Mathematical models of phase composition diagrams in multicomponent oxide systems and their applied significance

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Production of high-quality products requires knowledge of the phase composition of both the raw materials and the final product. Usually, phase diagrams are used for this purpose. However, they are usually three-component diagrams, while natural and man-made formations are multicomponent diagrams. In this paper, it is proposed to use mathematical models of phase composition diagrams for these purposes. Mathematical models have no restrictions on the number of oxides (or metals) presented in raw materials or finished product, they operate in a multidimensional space, not only in a three-dimensional one, where phase diagrams or physical properties are usually displayed. The authors have created mathematical models of a number of three-, four-, five- and six-component systems. The computer programs, which were created on the basis of the models, allow calculation of the numerical values of the phases with high accuracy. In this paper, mathematical models of one quinary $MgO-MnO-CaO-SiO_2-Al_2O_3$ and two six-component systems $CaO-SiO_2-Al_2O_3-MgO-FeO-Fe_2O_3$ and $CaO-MgO-FeO-Cr_2O_3-Al_2O_3-SiO_2$ were used to analyze the issue under discussion. They can describe the slag procedure of blast furnace and cupola smelting of cast iron, production of steel as well as silicon, manganese, chromium ferroalloys and slag-stone castings. The aim of the work is to develop and to apply mathematical models of phase composition for analysis and selection of the chemical composition of raw materials in manufacture of high-quality products, including slag casting and metallurgical slags. The work is aimed at creating numerical methods for calculating the phase composition of multicomponent systems and their use in optimizing processes such as cast iron making, steel making and ferroalloy production, as well as for solving the problems related to the creation of slag-cast products intended for storing and pumping acids, burying radioactive substances or lining of high-temperature zones in smelting furnaces.
Key words: rocks, slags, oxides, acidity, phase composition, diagram, mathematical model, computer program.
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Introduction

Industrial enterprises are aimed on manufacturing products with definite phase composition — just phase composition not chemical one, because it mainly determined the quality of fabricated components. The chemical composition, being a suitable tool, is used for stenciling of raw materials and manufactured products, calculation of cherge materials, accounting of extraction of the required elements in finished product. However, the important material propertieds are determined by the phase composition. This work proposes a numerical method for selection of raw material chemical composition via the preset phase composition of a casting. It is examined mainly on the example of slag-stone castings, which ar characterized by high strength, wear resistance, thermal resistance, acid resistance, providing thereby competitiveness with many materials (including steel and cast iron). Ability of slag-stone castings to withstand to the effect of durable and powerful radio emission should be especially emphasized [1, 2]. The main products of slag-stone castings are wear-resistant and corrosion resistant planches of different sizes for lining, paving stones, edge stones, pipes, angle pipes, gutters, multicyclones and other shape components [3, 4]. Mul lines and coke battery ramps, which are lined by stone cast planches, have service life at least 10 years (in comparison with 2 years for other equipment).

Availability of raw materials for manufacture of cast products is usually evaluated using scidity coefficient (K) and pyroxene module (M_{py}) [5]. They are based on examination of a large scientific and industrial experience of stone castings made of different raw materials and promored development of of stone casting science itself. However, they don't allow direct calculation of phase composition of products, which determines mainly their service properties. Thus, building of various special diagrams and consideration of phase equilibrium diagrams was rather natural. But most part of these diagrams are binary or ternary ones, while natural or technogenous eaw material is identified as multicomponent one. Thereby, to analyze formation of phases of the same material, just several ternary diagrams are used, e.g. the diagrams $CaO-Al_2O_3-SiO_2$, $MgO-Al_2O_3-SiO_2$, $CaO-MgO-SiO_2$, $CaO-FeO-SiO_2$ [6], with revealing each phase via geometrical building. Complication of this procedure and insufficient accuracy of measuring difital phase values from the diagrams is evident. Indeed, we need the diagram of quinary system $CaO-SiO_2-Al_2O_3-MgO-FeO$, but it can't be reflected correctly in 3D space (which is usual dir diagram building) and can't be used on the base of geometrical buildings. To obercome this difficulty, it is suggested in this research to use the mathematical models of phase composition ndiagrams for multo-component systems (these models were developed by the authors). Principally, mathematical models have no restrictions on amount of oxides (presented in raw materi al or in finished product), they operate in multi-dimensional space, not only in 3D, where phase equilibrium diagrams or physical properties are usually displayed. The aim of this research is development of mathematical models for multi-component oxide systems and reveal of the features of their use for solving applied problems.

