Development the means of modeling the processes and the systems of alumina production

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Abstract

The development of chemical and metallurgical industries today considers one of the most important issues all over the world. The primary task of a modern technological enterprise is to ensure unprecedented efficiency in the environment of unstable external factors. Against the background of a progressive imbalance between countries and companies, a new type of industrial enterprise, "adaptive production," the technology of which is based on precise mathematical algorithms and quickly transformed to new conditions, is emerging in natural resource reserves, rising costs, and instability in commodity markets. Analysis of the current situation points to the rapid evolution of the methods of mathematical modeling, software, automated systems, computer and telecommunication technologies that create the prerequisites for a fundamental reform in the methodology of optimization and management of industrial enterprises in the coming years. This review examines the methods and tools to adapt the technology of complex enterprises in optimal conditions. The current trends in the development of specialized software, high-performance computing, cloud technologies are analyzed, special attention is paid to the development of key methods of mathematical modeling, including block-structural modeling, computational fluid dynamics, and industrial analytics. The economic, administrative, algorithmic, and hardware problems of integrating mathematical models into the structure of enterprise management are formulated. The ideas of construction and development of software-hardware and man-machine complexes of adaptive productions are proposed.

Keywords: mathematical modeling of the process, software, digital double.

1. Introduction

The development of chemical and metallurgical industries today in the world is in a difficult situation due to the imbalance between the decline in a quality of raw materials and a complexity of its composition, requirements for product quality, safety of the production cycle, increasing competition and a cost reduction. To ensure the sustainable operation of enterprises in the industry, it is necessary to modernize them and move on to the so-called. "Adaptive production", which in a relatively short time is able to adapt to changes in the resource base, without reducing the volume and quality of products, respond flexibly and in a timely manner to changes in consumer requirements.

Necessary conditions for the transition to adaptive production are: 1) a high level of automation based on mathematical algorithms that allows you to quickly and efficiently respond to changes in the conditions of technological processes; 2) pre-predicted options for changes in the production cycle and the readiness of the factories to the reorganization with due allowance for possible changes.

Previously, for solving these tasks, the factory's pilot shop was used, where changes in the parameters of processing when using new production conditions was studied. This approach is accurate but costly. There was no other way at that time due to small amounts of factory's statistics data and low-powered and not so common means of computer. Currently, these problems have been solved, and companies are moving to a virtual experiment and special programs that allow working with databases.

The mathematical model, which is technically virtual clone of a factory, is the safest option which does not require significant expenses at testing scenarios of the functioning of a factories and the industry as a whole. The "virtual clone" created is not characterized by risks, so it is possible to work out any production modernization scenarios on it, assessing their effectiveness and safety in advance.

Analysis of the current situation points to the rapid development of mathematical modeling methods, software, automated systems, computer and telecommunication technologies, which create prerequisites for a fundamental reform in the methodology of optimization and management of industrial enterprises in the coming years. The number of enterprises with their full-fledged mathematical model is increasing.

2. Basic Principles and Objectives of Modeling Metallurgical Processes and Systems

The mathematical model is a system of mathematical equations that reflect the essence of the processes occurring in the object under study. In addition to the system of equations, it is also necessary to specify a modeling algorithm that allows one to investigate the behavior of an object under various operating conditions. Thus, it is necessary to consider three aspects of mathematical modeling of the process and, accordingly, the task of creating a mathematical model of the object:

- The semantic side of the mathematical model is a formalized description of the nature of the processes occurring in the object, allowing to establish internal links of the system objects and create on this basis their mathematical description;
- Analytical side - mathematical equations describing the process in accordance with the formalized description;
- Computational side - a modeling algorithm representing a sequence of mathematical operations that must be performed for solving the equations of a mathematical model and, thus, study the behavior of an object at different parameters corresponding to various working conditions.

In the 1960s, D.A. Diomidovsky proposed a generalized (formalized) structural diagram of the metallurgical process shown on the Figures 1 and 2 [1].

