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NEW APPROACH TO EVALUATING THE THERMODYNAMIC CONSISTENCY OF MELTS IN THE ‘METAL–SLAG’ SYSTEM BASED ON INTERATOMIC INTERACTION PARAMETERS

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The article presents a new approach to evaluating the thermodynamic state of the ‘metal–slag’ system during metal smelting in oxidizing-reducing conditions. The interaction between the metal and slag is analyzed using the model of the structure of metallurgical melts, which considers cooperative ion exchange processes and interatomic interaction parameters. As a result of analyzing experimental data on the compositions of reacting melts during pig iron and steel smelting, criteria were developed for assessing the degree of achieving the equilibrium in the system regarding sulfur. The charge state parameters of the metallic system Z^Y and the slag system Δe, the slag stoichiometry index ρ, and the charge state parameter of the melt components Zi were used. The regularity of a consistent formation of metallic and slag melts has been established, which is evidenced by a significant correlation between the chemical equivalent of the metal composition Z^Y and the slag Δe. Analytical dependences were obtained in the form of $Z^Y = f(\Delta e, \rho)$. The identified patterns and criteria can be integrated into automated process control systems for regulating the slag regime and producing high-quality pig iron and steel.

Keywords: ‘metal–slag’ system, interatomic interaction parameters, charge state of the system, sulfur equilibrium, thermodynamic consistency of melts

1. Introduction

In the theory of metallurgical processes, one of the most important issues that remains unresolved is the influence of chemical composition on the thermodynamic characteristics and structure of melts, as well as on the results and the degree of completeness of their interaction under reducing and oxidizing conditions during metal smelting. Despite significant achievements in the field of physical materials science and the theory of chemical bonding, a fundamental theory of multicomponent melts that would allow calculating thermodynamic and physicochemical characteristics based on the known properties of pure components of a given composition of real metallurgical systems has not been created to this day.

Existing theoretical concepts and models of the structure of metal and slag systems do not yet provide a unified understanding of the physical-chemical essence of the analyzed processes, since they often rely on simplified representations of the electronic structure of substances. In particular, the results of representative theoretical and experimental studies of the charge state of cations and anions in ionic compounds show that the assumptions of the ion model about the integer charge multiplicities of ions and the spherical symmetry of their electron clouds do not correspond to reality.

Known models of modern liquid state theory of solutions (ideal, regular, subregular, associated, etc.) satisfactorily describe individual properties of simple systems and in some cases are applicable to multicomponent systems. However, obtaining practically valuable results using them in applied research for real metallurgical melts is quite challenging.

2. A review of recent studies and publications

The processes of interaction in the 'metal–slag' system have been studied in many scientific works, most of which consider equilibrium conditions for metal smelting [1–7]. To describe the results of interaction, criteria such as binding energy, activity coefficients, and interaction parameters of the components in the melts are considered. Equilibrium constants for the reactions occurring at the metal–slag interface are mainly obtained experimentally, and the expressions for their calculation depend on the authors' choice of model representations of the mechanism of interaction of structural particles in melts. In metallurgy practice, calculations of activities based on interaction parameters (Wagner parameters) [8] have gained the most widespread use.

Various models have been proposed for slag systems, including the model of regular ionic solutions by Kojevnikov [9, 10], the model of slag as a phase with collective electrons by Ponomarenko [11], the model of perfect ionic solutions by Temkin [12], and others. However, these models can only be applied within a narrow range of concentrations, and their implementation in automated control systems for metal smelting is associated with significant difficulties. In Ref. [13], a comparison of these methods led to the conclusion that the method proposed by Ponomarenko is the most suitable for real steelmaking slags.

The applicability of known models for modern metal smelting conditions has been analyzed in many scientific publications. In Ref. [14], it is noted that the implementation of these models (ionic model and regular solution model) in computational thermodynamics programs allows for complex calculations of the equilibrium between slag and metal in steelmaking. However, at present, there are still difficulties in calculating the thermodynamic properties of slags due to the lack of an adequate physicochemical model that could satisfactorily describe the structure of slags.

In Ref. [15], a physical-chemical model for the distribution of sulfur in the 'metal–slag' system was developed based on the mixed structure theory of slags. It allows determining the sulfur content in the metal in a steelmaking unit using the proposed complex thermodynamic parameters of metallic and slag melts. For the conditions of oxidizing smelting, a thermodynamic model of a multicomponent liquid slag with the valency of its components taken into account was proposed [16], based on the calculation of the activity coefficients of chemical elements in the slag. The authors showed that this model works over a wide range of concentrations and can be implemented in automated control systems for steelmaking processes.

The thermodynamic model of the condensed phase presented in Ref. [17] is based on quantum mechanical concepts and Gibbs distribution. Like most of similar statistical models, the successful implementation of this model is dependent on the availability and tuning of its parameters, which describe the behaviour of elements in the Fe–O binary system and Fe–Me–O ternary systems, where Me is a metal. Although satisfactory results have been obtained for calculating the parameters of a binary system, the development of a general thermodynamic model of 'metal–slag–gas' is required for more complex systems.

Some researchers use information about the thermodynamic characteristics of various reactions occurring in the 'metal–slag' system from reference books by different authors, which are often used in many computer programs (Astra, Plasma, Terra, etc.) [18].

Thus, it is evident that most studies of interaction processes in the metal–slag system are carried out using traditional thermodynamic tools that are capable of predicting equilibrium compositions. However, in real metallurgical processes, equilibrium is hardly ever achieved. Metallurgical melts are complex multicomponent systems with actively occurring interatomic physicochemical processes. Therefore, the study of the regularities of formation of the structure and properties of metallic and slag melts and the results of their interaction should be based on considering them as chemically unified systems, the changes in the composition of which affect all properties through the variation of electronic structure parameters.