Research methods

Creation of a diagram begins from dividing the examined system to elementary polytops (triangles, tetrahedrons, pentatopes, hexatopes etc.) in equilibrium to the existing phases. This research uses for this case the method of minimization of Gibbs free energy variation for reacting compounds [7, 8]. Then the mathematical model of a phase composition diagram is created. The authors used their self method for this research [9], it is based on balance of distribution of slag oxides according to the forming phases. The computer programs were created on the base of obtained models. They were used for analysis of slag conditions in manufacture of different metals and slag-cast products. The obtained data were applied for improvement of technological processes.

Results of the researches

Mathematical models of the phase composition diagrams were created in this research for one quinary system $MgO-MnO-CaO-SiO_2-Al_2O_3$ and two six–component systems $CaO-SiO_2-Al_2O_3-MgO-FeO-Fe_2O_3$ and $CaO-MgO-FeO-Cr_2O_3-Al_2O_3-SiO_2$. The first system included 34 pentatopes (five-vertex) and in the second and third systems – 126 and 121 hexatopes (six-vertexes) respectively. Mathematical model is created for each polytope. For this purpose, distribution of initial oxides in the forming phases is described for each polytope. For better suitability, they were signed as CaO–C_0, SiO_2–S_0, FeO–F'_0, Fe_2O_3–F_0, $CaO{\cdot}SiO_2$–CS, $2CaO{\cdot}Al_2O_3{\cdot}SiO_2$–$C_2AS$, $2CaO{\cdot}FeO{\cdot}2SiO_2$–$C_2F'S_2$ etc. So, the following distribution equations of initial oxides in the forming phases were presented in the hexatope N126 CS–CMS_2–$CF'S_2$–CAS_2–F′F–S of the phase composition diagram for the system $CaO-SiO_2-Al_2O_3-MgO-FeO-Fe_2O_3$:

$$C_0 = 0.2593 \cdot CMS_2 + 0.2014 \cdot CAS_2 \quad (1)$$

$$S_0 = 0.6 \cdot MS + 0.555 \cdot CMS_2 + 0.4317 \cdot CAS_2 + 1 \cdot S \quad (2)$$

$$A_0 = 0.3669 \cdot CAS_2 \quad (3)$$

$$M_0 = 0.4 \cdot MS + 0.1857 \cdot CMS_2 \quad (4)$$

$$F'_0 = 0.3103 \cdot F'F \quad (5)$$

$$F_0 = 0.6897 \cdot F'F + 1 \cdot F \quad (6)$$

where the coefficients at the phases mean content of oxides in these phases in mass fractions.

Their joint solution allows obtaining of the equations (7)–(12) for calculation of the phases based on the known material chemical composition:

$$CS = 2.070 \cdot C_0 - 1.136 \cdot A_0 - 2.898 \cdot M_0 - 1.613 \cdot F'_0 + 0.725 \cdot F_0 \quad (7)$$

$$CMS_2 = 5.399 \cdot M_0 \quad (8)$$

$$CF'S_2 = 3.448 \cdot F'_0 - 1.551 \cdot F_0 \quad (9)$$

$$CAS_2 = 2.725 \cdot A_0 \quad (10)$$

$$F'F = 1.449 \cdot F_0 \quad (11)$$

$$S = -1.070 \cdot C_0 \cdot 1 \cdot S_0 - 0.589 \cdot A_0 - 1.500 \cdot M_0 - 0.834 \cdot F'_0 + 0.375 \cdot F_0 \quad (12)$$

Such mathematical models were created for 34 pentatopes of the system $MgO-MnO-CaO-SiO_2-Al_2O_3$. 126 hexatopes of the system $CaO-SiO_2-Al_2O_3-MgO-FeO-Fe_2O_3$ and 121 hexatopes of the system $CaO-MgO-FeO-Cr_2O_3-Al_2O_3-SiO_2$; 75,756 and 726 equations were obtained and solved for the first, second and third systems respectively.