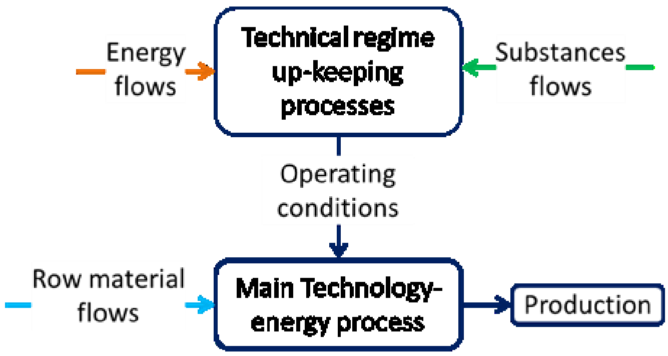

Figure 1. Generalized structure of the metallurgical process: the first approximation scheme.

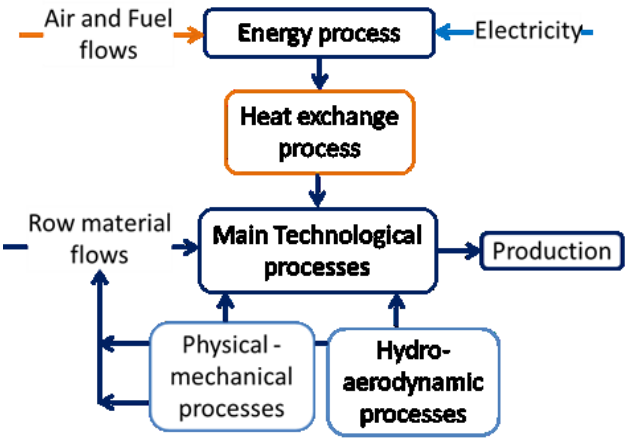

Figure 2. Generalized structure of the metallurgical process: the detailed scheme.

Although this scheme was originally proposed for pyrometallurgical processes, it turned out later that it is applicable to other types of processes. The central place in this scheme is occupied by the technological process, which is the object of control, while the remaining processes ensure its necessary functioning.

The foundations of the mathematical apparatus used to calculate systems of equations were developed in the 1980 - 1990s, but the development of these methods continues today [2, 3]. The calculation of real technological schemes is very complex and labor intense for such calculation due to their multithreading including the return of materials to earlier technological stages that makes the calculation of unknown's values cyclically interdependent. To open the cycle, a gap needs to be set, which will make the calculation consistent [4]. Multiprocessor computers and decision making matrix allow carrying out calculations of material and thermal balances by a ways of 1) multithreading, but now this method does not have the desired stability and does not provide a multiple increase in performance [5-8]; 2) extensive calculation with using of external program that based on the well-known sequential quadratic programming method (SQP), adapted for the tasks of chemical technology [9, 10] and finds the optimum by iterating through the parameters of a mathematical model; 3) using computing cluster and cloud resources [11, 12].

The developers of mathematical modeling programs try to make the interface as simple and clear as possible. The most successful option is a visual interface that allows to set the technological schemes of the plant with the help of lines and blocks almost duplicating the interface of common SCADA systems. The development of mathematical modeling systems goes in two main directions: 1) Advanced Process Control Systems and 2) creation of factory virtual clones based on Lumped Systems modeling principles.

With the use of advanced process control systems (APCS) the problems of optimizing the technology of existing and designed enterprises, determining the capital value of construction, production planning are solved. APCS allows optimizing the functioning of multi parameter objects by a given criterion, operating with several control channels (MIMO – Multi Input Multi Output). At existing factories, with their help, the searching and studying of bottlenecks, reassessment of equipment utilization ratios, and diagnostics of the causes of reduction of key indicators of the technological process are performed. The work of APCS based on building regression models that do not take into account the nature of the process. Therefore, the effectiveness of APCS is laid when it is set up - this is the most complex, lengthy and expensive stage of creating a system by a specialist. Adjustment errors lead to control instability: deviation from the optimum, self-oscillations, and the inverse response of the object to the applied effect [13]. The deterministic mathematical model of the technology enables the detection and timely correction of inaccurate data, both during the setup stage and during the operation of the control system [14, 15] so in the perspective of several years, an increase in the use of APCS as simulators for operational personnel of enterprises and as dynamic simulators when setting up automated control systems is expected.

