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].

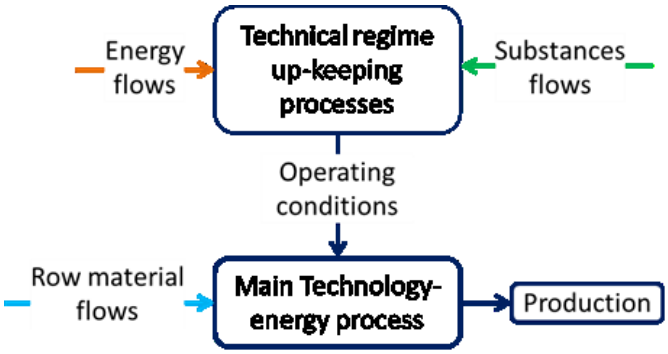

Figure 1. Generalized structure of the metallurgical process: the first approximation scheme.

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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7. References

1. D.A. Diomidovskyi, *Control and automation of processes in non-ferrous metallurgy. Part 2*. *Automation of metallurgical processes*. Moscow, Metallurgy. (1967). 404 p.
2. J. Perregaard, E.L. Serensen, Simulation and optimization of chemical processes: numerical and computational aspects, *European Symposium on Computer Aided Process Engineering*. (1992). P. 247-254.
3. W.F. Ramirez, *Computational Methods for Process Simulation. Second edition*. 1997. Oxford, Reed Educational and Professional Publishing Ltd. (1997). 461 p.
4. H. Elmqvist, M. Otter, Methods for tearing systems of equations in object-oriented modeling, *Proceeding of European Simulation Multiconference, ESM'94*. Barcelona. Spain. June 1-3. 1994. pp. 326-332.
5. S.A. Stage, Comments on An Improvement to the Brent's Method, *International Journal of Experimental Algorithms.* Vol. 4. Iss. 1. (2013). P. 1-16.
6. D. Metzger, Adaptive damping for dynamic relaxation problems with non-monotonic spectral response, *International Journal for Numerical Methods in Engineering*. Vol. 56. Iss. 1. (2003). P. 57–80.
7. J. Jeffers, J. Reinders, A. Sodani, *Intel Xeon Phi Processor High Performance Programming (Second Edition)*. Knights Landing Edition. 2016. P. 297–314.
8. S. Stoykov, S. Margenov, Scalable parallel implementation of shooting method for large-scale dynamical systems. Application to bridge components, *Journal of Computational and Applied Mathematics*. Vol. 293. (2016). P. 223-231.

9. D.B. Leinewebera, I. Bauer, H.G. Bock, An efficient multiple shooting based reduced SQP strategy for large-scale dynamic process optimization. Part 1: theoretical aspects, *Computers & Chemical Engineering*. Vol. 27. Iss. 2. (2003). P. 157–166.
10. D.B. Leinewebera, I. Bauer, H.G. Bock, An efficient multiple shooting based reduced SQP strategy for large-scale dynamic process optimization. Part II: Software aspects and applications, *Computers & Chemical Engineering*. Vol. 27. Iss. 2. (2003). P. 167–174.
11. J. Aipeng, J. Zhushu, H. Jingtao, W. Jian, Research of Large-Scale Reduced SQP Algorithm for Chemical Process System Optimization, *IFAC Proceedings Volumes*. Vol. 41. Iss. 2. (2008). P. 11034–11040.
12. D. Wu, J. Terpenny, W. Gentzsch, Cloud-Based Design, Engineering Analysis and Manufacturing: A Cost-Benefit Analysis, *Procedia Manufacturing*. Vol. 1. (2015). P. 64–76.
13. I. Ari, N. Muhtaroglu, Design and implementation of a cloud computing service for finite element analysis, *Advances in Engineering Software*. Vol. 60–61. (2013). P. 122-135.
14. H. Zhao, M. Harmse, J. Guiver, W.M. Canney, Subspace identification in industrial APC applications – A review of recent progress and industrial experience, *IFAC Proceedings Volumes*. Vol. 39. Iss. 1. (2006). P. 1074-1079.
15. I.S. Moreira, G.A. Neumann, A.T.M. Oliveira, Why some APC applications lose performance over time and how you can avoid it., *IFAC Proceedings Volumes*. Vol. 46. Iss. 32. (2013). P. 833-836.
16. S.P. Rosenberg, S.J. Healy, A thermodynamic model for gibbsite solubility in Bayer liquors, *4-th Int. Alumina Quality Workshop*, Darwin. (1996). P. 301-310.
17. I. Livk, D. Ilievski, Macroscopic agglomeration kernel model for gibbsite precipitation in turbulent and laminar flows, *Chemical Engineering Science*. Vol. 62. Iss. 14. (2007). P. 3787-3797.
22. V.N. Brichkin, D.A. Kremcheeva, V.A. Matveev, Quantitative influence of the seed on the indicators of mass crystallization of chemical precipitation, *Journal of Mining University*. Vol. 211. (2015). P. 64-70.
19. D. Ramkrishna, *Population balances. Theory and Applications to Particulate Systems in Engineering*. London.: Academic Press. (2000). 355 p.
20. M.J. Hounslow, J.D. Litster, D.J. Smit, Adjustable Discretized Population Balance for Growth and Aggregation, *AlChE Journal*. Vol. 41. Iss. 3. (1995). P. 591-603.
21. V.O. Golubev, D.G. Chistiakov, V.N. Brichkin, T.E. Litvinova, Systems and aids mathematical modeling of the alumina refinery methods: problems and solutions, *Non-ferrous Metals*. No 1. (2019). P. 40-47.