The aim of this study is to develop a new approach to assessing the thermodynamic state of the 'metal–slag' system from the perspective of cooperative ion exchange processes and the consistency formation of the chemical composition of the metallic and slag melts under reducing and oxidizing conditions during metal smelting.

3. Principles of physical-chemical modelling of metallurgical systems

A new model of the structure of metallurgical melts has been developed at the Iron and Steel Institute of the National Academy of Sciences of Ukraine [19–21], according to which the description of the nature of chemical bonding in metallic and slag melts is based on a unified methodological basis of physical-chemical modelling theory, taking into account the determining role of the directionality of interatomic interactions.

The developed approach is based on the mathematical apparatus of the concept of directed chemical bonding [19–20], the basic core of which is the description of the physicochemical act of elementary interaction. The model of pairwise interatomic interaction is based on the use of the concept of ion radius (*Ru*), expressed through the tabulated parameters of the system of non-polarized ionic radii (SNIR) Ru^0 and tgα of each element. These parameters satisfy a set of equations:

$$\lg Ru_i = \lg Ru_i^0 - Z_i \cdot \mathrm{tg}\,\alpha_i. \tag{1}$$

Equations (1) describe the change in the radius of a polarized ion Ru_i depending on the effective charge Z_i, atomic radius Ru_i^0 and a parameter $\mathrm{tg}\alpha_i$ that characterizes the change in the ion radius from its charge.

The values of unpolarized atomic radii Ru_i^0 characterize their 'original' non-ionized state. These values are obtained by a deductive method as quantities that are interconnected with the basic characteristics of atoms and ions – mass, ionization potential, number of electrons on the outer orbit, electronegativity, etc. [19]. The parameters Ru^0 and tgα are the 'convolution' parameters of this information. In a complex form, they take into account all the properties that, according to modern concepts, determine the nature and results of interatomic interaction. The coefficients Ru^0 and tgα of equations (1) change systematically depending on the position of elements in the periodic table [19].

Using equations like (1), effective charges (Z_{ij}) and radii (Ru_i) are calculated depending on the interatomic distance (*d*) (Fig. 1).

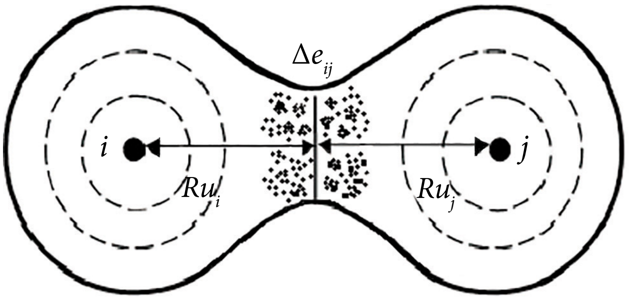

Fig. 1. Scheme of interatomic interaction.

The interaction between atoms *i* and *j* is described by the following system of nonlinear equations:

$$\begin{cases} Ru_j + Ru_j = d, \\ \lg Ru_i = \lg Ru_i^0 - Z_{ij} \cdot \mathrm{tg}\alpha_i, \\ \lg Ru_j = \lg Ru_j^0 - Z_{ji} \cdot \mathrm{tg}\alpha_j, \end{cases} \tag{2}$$

Here, *d* is the interatomic distance (bond length) between atoms *i* and *j*, Ru_i and Ru_j are the radii of the polarized ions *i* and *j*, Ru^0_i and Ru^0_j are the atomic radii of the non-polarized ions, and Z_{ij} and Z_{ji} are the effective charges of ions *i* and *j*, respectively, which are calculated using Eqs. (3) and (4), where Δe_{ij} is the number of electrons involved in the formation of bond *i*–*j*:

$$Z_{ij} = \frac{\lg \dfrac{Ru_i^0 \cdot \mathrm{tg}\alpha_i}{Ru_j^0 \cdot \mathrm{tg}\alpha_j}}{\mathrm{tg}\alpha_i + \mathrm{tg}\alpha_j} + \Delta e_{ij} \cdot \frac{\mathrm{tg}\alpha_i}{\mathrm{tg}\alpha_i + \mathrm{tg}\alpha_j}, \tag{3}$$

$$Z_{ji} = \frac{\lg \dfrac{Ru_i^0 \cdot \mathrm{tg}\alpha_i}{Ru_j^0 \cdot \mathrm{tg}\alpha_j}}{\mathrm{tg}\alpha_i + \mathrm{tg}\alpha_j} + \Delta e_{ij} \cdot \frac{\mathrm{tg}\alpha_j}{\mathrm{tg}\alpha_i + \mathrm{tg}\alpha_j}. \tag{4}$$

When developing a physical-chemical model of the electronic structure of metallic melts [19], the assumption was made that in any form of recording the conditions for the stability of such melts structure, the charges of atoms of all components (Z_i) during their interaction should be considered as functions of *d* and the physicochemical properties of their partners. The implementation of this thesis showed the expediency of using the VCC (volume-centered cubic lattice) structure model as the first approximation. In this case, it is assumed that the relationship between the effective charges for the first (Z^X) and second (Z^Y) coordination spheres is described by the equation:

$$4Z^X = -Z^Y. \tag{5}$$

In the case of multicomponent systems, the left and right sides of this equation are deciphered taking into account the probability of forming all possible pairs of interacting atoms:

$$Z^Y = \sum_{i=1}^{m}\left(\lg Ru_i^0 - \lg\frac{a}{2}\right)\mathrm{tg}\alpha_i n_i + \sum_{i=1}^{m}\sum_{j=1}^{m}2\Delta e_{ij} n_i n_j. \tag{6}$$

The indices i and j indicate the paired bond between cations i and j with the bond length a, and n_i, n_j are their atomic percentages in the melt. Z^X is calculated in a similar way to Eq. (6) with the bond length d. The relationship between a and d in the equations is $d = 0.866a$. The solution to Eq. (5) using Eq. (6) is found by the method of successive approximations (by selecting an a that satisfies condition (5) for a given specific composition).