Creating a "factory's virtual clones" the principle of Lumped Systems modeling is used. Computer programs of this type use the general principle of block-structural modeling, which combines the convenience of presenting the technological process as a process flow diagram (PFD) or Process and Instrument Diagrams with the power of computational tools, enclosed in functional units, depicted as industrial facilities as it shown on Figure 3.

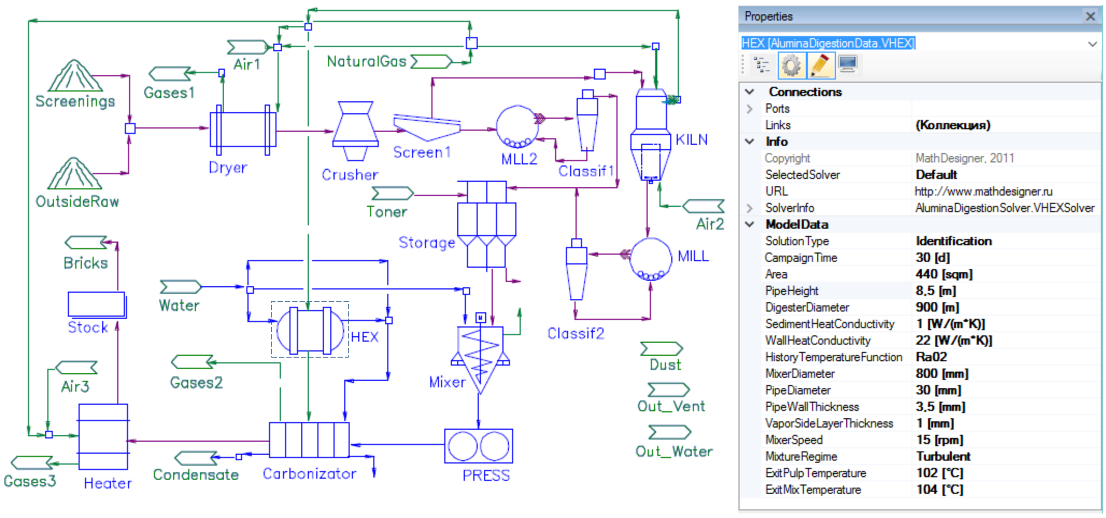

Figure 3. An example of a calculation and technological scheme and specification of the source data of the device in a program of block-structural modeling.

Today, there are several dozen different software products on the market for creating models based on the method of systems with lumped parameters. They are oriented to the tasks of oil and gas processing, pulp and paper industry, or they model only separate processes, for example: crushing, separation and classification, heap leaching, flotation, etc.

3. Features of Mathematical Modeling of Alumina Production

Today, the mathematical description of the individual stages of the technological process can be attributed to the well-developed questions of mathematical modeling of metallurgical processes based on the patterns of heat and mass transfer, as well as patterns of chemical kinetics. This allows the synthesis of models of a significant number of technological objects. At the same time, there is an acute shortage of programs adapted to the conditions of the alumina industry. Essentially, the choice is limited to the only SysCAD software product from KWA Kenwalt Pty Ltd (Australia), which designed and intended for use in alumina refineries that using the Bayer method. The program is based on equations describing the processing of high grade bauxite raw materials. The compositions of the solutions in alumina refineries largely depend on the composition of the raw materials and the method of its processing. When processing low-quality bauxite raw materials using the parallel Bayer-Sintering method, significant amounts of sulfur compounds are added to the components of the solution listed for the Bayer method. In the production of alumina from nepheline by the sintering method up to 30 % of sodium in solutions, it can be replaced by potassium. Thus, the coefficients in the equations for calculating the density must be determined on the basis of an experiment for each plant individually.

