance of the basic system state in conditions of silica accumulation in it, which essentially changes equilibrium conditions and leads to formation of alkaline hydroalumosilicate precipitations with variable composition. As analysis of a $K_2O - Na_2O - Al_2O_3 - H_2O - SiO_3^{2-}$ system shows, its state is a complex function of alkaline component concentration, temperature and molecular ratio $(K_2O + Na_2O)/Al_2O_3$, as well as of anion composition of a solution, an additional complication of which is a result of formation of alumosilicic complexes with variable composition $[SiAl_nO_{2(n+1)}(OH)_m]^{(m+n)}$ [10]. This makes it practically impossible to describe the system in a wide range of the mentioned factors and causes the need to study it as applied to frequent cuts for technologically significant compositions, for example, in concrete conditions of processing of bauxite, nepheline and other aluminic raw materials. The compositions which meet a $K_2O - Na_2O - Al_2O_3 - H_2O - CO_3^{2-}$ system at reduced content of Al_2O_3 and hydroxyl ion, should be marked out as a second boundary state. Such a state is typical for solutions in conditions of their neutralization (carbonization) by carbonic-acid gas, in connection with precipitation of aluminum hydroxide, deposition of soda, soda-potash, potash and other precipitations, as well as solving the questions of concentration and extraction of raw metals and removal of impurities. Thus, the importance of developing mathematical models for ascertainment of equilibrium compositions of alumina production

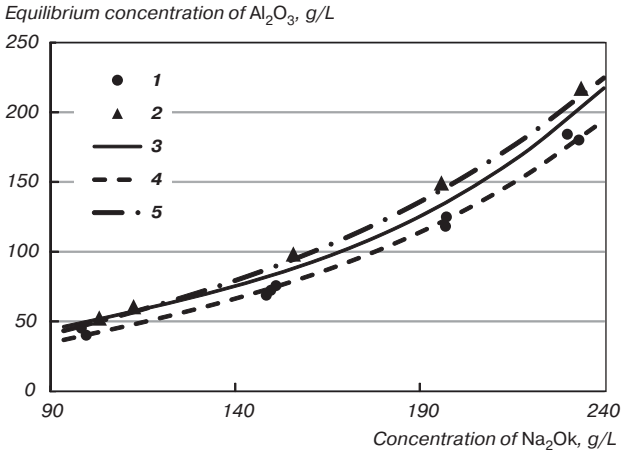

Fig. 4. The results of the laboratory data approximation by equilibrium dissolubility of aluminum hydroxide converted to its oxide at a temperature of 70 °C:
1 and *4* — test data and their approximations for solutions of RUSAL Kamensk-Uralsky (UAZ); *2* and *5* – that for solutions of RUSAL Krasnoturyinsk (BAZ); *3* — results of calculations with the formula from [12]

systems is difficult to overestimate. This fact has predetermined their evolution since 1980s and has resulted in creation of a thermodynamic model for solutions in Bayer method, published in 1996 [11–12]. This model has demonstrated sufficiently high efficiency in alumina production by the Bayer process and at the same time the vulnerability, connected with a large number of the empiric coefficients to be experimentally determined depending on concrete ratio of impurities, ionic force of solution, temperature and concentration conditions of manufacturing method and some other factors [12]. Table 1 contains the coefficients for two refineries of UC RUSAL refined in such a way in comparison with data obtained on Wersley Plant and used for developing the original model. The results of experimental data approximation in comparison with original model are plotted in Fig. 4. It is clear that elaboration of this thermodynamic model on the assumption about single type of equilibrium in aluminate solutions involving complex anion $Al(OH)_4^-$ and $Al(OH)_3$ is one of its fundamental restrictions, since

it does not comply in full measure with modern conceptions, allowing the following sequence of changes in ion composition [13]:

$$Al(OH)_6^{3-} = Al(OH)_5^{2-} + OH^- = Al(OH)_4^- + OH^- =$$
$$= AlO(OH)_2^- + H_2O = Al_2O(OH)_6^{2-} = AlO_2^- + H_2O$$

The second natural limitation of the Rosenberg – Healy thermodynamic model is its applicability in relation to the equilibrium with a single solid phase and in the absence of potassium. This does not allow its use for a number of important systems and processes of alumina production, including on the processing of nepheline, alunite and other types of potassium-containing raw materials. The stated considerations let us speak about high topicality of the studies devoted to creation of a wide range of mathematical models for the description of equilibriums in the alumina production systems, as an element of simulation and optimization of the corresponding technological processes.