The equations of (7)–(12) kind followed from the equations (1)–(6), but both systems have theit independent importance. The equations (1)–(6) allow colculation of the required chemical composition of initial raw materials via preset phase composition of a component, while the equations (7)–(12) make it possible to determine phase composition of raw materials or castings via preset chemical composition.

So, slag-cast products are created for definite tasks, e.g. for storage and pumping of acids, buring radioactive substances of lining of high-temperature areas in melting furnaces. Of course, phase composition of castings in these cases should be equal and raw material should be chosen according to these requirements. To solve such problems, it is suitable to use equations of (1)–(6) kind. Thus, if the casting consists only of diopside (CMS_2), then content of calcium oxide (C_0), silicon oxide (S_0) and magnesium oxide (M_0) in charge material should constitut, according to the equations (1)–(6), the following values (mass. %):

$$C_0 = 0.2593 \cdot CMS_2 = 0.2593 \cdot 100 = 25.93$$

$$S_0 = 0.5550 \cdot CMS_2 = 0.5550 \cdot 100 = 55.50$$

$$M_0 = 0.1857 \cdot CMS_2 = 0.1857 \cdot 100 = 18.57$$

Consumption of limestone, chalk, quartzite and dolomite can be determined practically via the obtained numerical data. In such way light stone casting is obtained [10].

Melilite provides high level of operating parameters in castings. It is a solid solution of helenite (C_2AS) and akermanite (C_2MS_2). Raw material for manufacture of castings with melilite can be chosen iding the equations (13)–(18) of hexatope N83 C_2MS_2–C_2AS–CAS_2–MA– F′F– F.

$$C_0 = 0.4118 \cdot C_2MS_2 + 0.409 \cdot C_2AS + 0.2014 \cdot CAS_2 \quad (13)$$

$$S_0 = 0.4412 \cdot C_2MS_2 + 0.219 \cdot C_2AS + 0.4317 \cdot CAS_2 \quad (14)$$

$$A_0 = 0.372 \cdot C_2AS + 0.3669 \cdot CAS_2 + 0.7183 \cdot MA \quad (15)$$

$$M_0 = 0.147 \cdot C_2MS_2 + 0.2817 \cdot MA \quad (16)$$

$$F'_0 = 0.3103 \cdot F'F \quad (17)$$

$$F_0 = 0.6897 \cdot F'F + 1 \cdot F \quad (18)$$

Helenite and akermanite are characterized by various melting temperatures. The suggested equations allow preparing charges with different relationship of these phases, in order tro select e.g. melting equipment. Thus, when manufacturing the casting with melilite containing of 50 % helenite and 50 % akermanite, raw material should contain the following amounts of oxides (mass. %):

$$C_0 = 0.4118 \cdot 50 + 0.409 \cdot 50 = 41.04$$
$$S_0 = 0.4412 \cdot 50 + 0.219 \cdot 50 = 33.01$$
$$A_0 = 0.372 \cdot 50 = 18.6$$
$$M_0 = 0.147 \cdot 50 = 7.35$$

Uncluding these data finalizes in the equations (19)–(24), which were obtained from the equations (13)–(18):

$$C_2MS_2 = 0.692 \cdot C_0 + 0.648 \cdot S_0 - 1.143 \cdot A_0 + 2.915 \cdot M_0 \quad (19)$$
$$C_2AS = 2.794 \cdot C_0 - 1.995 \cdot S_0 + 0.767 \cdot A_0 - 1.957 \cdot M_0 \quad (20)$$
$$CAS_2 = -2.125 \cdot C_0 + 2.645 \cdot S_0 + 0.779 \cdot A_0 - 1.986 \cdot M_0 \quad (21)$$
$$MA = -0.361 \cdot C_0 - 0.338 \cdot S_0 + 0.596 \cdot A_0 + 2.028 \cdot M_0 \quad (22)$$
$$F'F = 3.222 \cdot F'_0 \quad (23)$$
$$F = -2.222 \cdot F'_0 + 1 \cdot F \quad (24)$$

It provides 50 % helenite and 50 % akermanite in this casting. I.e. melilite with the preset composition. It is known that mililite is contained in various slags during ironmaking in bkast furnaces. High-temperature refractories are required in the industry, and they can be fabricated via casting from natural or technogenous materials. The required chemical composition of technogenous materials can be determined via the mathematical models which were developed in this research. So, initial and final equations for analysis of forming in the hexatope N108 A_3S_2–CAS_2–$M_2A_2S_5$–$F'_2A_2S_5$–$F'A$–$F'F$ look like the equations (25)–(30) and (31)–(36).