The main parameters of the metallic melt model are the effective charges of the components Z_i (Table 1), its chemical equivalent of composition Z^Y, which combines data on the charges of the components taking into account the probabilities of forming different types of bonds, and the structural parameter d, which characterizes the mean statistical distance between atoms in the quasi-chemical approximation.

The model of the structure of slag melts was developed based on the models of ordered structures of crystalline and molecular compounds [19]. In accordance with the basic hypothesis, it is represented as an anionic framework, with some of the octahedral and tetrahedral interstices being filled with cations. This assumption takes into account the absence of a stationary anionic environment around the cations and assumes that the effect of the cationic composition on properties is reflected through changes in the size and nature of the jointing of anionic polyhedra.

The stability condition of the electronic structure of oxide melts is expressed in the form of a system of equations (7–8):

$$Z_{\mathrm{K(K-A)}} - Z_{\mathrm{K(K-K)}} = \frac{Ru_{\mathrm{A}} / Ru_{\mathrm{K}} - 0.53}{15.45\cdot(\mathrm{tg}\alpha_{\mathrm{K}})^{1.507}} + 0.51, \tag{7}$$

$$Z_{\mathrm{A(A-K)}} - Z_{\mathrm{A(A-A)}} = \frac{Ru_{\mathrm{K}} / Ru_{\mathrm{A}} - 0.485}{6.067\cdot(\mathrm{tg}\alpha_{\mathrm{A}})^{0.193}} + 0.275. \tag{8}$$

The first equation describes the condition of equilibrium of forces acting on an atom in the cationic sublattice K, while the second is for those acting in the anionic one A. To solve this system, the composition of the melt is expressed as $\mathrm{K}_\rho\mathrm{A}$, where ρ is the stoichiometry index, determined by the ratio of the number of cations K (Fe, Cr, Al, Si, Mn...) to the number of anions A (O, S, ...) in 100 grams of the melt, calculated using the formula

$$\rho = \sum_{i=1}^{l}[m_i\cdot(K_{m_i}\cdot A_{n_i})/M_i] / \sum_{i=1}^{l}[n_i\cdot(K_{m_i}\cdot A_{n_i})/M_i], \tag{9}$$

where K_{m_i}, A_{n_i} is the content of the slag component in mass percent (here K is cation and A is anion), M_i is the molecular weight of the component, and m_i and n_i are the stoichiometric coefficients of the component.

By solving the system of Eqs. (7) and (8) using the method of successive approximations, the interionic distance d is determined implicitly. Then, the Z charges and Ru radii of the components are calculated based on the interionic distance d, $d_{A\text{-}A}$, $d_{B\text{-}B}$ and the corresponding bond lengths, from

Table 1. Chemical composition and model parameters of metallic melts.

Chemical composition of the metal, %								Integral parameters and average charges			
C	Si	Mn	Ni	Cr	Mo	V	Ti	d, 10^{-1} nm	Z^Y, e	Z_{C}, e	Z_{Si}, e
0.38	0.33	0.63	0.19	3.03	0.87	0.24	–	2.765	1.314	–3.377	–1.810
0.50	1.01	1.19	0.18	5.28	3.4	0.76	0.44	2.752	1.491	–3.341	–1.759
0.40	0.20	0.65	0.25	3.0	1.0	–	–	2.765	1.310	–3.378	–1.812
0.31	0.17	1.10	0.20	0.20	–	–	–	2.773	1.202	–3.402	–1.846
0.33	0.17	1.14	1.19	1.29	0.21	–	–	2.773	1.258	–3.399	–1.842
0.15	0.29	0.52	0.15	0.42	1.13	0.29	–	2.799	1.219	–3.435	–1.882

the system of equations describing the elementary interaction of atoms K and A.

Since information about the charges of the elements in a complex form is taken into account by the parameters Δe, a parameter Δe_{sl} is introduced to characterize the interaction of cation–anion in slag melts, which is calculated as

$$\aleph e_{sl} \quad \sum_{i=1}^{n} m_{\mathrm{a}_i} \sum_{j=1}^{m} m_{\mathrm{k}j} \quad e_{\mathrm{K}j-\mathrm{A}_i}. \tag{10}$$

The individuality of the cation sublattice of the melt is taken into account by the weighted average parameter tgα. The values of the weighted average charges and radii of cations in the sublattice K, anions in the sublattice A, as well as in the direction of the bond K–A and A–K are calculated using the formulas

$$\begin{aligned} Z_{\mathrm{K(K-A)}} &= \sum_{i=1}^{m} m_{\mathrm{k}_i} \sum_{j=1}^{n} m_{\mathrm{a}j} Z_{\mathrm{K}_i-\mathrm{A}_j}, \\ Z_{\mathrm{K(K-K)}} &= \sum_{i=1}^{m} m_{\mathrm{k}_i} \sum_{j=1}^{n} m_{\mathrm{k}j} Z_{\mathrm{K}_i-\mathrm{K}_j}, \end{aligned} \tag{11}$$

$$\begin{aligned} Z_{\mathrm{A(K-A)}} &= \sum_{i=1}^{m} m_{\mathrm{a}_i} \sum_{j=1}^{n} m_{\mathrm{a}j} Z_{\mathrm{A}_i-\mathrm{K}_j}, \\ Z_{\mathrm{A(A-A)}} &= \sum_{i=1}^{m} m_{\mathrm{a}_i} \sum_{j=1}^{n} m_{\mathrm{a}j} Z_{\mathrm{A}_i-\mathrm{A}_j}. \end{aligned} \tag{12}$$

Here, the indices k and a indicate the bond between cation K and anion A, m is the number of cations, n is the number of anions, and m_{k_i} and m_{a_i} represent their atomic fractions.