Integral elements of mathematical description of technological processes are calculation and consolidation of material flows, which operate with the bulk flow units, while the production flows of hydrometallurgical operations are measured in that of volume flow, which causes the necessity of corresponding converting with the use of the solution density values. It is clear that the process solution density plays is of more importance in mathematical models of alumina manufacturing processes. The density value is widely used for the transition from weight to volume concentrations, to give control over the degree of solutions evaporation, as well as when performing hydrodynamic and thermal design, along with the other characteristics of solutions. In actual practice of alumina production by the Bayer method, a Mulloy-Donaldson formula has made a good showing in determination of solution densities, provided fitting of 10 experimentally determined constants [14]. With regard to the solutions formed during the bauxite and other alumina-containing raw stuff processing by sintering, it gives essential errors resulting in the need to use a more general equation in which the solvent (water) density is amended to take into account the solute mass fractions, the calculation of which requires the creation of a large library of experimental data [14]:

$$\rho_t = \rho_{w.25} \cdot (1 + \Sigma D_i) \qquad D_i = a_i C_i + b_i C_i^2 + ... + d_n C_i^n$$

where: ρ_t and $\rho_{w.25}$ are the water densities at the desired temperature and 25 °C, kg/m^3; D_i is a correction for the i^{th} solute depending on its mass concentration C_i in a solution; a_i, b_i, ...d_n are the coefficients of polynomial equation for calculating the correction value.

Kinetic models of chemical interactions in the alumina production systems are the most important part of its digital description, as they allow to determine the leading technological indicators and predict their change depending on the conditions of the processes implementation, where previously considered models act as subsystems. At the same time, in the overwhelming majority of cases we have to talk about the kinetics of heterogeneous interactions, corresponding to two multi-directional processes. One of them is associated with conversion of the solid phase components into solution, i.e. with digestion, and the second one is responsible for separation of components from the solution in the batch crystallization process. In actual practice of their implementation, a series-parallel mechanism is gaining development, but it is complicated by side and secondary interactions, which significantly impedes kinetic simulation of such processes [11].

Digestion of, including bauxite and leaching aluminum sinters, can be attributed to the well-studied objects, to which are applicable both formal kinetic approaches and the models taking into account the geometry, size, unsoundness, surface interactions and internal structure of the particles [15]. This made it possible to propose a number of simple and more complex kinetic models, the adaptation of which to the real-life refinery environment is quite realistic, but is associated with the processing of a large amount of information, which was shown by V. Ya. Abramov on an example of bauxite and nepheline cakes leaching [16]. At that, one should take into account the characteristics of the materials formed at the adjacent technological stages, as well as the indicators adopted in production conditions: duration of stay in the apparatus, material consumption, concentration of solids in the pulp, flow hydrodynamics, compositions and modules of solutions, temperature regimes of the apparatus and a number of others [15–19].

Among the processes of alumina production, one of the most difficult for modeling is precipitation of aluminate solutions, which in accordance with the existing classification can be attributed to the polythermal batch crystallization on a seed, accompanied by a chemical impact in the form of a hydrolysis reaction of aluminate ions. The modeling of this process solves not only the problem of describing the aluminum hydroxide precipitation rate and depth, but also ensures the required particle distribution by size to achieve the specified the seed aluminum hydroxide recycling parameters and to obtain the commodity output of proper quality. Notwithstanding the fact that the modern theory of crystallization is a highly developed doctrine with a many years' history, a number of phenomena and processes in the context of this doctrine has no rigorous mathematical description and its compliance with practice yet. This is because of the great complexity and diversity of the processes accompanying crystallization and occurring at the micro-, nano- and even atomic levels, which is connected with the implementation peculiarities of the precipitation process. For this reason, the simulation mainly uses empirical and semi-empirical equations, which allow us to describe

the known phenomena and regularities within the framework of basic theoretical theses, taking into account the additionally introduced and experimentally determined coefficients. A typical example of this kind is the use of a universal empirical equation (1) for crystallization kinetics description, as well as equations (2), (3) based on it and their modifications to simulate a precipitation under conditions of the layer growth of aluminum hydroxide particles [15, 20]:

$$j = \mathrm{d}m/\mathrm{d}\tau F = K(C - C_0)^n \quad (1)$$

$$\mathrm{d}A/\mathrm{d}\tau = K_0(A - A_0)^2 F \quad (2)$$

$$\mathrm{d}A/\mathrm{d}\tau = K_0'[(A - A_0)/N)]^2 F \quad (3)$$

where: j — crystallization flow; m and F are respectively the mass and surface of a crystallizing substance; τ — time; n is a kinetic parameter that does not coincide with the chemical reaction order; C, C_0 — concentration of supersaturated and equilibrium solutions by crystallizing phase; A, A_0 — concentration of Al_2O_3 in a supersaturated and equilibrium solution; N is the caustic alkali total concentration in terms of Na_2O; K, K_0, K_0' — constants.