Thje equations of oxides distribution to phases:

$$C_0 = 0.2014 \cdot CAS_2 \quad (25)$$
$$S_0 = 0.282 \cdot A_3S_2 + 0.4317 \cdot CAS_2 + 0.5137 \cdot M_2A_2S_5 + 0.463 \cdot F'_2A_2S_5 \quad (26)$$
$$A_0 = 0.718 \cdot A_3S_2 + 0.3669 \cdot CAS_2 + 0.3493 \cdot M_2A_2S_5 + 0.3148 \cdot F'_2A_2S_5 + 0.5862 \cdot F'A \quad (27)$$
$$M_0 = 0.137 \cdot M_2A_2S_5 \quad (28)$$
$$F'_0 = 0.2222 \cdot F'_2A_2S_5 + 0.4138 \cdot F'A + 0.3103 \cdot F'F \quad (29)$$
$$F_0 = 0.6898 \cdot F'F \quad (30)$$

The equations for calculating phases via content of oxides in raw material:

$$A_3S_2 = -2.537 \cdot C_0 - 7.705 \cdot S_0 + 1.392 \cdot A_0 - 3.550 \cdot M_0 - 1.937 \cdot F' + 0.887 \cdot F \quad (31)$$
$$CAS_2 = 4.965 \cdot C_0 \quad (32)$$
$$M_2A_2S_5 = 7.299 \cdot M_0 \quad (33)$$
$$F'_2A_2S_5 = -3.084 \cdot C_0 + 2.159 \cdot S_0 - 0.848 \cdot A_0 - 5.955 \cdot M_0 + 1.201 \cdot F' - 0.540 \cdot F \quad (34)$$
$$F'A = 1.656 \cdot C_0 - 1.159 \cdot S_0 + 0.455 \cdot A_0 + 3.187 \cdot M_0 - 1.771 \cdot F' - 0.796 \cdot F \quad (35)$$
$$F'F = 1.449 \cdot F \quad (36)$$

It can be seen that the rquations are valid for selection of chemical composition for initial charge (used in production of both mullite refractories A_3S_2 – $3Al_2O_3{\cdot}2SiO_2$ and cordeirite refractories $M_2A_2S_5$ – $2MgO{\cdot}2Al_2O_3{\cdot}5SiO_2$. In order to manufacture combined casr refractorym containing 70 % of mullite and 30 % of cordierite, the charge have to contain:

$$S_0 = 0.282 \cdot 70 + 0.5137 \cdot 30 = 19.74 + 15.41 = 35.15$$
$$A_0 = 0.718 \cdot 70 + 0.3493 \cdot 30 = 50.26 + 10.48 = 60.74$$
$$M_0 = 0.137 \cdot 30 = 4.11$$

When substituting the obtained data in the equations (31)–(36), it can be seen that cast refractory with preset phase composition is obtained. If required, magnetite ($F'F$), hercynite ($F'A$), anortite (CAS_2) can be introduced as a selected phase, in addition to mullite and cordierite.

The cast products made of oxide materials are not manufactured in Kazakhstan, though appr. 2 mln. t of slags is produced. Their availability for manufacture of slag-cast products was assessed using calculation of phase composition. Establishment of the polytope related to location of raw material (preset with remote control pulpit) is difficult, because it is impossible to reflect correctly a six-component system in 3D space. This problem can be solved in the following way. Chemical composition of raw material is preset using remote control pulpit and then automatically substituted in all polytopes. When all phases in any polytope are characterized by positive numerical values (summarized as 100 %), calculation is finished. Such polytope is inique for any concrete raw material. Then, without stopping the calculation procedure, the number of the required polytope and phase composition of raw material (or product) is sent to a monitor or a printer in 5 (mass.) (**Fig. 1**).

