Instrumented system “Engineering-Metallurgy” for solving a wide class of engineering tasks

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Abstract. The instrumented system “Engineering-Metallurgy” is presented in the form of a set of programs and databases adapted for a number of metallurgical technologies that helps to perform multivariate calculations, conduct research, solve various optimization problems and determine the best conditions for implementation of metallurgical processes.

1. Introduction
One of the most important problems that ferrous and non-ferrous metallurgy industries are currently facing is the reduction in the costs per unit of raw materials and energy per unit of output, that is, the problem of creating energy and resource-saving technologies [1]. The development of new resource-saving technologies is impossible without computational experiments that allow the states and processes to be analyzed and conclusions about the behavior of the objects under investigation to be drawn on the basis of model representations. Therefore, at the present time it is actual to create instrumental systems that implement mathematical models and allow calculations, studies to be efficiently performed and various optimization problems to be solved. To solve these problems with the use of MS Excel and Delphi, the instrumented system “Engineering-Metallurgy” was created, which performs the tasks determining the optimal conditions for the implementation of metallurgical technologies, in which a mathematical description of the interconnection of flows and process parameters is implemented using a set of mathematical deterministic models, based on the first and second laws of thermodynamics [2 - 4].

2. Structure, functions and purpose of the instrumented system
The instrumented system, the structural diagram of which is shown in figure 1, is a set of programs adapted for a number of metallurgical technologies. The programs include a set of standard blocks: “Input data”, “Balances”, “Enthalpies”, “Activities”, “Reactions”, “Technical and economic indicators”, “Optimization”, “Graphic”, “Research”, in which the following databases are used: “Chemical composition of materials”, “Thermal properties of individual substances”, “Parameters of interaction of the first order”, “Atomic parameters”, “Thermodynamic characteristics of reactions of phase transitions and dissolution of elements”.

The algorithm for calculating the optimal modes of metallurgical processes in the “Engineering-Metallurgy” system is shown in figure 2.

Data of thermodynamic functions of substances are used for the calculation using the database “Thermodynamic properties of individual substances”.

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In the “Activities” block, the activities of metal components are calculated using the apparatus of interaction parameters, slag – according to the theory of collectivized electrons and partial pressures of the gas phase. When calculating activities, the databases “Parameters of interaction of the first order” and “Atomic parameters” are used. Thermodynamic analysis of chemical reactions is carried out by the constant method in the “Reactions” block. The list of independent reactions is formed using the methods of thermodynamic modeling in the result of analysis of all possible reactions of the system transition from the initial state to the final one. The scheme for calculating thermodynamic characteristics of the main types of metallurgical reactions is shown in figure 3. For reactions of combustion, reduction, oxidative refining and reactions between individual substances, a change in the isobaric-isothermal potential and the equilibrium constant are calculated. For this purpose, we use data on the calculation of thermodynamic functions of individual substances using a directory on the thermal properties of substances and databases on the thermodynamic characteristics of reactions of phase transitions and the reactions of dissolution of elements in liquid iron.

An estimate is made of the degree of reactions deviation from thermodynamic equilibrium by analyzing the ratio of the product of the activities of the reacting substances to the equilibrium constant. For this purpose, data on the activity of metal and slag components are used.

The block “Technical and economic indicators” is presented by the table of calculation of the unit’s productivity, unit costs of materials, cost and energy intensity of the product. In this case, a database of values of specific energy intensities of materials is used.
Figure 2. Algorithm for calculating the optimal modes of metallurgical process in the instrumented system “Engineering-Metallurgy”.
Figure 3. Calculation scheme of thermodynamic characteristics of chemical reactions.

In the “Optimization” block the problem of determining the optimal technological modes of metallurgical processes is solved, which consists in calculating control actions for obtaining a product with specified properties while optimizing one of the criteria. The following indicators can be chosen as criteria: total consumption of charge materials; the cost per unit of output, the cost of production, the energy intensity of the process or the capacity of the unit.

The solution of the optimization problem consists in determination of the extremum of one of the above criteria when performing limitations on the ranges of change in the flow components of the input streams; observance of the law of mass conservation at the level of flows, substances and elements; observance of the law of conservation of energy; compliance with restrictions on the parameters of the finished product; fulfillment of the normalizing relations and fulfillment of the target conditions by the remaining criteria.

The scheme for setting and solving the optimization problem is shown in figure 4. The problem is solved by the method of nonlinear programming – the generalized reduced gradient.
Figure 4. The scheme for solving the optimization problem.

In the “Optimization” block the summary results of the calculation are also presented: material balance by flows, total heat balance, technical and economic indicators and compositions of metal, slag and gas. In the “Visual content” block the graphical representation of the results in the form of histograms, pie charts and graphs is realized provides a full analysis of the results.

In the “Research” block a summary table with the results of multivariate studies is formed, followed by the possibility of plotting, including the values of unit costs of materials, technical and economic indicators, parameters of metal, slag and gas, and other necessary parameters for the chosen technology option.

The modules “Enthalpies”, “Activities”, “Reactions”, “Optimization”, “Graphics” and “Research”, as well as the databases used are standard and can be used to calculate all types of processes by coordinating data with the “Input data” and “Balances” blocks, which, like the module “TEI”, are adapted to the specific technology option.

In the software complex, various directories are implemented in the form of databases, the main of which is a directory on the thermodynamic properties of individual substances. It includes the following information: the chemical formula of the substance with the indication of the phase state, molar mass, enthalpy of formation and entropy of the substance at standard temperature, the temperature and the change in the enthalpy of phase transitions, and the coefficients of the approximation equation for the reduced Gibbs energy. The database of the software complex “Terra” [5] and the handbook on thermodynamic properties of individual substances “TSIV” [6] are taken as a basis.

The instrumented system includes a set of programs for the following technology options: oxygen-converter process, electric steelmaking process, steel alloying processes in the ladle, direct metal production from iron-containing materials, processing of titanium-magnesium concentrates and
manganese ores, direct reduction of iron with co-production of synthesis gas in the unit of a jet-emulsion type, combustion processes of various types of fuel in the vortex adiabatic furnace, the process of obtaining copper in the anode furnace, process for the production of siliconmanganese and a manganese production process in the plasma furnace. The developed software package was registered by the Federal Service for Intellectual Property of the Russian Federation (No. 2017617445).

3. Conclusion
Thus, the created instrumented system “Engineering-metallurgy” makes it possible to carry out multivariate calculations, conduct research and solve a complex of interrelated optimization problems for determining the best conditions for metallurgical processes [7 - 10]. The use of this software tool allows the labour productivity of researchers to be significantly increased and conditions for objective assessment of the obtained results reliability to be created.

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