As practice shows, equations (2), (3) are of the second order and on the basis of this they do not correspond to stoichiometry used in the equilibrium thermodynamic modeling in a $Na_2O - Al_2O_3 - H_2O$ system [12]. This suggests a lack of understanding of the real mechanism of this process and possibility of its use for creating kinetic models with physical meaning. Even greater uncertainty refers to formation of the aluminum hydroxide precipitate granulometric composition as a result of cumulative influence of the factors of heterogeneous and homogeneous nucleation, linear growth of the particles and its violation, agglomeration, classification, recrystallization, mechanical failure, and the others [11, 15, 21]. In this connection, it is common practice to model a precipitation using the population balance equation, which takes into account most of the listed factors [22]. For its integration over time, there have been developed special algorithms, which differ in the form of computational grid, order and method of solving the difference scheme [23]. Within the population balance, contribution of a particular factor to the particle distribution by size is estimated by individual functions and models created for each of the above mentioned processes [20, 22–24]. Applicability of such an approach and corresponding models is confirmed by the factory practice of foreign enterprises working on low-modulus aluminate solutions ($\alpha_k < 1.4$) with agglomeration tanks. When processing refractory raw materials at domestic alumina refineries, they receive the aluminate solutions with a higher caustic module ($\alpha_k = 1.68 \div 1.71$), which reduces the agglomeration efficiency at a temperature of 75–85 °C. Regardless of this, the particle linear growth rate law equation can be adjusted to adequately evaluate the aluminate solution productivity in accordance with the refinery data. Unfortunately, the models of nucleation and agglomeration in these conditions do not allow one to reproduce particle size distribution (PSD) of the product hydrate, intrinsic to domestic alumina refineries, which does not prevent to correctly predict the change in content of one characteristic fraction, i.e., –45 μm, when the external process conditions changing (Table 2).

The use of carbonization processes for decomposition of aluminate solutions is significantly less important in the world practice of alumina production, although it plays a significant role in the domestic metallurgy, allowing one to obtain about 40% of the produced alumina. This has caused a depressed interest of researchers to the modeling aspects of this process, which by its nature fundamentally differs from decomposition and in the first approximation can be defined as isothermal batch crystallization at chemical interaction, accompanied by hydrolytic precipitation of $Al(OH)_3$. At that, the system becomes conditionally four-component $Na_2O - Al_2O_3 - CO_2 - H_2O$ and the three-phase one, which essentially complicates the mechanism of the structure and precipitation granulometric composition formation as well as makes the known precipitation population balance equations not applicable in these conditions [26]. This allows us to highlight as one of the priorities the development of an original model of carbonization process, the topicality of which is determined by the increasing role of regional non-bauxite raw materials in the balance of alumina production.

Despite the existing problems in creating a complete digital twin for alumina refinery, which has a predictive capability when changing any parameters of the technology, the United Company RUSAL has already been

Table 2
Ratio errors in the precipitation factor calculation by results of the population balance model tuning

Grain-size class, μm	UAZ	BAZ
	Ratio error in predicting the solution productivity, %	
	0.6	0.5
	Ratio error in calculating the class content, %	
–5	91.3	85.6
–10	68.6	60.5
–20	29.0	24.7
–45	0.0	0.0
–63	1.1	1.3
–100	3.6	4.2
–125	5.3	6.1

using the models of its alumina refineries for more than 10 years. The functionality of the models is implemented in the Windows environment with the use of SysCAD software, which makes it possible to obtain information on properties of any material flow, parameters of each technological apparatus and to solve a complex of issues, including [27]:

– playing over the scenarios with different settings of the manufacturing method (raw material composition, aluminum and alkali concentration, temperature and duration of digestion, temperature profile for precipitation, etc.);

– search for operational benefits, i.e. optimum at prime cost, which is achieved due to the change of regime indicators and hardware-process solutions;

– planning the demand for raw and materials taking into account the changes in the composition of raw materials and the schedule of repairs;

– optimization of capital outlays and calculation of technological effect by appointing the expansion of production order and selection of objects for modernization based on the results of determining the aggregate economic effect, as well as some other tasks.

A necessary element of further improving the efficiency of digital models is their use in improved control systems, as part of MES (Manufacturing Execution System) for automated making up and coordinating balances of materials and energy supply, in the systems of alumina plant multiparameter optimization, etc. [28–30]. At the same time, the issue of access to computing resources becomes crucial for solution of these problems and it depends on technical capabilities to organize supercomputer centers and computing clouds [31].

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Conclusions

1. The development of systems and means of mathematical modeling of processes technologies is an integral part of effective functioning of modern alumina enterprises, the specifics of the production scheme of which makes it difficult or even excludes the possibility of a unified approach to construction of their digital twins and necessitates flexible combining the individual and universal approaches.

2. Until the present time the relevance of profound understanding of the nature of the laws, phenomena and processes occurring in the systems of alumina production, as well as the creation of their digital databases and libraries of experimental data to make it possible to develop physical and chemical models with the increased universality in solving problems of mathematical modeling.

3. Further improvement of mathematical tool is associated with the need to improve the efficiency of multithreaded calculations in design of technological systems, which being combined with an access to powerful computing resources creates the conditions for transition to a new level of solving production technological problems, including multiparametric optimization of alumina refineries and others.

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