Chemical and calculated phase compositions of several slags from Kazakhstan works are presented in the **Table 1** and **Table 2** respectively.

Based on the data from the Table 2, we can state that blast furnace slag from "Qarmet" metallurgical works (Temirtau) consists for 90 % of helenite ($2CaO{\cdot}Al_2O_3{\cdot}SiO_2$), magnesial spinel ($2CaO{\cdot}MgO{\cdot}2SiO_2$) and ferriferous akermanite ($2CaO{\cdot}FeO{\cdot}2SiO_2$). They form together a solid solution of melilite. In other words, blast furnace slag from "Qarmet" metallurgical works is practically a miulti-phase compound, what provides heterogeneity of its properties through a whole ingot volume.

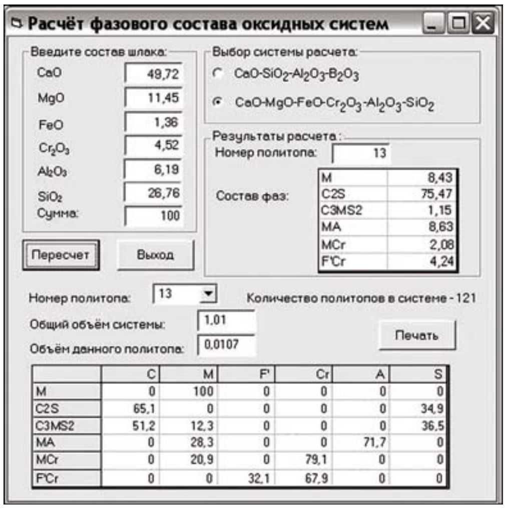

Fig. 1. The program window screenshot for calculation of phase composition

Table 1. Parameters of metallurgical slags from Kazakhstan works

Slag	Content of the components. %							
	CaO	SiO_2	Al_2O_3	MgO	FeO	MnO	Cr_2O_3	Fe_2O_3
Blast furnace slag “Qarmet”	40.2	37.2	13.8	8.3	0.50	–	–	–
Melting of SiMn	22.94	47.26	9.76	2.44	0.46	17.14	–	–
Melting of carbonaceous ferrochromium	0.8	33.4	17.1	44.8	–	–	3.9	–
Melting of copper matte	3.2	36.3	4.0	0.5	52.21	–	–	3.79

Table 2. Phase composition of slags from Kazakhstan works

1	Blast furnace slag «Qarmet»					
	Phase composition. % (mass.)					
	Wollastonite	Helenite	Akermanite	Ferroakermanite	Anorthite	
	$CaO{\cdot}SiO_2$	$2CaO{\cdot}Al_2O_3{\cdot}SiO_2$	$2CaO{\cdot}MgO{\cdot}2SiO_2$	$2CaO{\cdot}FeO{\cdot}2SiO_2$	$CaO{\cdot}Al_2O_3{\cdot}2SiO_2$	
	4.26	31.93	56.46	2.11	5.24	
2	Melting of silicomanganese slag at Aksusky plant of ferroalloys					
	Phase composition. % (mass.)					
	Wollastonite	Manganese monosilicate	Tephroite	Diopside	Anorthite	
	$CaO{\cdot}SiO_2$	$MnO{\cdot}SiO_2$	$2MnO{\cdot}SiO_2$	$CaO{\cdot}MgO{\cdot}2SiO_2$	$CaO{\cdot}Al_2O_3{\cdot}2SiO_2$	
	29.31	25.48	5.43	13.12	26.66	
3	Melting of carbonaceous ferrochromium slag at Aktyibinsky plant of ferroalloys					
	Phase composition. % (mass.)					
	Forsterite	Anorthite	Cordierite	Magnesial spinel	Alumochromite	
	$2MgO{\cdot}SiO_2$	$CaO{\cdot}Al_2O_3{\cdot}2SiO_2$	$2MgO{\cdot}2Al_2O_3{\cdot}5SiO_2$	$MgO{\cdot}Al_2O_3$	$MgO{\cdot}Cr_2O_3$	
	65.6	3.96	7.17	18.3.4	4.93	
4	Melting of matte slag in a Vanyukov furnace at Balkhash copper-smelting plant					
	Phase composition. % (mass.)					
	Fayalite	Ferrosilite	Hedenbergite	Diopside	Anorthite	Magnetite
	$2FeO{\cdot}SiO_2$	$FeO{\cdot}SiO_2$	$CaO{\cdot}FeO{\cdot}2SiO_2$	$CaO{\cdot}MgO{\cdot}2SiO_2$	$CaO{\cdot}Al_2O_3{\cdot}2SiO_2$	Fe_3O_4
	41.87	37.69	1.35	2.70	10.9	5.5