As our many years of experience have shown, the use of parameters Δe, ρ and d (Table 2) is an effective means of 'collating' information about the composition of multicomponent oxide melts when studying the patterns of their property formation [22]: viscosity at different temperatures, surface tension, electrical conductivity, density, and slag melting.

The information support for modelling the properties of melts is based on the databases of fundamental experimental data on the properties of slag melts, iron ore materials, slag-forming mixtures, and the distribution of elements during real metallurgical processes (databases 'Slag', 'Slag-forming mixtures', 'Iron ore materials' and 'Metal–Slag–Gas'), which are developed at the Iron and Steel Institute in accordance with the main concept of forming the 'Metallurgy' database DBMet [22]. In particular, the 'Slag' database currently contains more than 500 documents with information on the properties of over 8,000 compositions of slags of various purposes. The database of experimental data in 'Metal–Slag–Gas' contains information on the distribution of impurity elements (S, P, C, H and N), elements of variable valency (Fe, C, Cr and Mn), as well as Al, Si and others between the slag and metal or the slag and gas phase. The calculation of integral parameters of iron and slag is carried out based on the initial chemical composition of the system using computer systems 'Slag' and 'Metal'.

4. Modelling the interaction between metal and slag as a cooperative ion exchange process

The distribution coefficients L_{S}, L_{Mn}, L_{Si} and L_{P} are the main thermodynamic parameters that determine the efficiency and completeness of ion exchange processes in the 'metal–slag' system. Since thermodynamic characteristics that quantitatively describe a process are applicable only in the case of equilibrium processes, the issue of equilibrium and the assessment of its achievement when determining possible areas of application of thermodynamics for quantitative characterization of real processes is currently relevant.

Table 2. Model parameters of steelmaking slags.

Chemical composition of the slag, %										Integral parameters		
CaO	SiO_2	MgO	MnO	Al_2O_3	P_2O_5	FeO	CaS	CaF_2	Fe_2O_3	d, 10^{-1} nm	$-\Delta e$, e	ρ
50.64	17.15	10.9	–	1.07	1.09	19.14	–	–	–	3.088	2.598	0.847
51.74	14.41	6.18	0.62	19.56	0.1	0.72	1.39	5.28	–	2.667	1.364	0.783
41.39	12.17	10.47	0.33	6.67	0.11	0.5	3.25	25.1	–	2.909	1.565	0.743
35.7	11.2	9.2	5.1	2.7	2.6	12.7	0.05	–	4.2	3.228	2.961	0.831
46.0	14.98	7.35	6.47	2.06	2.63	11.9	0.014	–	9.9	3.201	2.928	0.816
55.0	10.0	5.0	–	25.0	–	–	–	5	–	2.449	0.746	0.793

The study of the equilibrium distribution of any component between metal and slag is reduced to experimentally determining the activities or activity coefficients and establishing the functional dependence on known factors. Researchers have not yet reached a consensus on the degree of equilibrium achieved in different processes. For example, early studies [23] found that the redistribution of sulfur, manganese and silicon in the 'metal–slag' system in the blast furnace does not reach the equilibrium. In the studies by Okhotsky it was concluded that the redistribution of manganese between metal and slag in the blast furnace process, although close to the equilibrium, does not occur completely [24]. The actual manganese content in iron is below the equilibrium value, while the redistribution of silicon corresponds to the equilibrium, and the redistribution of sulfur is very close to the equilibrium. Similar conclusions have been made by numerous studies analyzing steelmaking processes, which note that even in the conditions of an oxygen converter process, the equilibrium is not fully achieved.

With regard to the real metallurgical processes, these circumstances have led to the development of an alternative approach to evaluating the thermodynamic state of the 'metal–slag' system from the perspective of a cooperative ion exchange process and the consistency formation of the chemical composition of the metal and slag melt when the single system strives for equilibrium.

4.1. Investigation of the 'metal–slag' system under oxidizing conditions in metal smelting

At the initial stage of the research, actual data on the compositions of reacting melts during steelmaking were analyzed. Samples of metal and slag for analysis were taken during the blowing process on 25 heats in 50-ton converters and 43 heats in 130-ton converters, respectively. Similar domestic and foreign data on steelmaking in a large converter [22] were also used. Table 3 presents some of the compositions of metal and corresponding slags, as well as the calculated model parameters Z^Y, Δe and ρ based on their compositions. The graphical interpretation of the changes in these parameters during the heat indicates that as the liquid slag is formed and carbon and other impurities in the iron are burned off, the chemical equivalent of the slag increases and that of the metal decreases monotonically (Fig. 2). The consistency of the changes in the chemical equivalents of metal and slag is reflected by the following equations (R is the coefficient of correlation):

$$Z^Y = 2.01 – 0.17 \cdot \Delta e – 1.65 \cdot \rho \text{ for 300-ton converters,}$$

$$R = 0.85, \qquad (13)$$

$$Z^Y = 2.2 – 0.07 \cdot \Delta e – 1.49 \cdot \rho \text{ for 130-ton converters,}$$

$$R = 0.86. \qquad (14)$$

Deviations from these dependences for individual melts are due to fluxing additives, which lead to some discrepancies in the ratios between Z^Y and Δe. This is associated with the systemic influence of the stoichiometry parameter ρ on the reactivity of slags. Therefore, the additional consideration of ρ increases the accuracy of describing the coordinated changes in the chemical equivalents of metal and slag.