The question remains of an adequate description of the equilibria in the corresponding technological systems. The applicability of the widely used Rosenberg-Healey equation [16] is limited to soda-aluminate solutions, and in the conditions of such plants as “Pikalevo alumina refinery” or RUSAL Achinsk, where up to 25 % of alkali in the solution is potassium, it cannot be used. The development of a similar equilibrium solubility equation for alumina for such mixed solutions remains an urgent task. In the existing models the description of changes in the impurity composition of solutions and its influence on the alumina and soda losses remains unresolved. To overcome these difficulties, the software for modeling alumina production should contain data bank of state diagrams of chemical systems and tools for their use. In the software available on the market today, there are no such opportunities. The formation of the granulometric composition of precipitation is characterized by even greater uncertainty as the summary result of lot of factors affecting this process: heterogeneous and homogeneous nucleation, linear growth of particles and its violation, agglomeration, classification, recrystallization, mechanical destruction and other [17, 18]. For this reason, the simulation of the precipitation process for aluminate solutions, that is obtained from Bayer or Bayer-Sintering method, the population balance model which takes into account most of the listed factors is used [19, 20]. The accuracy of the mathematical description of the elementary stages of the technological process is determined by the level of modern development of the theory of these processes, which needs further development [21].

4. New Tendencies in Mathematical Modeling of Alumina Refineries

Over the past few years significant progress in the alumina industry has been noted in developing information and communication systems MES and ERP levels, organizing unified data centers that provide centralized online monitoring of industrial KPI and the state of equipment in alumina refineries and in direction of analysis and optimization of production processes. Such systems place high demands on the quality of the source data. The deterministic model of the technological process is an ideal object of comparison when checking the correctness of statistical hypotheses, rejecting erroneous values, filling in data losses. This model ensures complete coherence between all parameters of the alumina refinery. It can also act as a consumer of filtered data and an object of communication with users, since possesses much more information capacity than the system of field sensors and laboratory analyzes.

The solution of multi parameter optimization problems on the basis of mathematical models of plants today is carried out manually or through an external program that finds the optimum by enumerating the values of the parameters of a mathematical model. The optimal search algorithm that is well adapted to the tasks of chemical technology is the sequential quadratic programming method (SQP). To find the global optimum, it takes from several tens to several hundreds of independently converged model solutions. In the problem of multiparameter optimization of an alumina plant, the issue of access to computing resources becomes crucial, so it is proposed to build such systems on the basis of supercomputer centers and computing clouds [9-13]. Creating a model is accompanied by laboratory experiments that are required for its periodic updating, configuration and maintenance of health. A large amount of analytical measurements is required to adjust the coefficients of the models of mills, hydrocyclones, separators, heat exchangers, clarification of heat losses. At an average alumina refinery, from 2 to 5 thousand process parameters are measured, and the task of converting the calculation results with the fact is the main challenge for those who operate the model. To simplify the configuration process, an external interface is created that provides data collection, filtering, and transfer to the model. A configuration mode is added to the model; upon activation of which additional regulators are included that automatically adjust the most significant parameters.

In recent years, the joint work of the Saint Petersburg Mining University and UC RUSAL in the direction of creating a mathematical model of alumina production has yielded positive results. In 2013-2016, the sintering technology database was significantly supplemented, algorithms were developed, and existing models of existing productions were supplemented. Since 2018, the Department of Metallurgy has carried out a project with the financial support of the Russian Science Foundation under Agreement No. 18-19-00577, the purpose of which is to create digital technologies based on extensive fundamental knowledge and production data of alumina refineries enterprises.

5. Conclusions

The development of systems and tools for mathematical modeling of technological processes is an integral part of the effective functioning of modern alumina enterprises. The specificity of the production scheme makes it difficult to use a unified approach for creating their digital counterparts and requires a flexible combination of individual and universal approaches.

The relevance of an in-depth understanding of the nature of the patterns, phenomena and processes occurring in the systems of alumina production. The creation of digital databases and libraries for experimental data is also relevant

Further improvement of the mathematical apparatus is associated with the need to improve the efficiency of multi-threaded calculations when calculating technological systems. When combined with access to powerful computing resources, creates the conditions for a transition to a new level of solving production technological problems, including multi-parameter optimization of alumina refineries.

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