Wollastonite ($CaO{\cdot}SiO_2$) is a dominating phase in slags of manufacturing of silicomanganese at the Aksusky plant of ferroalloys. But presence of diopside ($CaO{\cdot}MgO{\cdot}2SiO_2$) in these slags, which is mostly useful for slag-stone casting and which is able to accept bivalent cations, is rather interesting. Such cations can be presented by manganese, which is containing in slag in the form of silicates ($MnO{\cdot}SiO_2$ and $2MnO{\cdot}SiO_2$). This slag can also be characterized by forming of olivines $(Mg,Mn){\cdot}SiO_4$ and continuous set of solid solutions among Mg_2SiO_4 and Mn_2SiO_4, what can be considered as a positive sign in manufacture of cast products. It is known that Nikopol plant of ferroalloys had experience in manufacturing foundation blocks on the base of slags obtained during smelting of silicomanganese [11]. These slags differ slightly from the slags manufactured at the Aksusky plant of ferroalloys, thereby fabrication of cast products from Aksus ferroalloys can be realized.

Forsterite and magnesial spinel are considered as slag dominating phases during smelting of carbonaceous ferrochromium. Forsterite (65.6 %) prevails in this composition, while its sum with magnesial spinel (18.34 %) makes 83.94 %. They are combined of singular anions, and molten slag should have low viscosity. But both these two phases are gigh-temperature ones: $2MgO{\cdot}SiO_2$ is subjected to melting at 2163 K, while $MgO{\cdot}Al_2O_3$ $MgO{\cdot}Al_2O_3$ – at 2408 K, and thereby the temperature of slag crystallization is located within the range 1923–1973 K. Thus, slag is so-called “short” and is crystallized in this temperature range, what hampers obtaining of cast products directly from slag. So, correction of slag composition by additives is required.

A molten slag of copper matte at the Vanyukov firnace of Balkhash copper-smelting plant is acidic and consists mainly of silica (SiO_2) and iron monoxide (FeO), totally constituting 95–96 %. Calcium oxide (CaO) is also presented in small amount (up to 4 %) in these substances, while iron silicates (Fe_2SiO_4 and $FeSiO_3$) with total amount 79.56 % prevail in slag. We can hardly plan manufacture of cast products with these components. It is noted that the pilot site for fabrication of cast products from copper slags (but only with addfition of Kounrad diabases) operated at Balkhash plant still in 1960 [3].

Mathematical models of the above-mentioned systems can describe a slag procrdure for blast furnace of cupolsa furnace iron making, steel making and also manufacture of silicon, manganese and chromium ferroalloys. The slag procedure for producrion of several metals is analyzed and the measures for its improvement are suggested. It was established that problems on smelting of carbonaceous ferrochromium on the baze of Kazakhstan ores are connected with growth of magnesium oxide and transition of slags from the area of magnesial spinel ($MgO{\cdot}Al_2O_3$) crystallization to the area of forsterite ($2MgO{\cdot}SiO_2$) (**Table 3**).

The authors proposed to introduce low-melting flux in the charge for production of this ferroalloy. Based on the data of industrial testing, decrease of Cr_2O_3 content on slag by 0.35–0.48 %, increase of Cr content in the ferroalloy (from 66.9 to 67.45 %) and elevation of furnace productivity by 0.8 % were achieved [12].