Table 3. Changes in the composition and structure characteristics of slag and metal melts during the blowing process in 50-ton converters.

Chemical composition of the slag, %							Model parameters of the slags		Chemical composition of the metal, %				Model parameter of the metal Z^Y, e
SiO_2	CaO	MgO	FeO	Fe_2O_3	MnO	P_2O_5	$-\Delta e$, e	ρ	C	Mn	S	P	
32.6	33.9	6.6	7.1	1.5	17.1	0.316	3.70	0.749	3.98	0.40	0.066	0.052	1.372
32.2	44.9	4.8	5.0	1.5	11.6	0.408	3.13	0.755	3.32	0.39	0.060	0.034	1.345
25.8	44.6	9.2	7.4	3.1	8.3	0.792	3.03	0.786	1.57	0.37	0.060	0.022	1.261
31.5	43.4	8.5	3.4	1.6	10.1	0.410	3.06	0.759	3.14	0.52	0.050	0.036	1.334
25.0	46.4	9.6	5.4	2.4	8.7	0.690	2.92	0.792	1.16	0.52	0.040	0.027	1.226

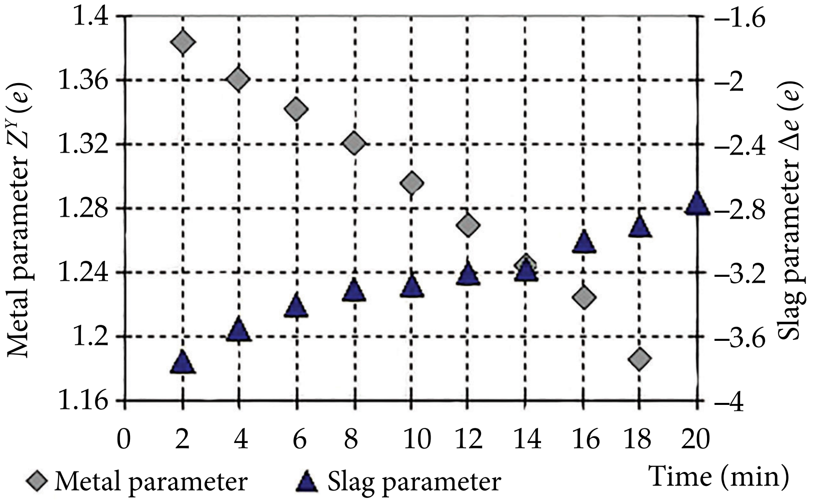

Fig. 2. Kinetics of changes in the parameters of metal (♦) and slag (▲) melts during the converter process.

4.2. Study of the 'metal–slag' system under reducing conditions in metal production

Similar studies have been carried out using actual data of blast furnace smelting products under reducing conditions. The final composition of pig iron and slag is formed as a result of the ion-exchange interaction of pig iron and final slag elements in the blast furnace hearth. To study the mentioned processes, the experimental equilibrium data by Kulikov [22] and the actual data from the production of pig iron in blast furnaces in Ukraine were investigated.

Based on Kulikov's data obtained from the study of the equilibrium between pig iron and slag in terms of sulfur, a dependence of element distribution coefficients on model parameters characterizing the metallic (Z^Y) and slag (Δe and ρ) systems was established. In particular, an equation was derived to predict the equilibrium sulfur distribution coefficient L^0_S:

$$\lg \mathrm{L}^0_S = 9.03 \cdot Z^Y + 18.53 \cdot \rho - 0.096 \cdot \Delta e - 24.27$$

$$(R = 0.93). \qquad (15)$$

The established dependence allows for an assessment of the degree of approximation of the 'pig iron–slag' system to the sulfur equilibrium under real conditions of blast furnace operation by comparing the actual sulfur distribution coefficient L_S to the equilibrium value L^0_S: $E_S = L_S/L^0_S \cdot 100\%$. The effectiveness of using the proposed criterion E_S for assessing the degree of sulfur equilibrium attainment is illustrated in Fig. 3. Production data from three furnaces operating under modern conditions with different fuel-energy additives are considered. Specifically, BF-A operated with natural gas injection, BF-B with a combination of natural gas and pulverized coal injection, and BF-C with only pulverized coal injection. The presented data indicates that under real smelting conditions, the sulfur distribution is below the equilibrium, and its deviation increases proportionally with the deviation of L_S from L^0_S. In addition, the best degree of sulfur equilibrium attainment is observed for BF-A, with an average E_S value of 74%, while for BF-B and BF-C, these values are 62 and 53%, respectively. This effect is explained by the fact that unburned coal particles litter the slag, increasing its viscosity, and complicate the interaction processes in the 'metal–slag' system.

Also, according to the data of Kulikov, the dependence of sulphur and silicon content in pig iron on the model parameters has been established:

$$[\mathrm{S}] = 0.346 – 0.136 \cdot Z^Y + 0.011 \cdot \Delta e - 0.162 \cdot \rho$$

$$(R = 0.93), \qquad (16)$$

$$[\mathrm{Si}] = -6588 + 34.19 \cdot Z^Y - 0.043 \cdot \Delta e + 26.38 \cdot \rho$$

$$(R = 0.87). \qquad (17)$$

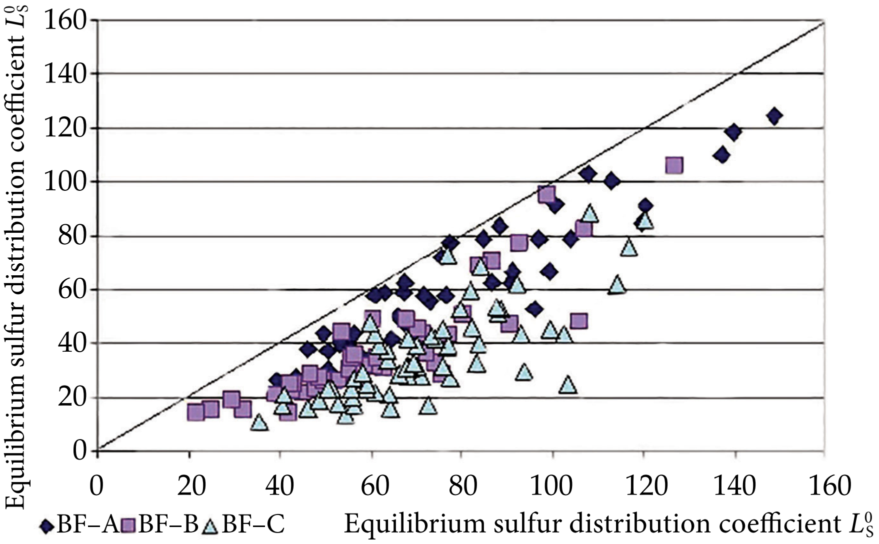

Fig. 3. Assessment of the degree of achieving the sulfur equilibrium in modern conditions of blast furnace operation with various fuel and energy additives: BF-A with natural gas injection, BF-B with natural gas and pulverized coal fuel and BF-C with pulverized coal fuel.

Equations (16–17) in their integral form reflect the classical understanding of how all components of the complex 'metal–slag' system influence the processes and outcomes of their interaction, including desulfurization of iron, silicon reduction, etc.

It has been previously established that the distribution of elements between the metal and the slag is significantly affected by the local environment of each component of the system, which is determined by the weighted average value of its effective charge (Z_{el}) [25, 26]. The change in the state of each component during the transition from one phase to another can be determined as the 'recharging' of diffusing ion element ΔZ_{el}, which is equal to the difference in the charges of the element in metal $[Z_M^{el}]$ and slag (Z_{Sl}^{el}): $\Delta Z_{el} = [Z_M^{el}] - (Z_{Sl}^{el})$. For equilibrium data, the introduction of an additional parameter ΔZ_{el} in models (16–17) did not improve the prediction accuracy for the sulpur and silicon content, since the 'iron–slag' system reached the equilibrium at long curing.

In order to verify the validity of the obtained dependences, iron output data were analysed under current operating conditions of blast furnaces using natural gas and pulverized coal BF-A, BF-B and BF-C.

In production conditions, when temperature conditions of melting, in particular the thermal state of the furnace, actively affect the processes in addition to the chemical characteristics of the 'pig iron–slag' system, less significant dependences similar to models (16–17) on the quality indicators of pig iron should be expected from the model parameters of metallic and slag melts.

As a result of data processing from more than 500 smelting outputs, there are the similar patterns of the influence of integral characteristics of melts on the quality indicators of blast furnace smelting, such as sulfur and silicon content in pig iron, as well as the distribution coefficients of these elements between pig iron and slag for BF-B using natural gas and pulverized coal (Tables 4–6).

The equations obtained take into account the integral parameters of cast iron and slag Z^Y, Δe and ρ, as well as the partial parameter 'recharging' ΔZ_{el}, the use of which significantly increases the accuracy of the calculation, estimated by the correlation coefficient R. For example, the equation for calculating the sulfur content in pig iron is as follows:

$$[S] = 1.83 - 0.94 \cdot Z^Y + 0.01 \cdot \Delta e - 0.68 \cdot \rho \ (R = 0.88). \quad (18)$$

Including the recharge parameter ΔZ_S,

$$[S] = 0.54 - 0.47 \cdot Z^Y + 0.01 \cdot \Delta e - 0.33 \cdot \rho - 0.21 \cdot \Delta Z_S \quad (R = 0.92). \quad (19)$$

Table 4. Chemical composition of pig iron and slag from the blast furnace DP-B operation using natural gas and pulverized coal as fuel.

No.	Composition of pig iron, %					Composition of slag, %									
	C	Si	Mn	P	S	SiO_2	Al_2O_3	CaO	MgO	MnO	FeO	S	K_2O	Na_2O	TiO_2
1	4.71	0.66	0.24	0.043	0.044	43.4	5.70	44.3	5.00	0.46	0.46	1.22	0.47	0.53	0.26
2	4.45	0.52	0.19	0.045	0.052	42.0	5.90	45.0	5.91	0.28	0.39	1.37	0.37	0.56	0.28
3	4.64	0.44	0.25	0.054	0.039	42.0	5.90	46.0	4.90	0.41	0.32	1.33	0.39	0.58	0.27
4	4.76	0.49	0.30	0.056	0.034	42.2	5.80	46.2	5.00	0.41	0.28	1.35	0.38	0.57	0.26
5	4.54	0.75	0.21	0.052	0.046	43.7	6.16	43.7	5.13	0.42	0.47	0.96	0.51	0.52	0.30
6	4.41	0.44	0.12	0.047	0.050	42.3	6.00	45.6	5.20	0.22	0.44	1.08	0.37	0.54	0.26

Table 5. Model parameters of pig iron and slag corresponding to the compositions in Table 4.