There is a problem of decomposition of high-basic slags to fine-dispersed powder, what causes environmental problems. It was established via calculations that bicalcium silicate (C_2S) is presented in slags in the p;rocess of manufacturing large amounts of refined ferrochromium grades (**Table 4**). This silicate transits from stable β-form to decomposed γ-form in the conditions of temperature decrease, with volume increase by 12 % and slag transformation in fine-dispersed dust.

It was suggested by the authors to introduce Kazakhstan borate ores in charge for manufacture of this ferroalloy, with the purpose to obtain 0.3–0.5 % B_2O_3 in slag. This technology was put into practice at the ferroalloy plant in Kazakhstan [13]. Slag is not decomposed after cooling, it is produced in a lumpy form and is used as rubble for road construction.

Thus, mathematical models of the diagrams of MgO–MnO–CaO–SiO_2–Al_2O_3, CaO–SiO_2–Al_2O_3–MgO–FeO–Fe_2O_3 and CaO–MgO–FeO–Cr_2O_3–Al_2O_3–SiO_2 systems are suggested in order to choose raw material for manufacture of slag-cast products and assessment of phase composition of these products. The models are realized as computer programs and can be useful also for assessment of a slag procedure during iron making, steel making and production of ferroalloys.

Conclusion

The mathematical models of phase composition for multi-component systems, which are presented in this research, open new possibilities for more exact forecast and noptimization of manufacturing processes for high-quality metallurgical products. Use of these models allows overcoming any difficulties in application of conventional equilibrium diagrams, which are usually restricted by three components. The developed mathematical models for the multi-component systems, such as MgO–MnO–CaO–SiO_2–Al_2O_3, CaO–SiO_2–Al_2O_3–MgO–FeO–Fe_2O_3 and CaO–MgO–FeO–Cr_2O_3–Al_2O_3–SiO_2, provide possibility of more precise selection of chemical composition for raw material in manufacture of various metals and slags.

The demontrated numerical method for selection of chemical composition for raw material on the base of presen phase composition of a casting is considered as an important tool for implementation of special tasks, such as manufacture of slag-cast products for storage of dangerous substances or for lining of high-temperature furnaces. Practical assessment of availability of metallurgical slags and proposed methods for solving the problems, which are connected with ferrochromium production of Kazakhstan chromium ores, ensures rise of efficiency and stability of metallurgical production processes.

Thus, the results of this research can be useful both for scientific investigations in the field of phase analysis and for practical use in metallurgy. It allows achieving high standards of quality and ecological safety during manufacture if finished products.

Table 3. Composition of slags in production of carbonaceous ferrochromium

No.	Years	Chemical composition, %			Phase composition, %		
		SiO_2	Al_2O_3	MgO	$MgO·Al_2O_3$	SiO_2	$2MgO·SiO_2$
1	1942–1945	39.5	29.0	31.5	40.4	24.6	35.0
2	1950–1952	32.7	28.5	38.8	39.8	12.2	47.9
3	1960–1963	34.9	23.9	41.2	33.4	11.2	55.4
4	1968–1969	33.4	21.9	44.7	30.6	6.5	62.9
5	1987–2000	35.1	18.0	46.9	25.0	5.0	70.0

Table 4. Chemical and phase composition of slags during manufacture of refined ferrochromium

No.	Composition. %														
	Chemical composition, %							Phase composition, %							
	CaO	SiO_2	Al_2O_3	MgO	Cr_2O_3	FeO	CaO/ SiO_2	M	C_2S	CCr	MA	MCr	fCr	CA	C_3MS_2
1	49.9	26.5	5.8	13.4	3.6	0.8	1.88	10.9	75.9	1.7	8.1	0.8	2.6	–	–
2	50.7	26.7	6.1	12.9	2.9	0.7	1.89	10.8	76.5	1.9	7.6	–	2.1	1.1	–
3	49.9	25.1	7.5	12.2	3.9	1.4	1.98	11.2	71.9	1.3	3.5	–	4.4	7.7	–
4	49.2	26.5	5.77	13.2	4.5	0.83	1.85	10.0	74.5	-	8.1	3.5	2.5	–	1.4
5	50.7	26.4	5.84	12.7	3.6	0.76	1.92	10.9	75.6	2.7	6.3	–	2.4	2.1	–

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