No.	Basicity of the slag CaO/SiO_2	Distribution coefficient		Parameters of pig iron			Parameters of slag				Parameters of recharge	
		L_S	L_{Si}	Z^Y, e	$Z_{[Si]}$	$Z_{[S]}$	$-\Delta e$, e	ρ	$Z_{(Si)}$, e	$Z_{(S)}$, e	ΔZ_{Si}, e	ΔZ_S, e
1	1.02	27.7	65.8	1.408	−1.119	0.149	2.593	0.702	−2.486	−1.373	1.367	1.522
2	1.07	26.3	80.8	1.395	−1.147	0.124	2.551	0.709	−2.486	−1.392	1.338	1.515
3	1.10	34.1	95.5	1.400	−1.130	0.139	2.515	0.709	−2.468	−1.369	1.338	1.508
4	1.09	39.7	86.1	1.406	−1.117	0.151	2.513	0.709	−2.467	−1.368	1.350	1.519
5	1.00	20.9	58.3	1.405	−1.135	0.134	2.616	0.700	−2.491	−1.377	1.356	1.511
6	1.08	21.6	96.1	1.391	−1.152	0.119	2.524	0.707	−2.466	−1.366	1.314	1.485

Table 6. Influence of the ‘recharging’ parameter on the distribution of elements in the ‘metal–slag’ system.

Indicator	Value of the correlation coefficient *R* of the predictive equation:	
	Indicator = $f(Z^Y, \Delta e, \rho)$	Indicator = $f(Z^Y, \Delta e, \Delta, \Delta Z_{el})$
Sulfur content in pig iron, % [S]	0.88	0.92
Silicon content in pig iron, % [Si]	0.75	0.9
Manganese content in pig iron, % [Mn]	0.65	0.72
Sulfur distribution coefficient L_S	0.83	0.86
Silicon distribution coefficient L_{Si}	0.71	0.86
Manganese distribution coefficient L_{Mn}	0.85	0.93

The influence of the parameter ΔZ_{el} is higher the further the system is from the equilibrium. Table 6 data show that the system is further from the equilibrium for silicon than for sulfur, since the introduction of the ΔZ_{Si} parameter into the model $L_{Si} = f(Z^Y, \Delta e, \rho)$ increases the correlation coefficient *R* from 0.71 to 0.86.

The influence of the parameter ‘recharging’ of sulfur ΔZ_S is significantly enhanced for the sample of these ‘bad’ outputs with a low value of the degree of achievement of the equilibrium by E_S <50%, for which the correlation coefficient *R* for the relationship $L_S = f(\Delta Z_S)$ is equal to 0.72 (Fig. 4). For this sample of ‘bad’ outputs the average sulfur content in pig iron is higher than in the whole array: [S] = 0.045% (Table 7). For ‘good’ outputs with a high value E_S >75% there is no influence of the ‘recharging’ parameter ΔZ_S on L_S (Fig. 4). In this case, the average sulfur content in pig iron [S] = 0.026%, which corresponds to the technical specifications for melting sulfur-containing pig iron. These results give grounds to use the ‘recharging’ parameter ΔZ_{el} as a criterion for the deviation of the system from the equilibrium in real conditions of blast furnace smelting.

In order to identify patterns and criteria describing the consistent formation of compositions of metal and slag melts under reducing conditions

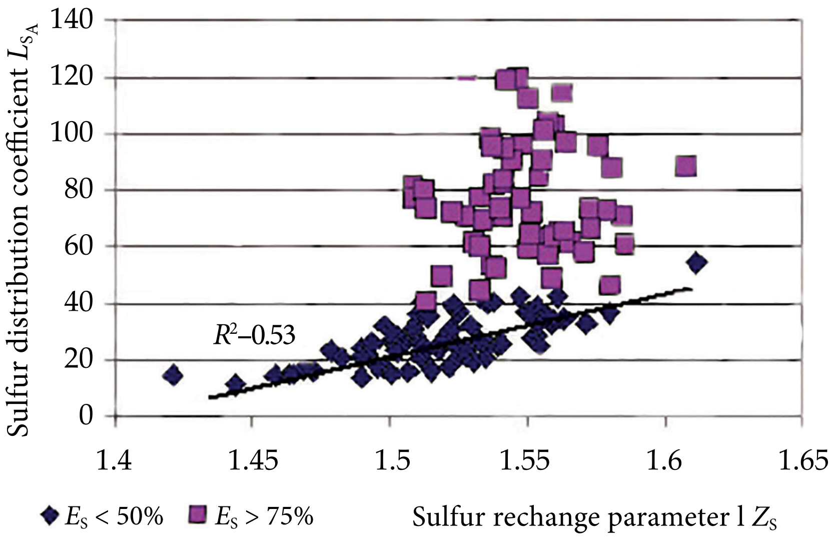

Fig. 4. The effect of the ‘recharging’ parameter ΔZ_S on the sulfur distribution coefficient between iron and slag under the conditions of BF-B operation.

Table 7. Performance indicators of the DP-B blast furnace for pig iron outputs with different values of the degree of attainment of the equilibrium for sulfur between metal and slag.

Indicator	Minimum	Maximum	Average
For pig iron outputs for the entire period ($N = 533$)			
Silicon content in pig iron, % [Si]	0.13	1.16	**0.48**
Sulfur content in pig iron, % [S]	0.010	0.126	**0.037**
Slag basicity CaO/SiO_2	0.91	1.28	1.09
Actual sulfur distribution coefficient L_S	6.0	119.0	40.2
Equilibrium sulfur distribution coefficient L_S^0	7.5	197.8	63.9
Degree of attainment of equilibrium for sulfur E_S	33.6	99.5	**61.7**
For pig iron outputs with a value $E_S > 75\%$ ($N = 80$)			
Silicon content in pig iron, % [Si]	0.13	1.16	**0.61**
Sulfur content in pig iron, % [S]	0.010	0.126	**0.026**
Slag basicity CaO/SiO_2	0.96	1.23	1.11
Actual sulfur distribution coefficient L_S	6.9	119.0	69.8
Equilibrium sulfur distribution coefficient L_S^0	7.5	155.9	83.8
Degree of attainment of equilibrium for sulfur E_S	75.0	99.5	**82.9**
For pig iron outputs with a value $E_S < 50\%$ ($N = 80$)			
Silicon content in pig iron, % [Si]	0.14	0.75	**0.41**
Sulfur content in pig iron, % [S]	0.013	0.079	**0.045**
Slag basicity CaO/SiO_2	1.00	1.28	1.11
Actual sulfur distribution coefficient L_S	11.6	93.0	28.5
Equilibrium sulfur distribution coefficient L_S^0	25.1	197.8	62.6
Degree of attainment of equilibrium for sulfur E_S	33.6	49.9	**45.6**

of blast furnace operation, a few published experimental data on the behaviour of melts in a blast furnace were analyzed.

In particular, the operation of two blast furnaces with a volume of 3200 m^3 was evaluated using Shepetovsky's data presented in the database 'Metal–Slag–Gas' [22]. The chemical composition of pig iron and final slag was investigated according to the actual data of iron output. Unevenness of this composition is formed along the diameter and height of the furnace during the accumulation of liquid products of melting. Smelting products were sampled every 10 min. The averaged results of 8 samples of iron compositions for one release, the corresponding slag compositions, and the calculated model parameters Z^Y, Δe and ρ based on them are presented in Tables 8 and 9. The consistent change of the model parameters of iron Z^Y and slag Δe taking into account the slag parameter ρ is expressed by the relationship

$$Z^Y = 0.66 + 0.11 \cdot \Delta e + 1.44 \cdot \rho \quad (R = 0.78). \qquad (20)$$

A similar relationship was obtained for the conditions of operation of a 1386 m^3 BF based on the data of Novokhatsky [27] for five heats. In each heat, seven samples of pig iron and slag were taken at equal time intervals. The chemical composition of the smelting products and the calculated model parameters are presented in Tables 10 and 11. The condition of the consistency of the composition change of pig iron and slag is determined by the relationship

$$Z^Y = 0.47 + 0.72 \cdot \Delta e + 1.07 \cdot \rho \quad (R = 0.79). \qquad (21)$$

The established dependences (20–21) between the chemical equivalent of the iron composition and the parameters of slag melt in the form of $Z^Y = f(\Delta e, \rho)$ can be characterized as a condition of consistency of the composition formation of the smelting products during the production of iron. The revealed regularity reflects the process of interaction of melts based on the measurements of several samples of pig iron outputs. Different values of measurements

Table 8. Composition and model parameters of pig iron by the cross-section of the hearth (D is the distance from the cut of tuyere and at the output of pig iron) according to Shepetovskiy.

No.	D, мм	Composition of pig iron, %						Integral indicators of pig iron	
		Si	Mn	S	P	C	Fe	d, 10^{-1} nm	Z^Y, e
1	500	1.06	0.23	0.131	0.04	2.74	95.8	2.470	1.347
2	1000	1.42	0.43	0.152	0.06	3.57	94.4	2.403	1.395
3	1500	1.66	0.92	0.074	0.09	3.87	93.4	2.383	1.419
4	2000	2.03	1.07	0.059	0.1	3.92	92.8	2.377	1.433
5	2500	1.97	0.78	0.053	0.1	4.28	92.8	2.353	1.437
6	3000	1.31	0.55	0.086	0.08	4.55	93.4	2.339	1.424
7	4000	0.83	0.48	0.09	0.07	4.6	93.9	2.339	1.412
8	output	0.76	0.86	0.024	0.1	4.55	93.7	2.344	1.414

Table 9. Composition and model parameters of slag corresponding to the composition of pig iron in Table 8.

No.	Composition of slag, %								Integral indicators of slag		
	SiO_2	CaO	Al_2O_3	Fe_2O_3	FeO	MnO	MgO	CaS	d, 10^{-1} nm	$-\Delta e$, e	ρ
1	19.17	16.87	5.36	8.18	24.34	0.68	7.46	0.2	3.32	3.704	0.736
2	24.18	23.93	9.31	4.97	19.81	1.17	7.81	0.41	3.198	3.339	0.749
3	33.19	33.27	7.19	2.19	10.17	0.91	8.64	0.53	3.046	2.98	0.727
4	35.02	35.97	8.26	0.23	16.19	0.48	8.19	0.44	3.055	3.005	0.734
5	32.26	35.13	10.08	0	15.43	0.51	7.12	0.57	3.033	2.917	0.736
6	33.18	34.41	8.02	0	18.62	0.34	7.76	0.55	3.077	3.057	0.739
7	32.74	33.3	6.18	0	21.17	0.31	8.93	0.64	3.121	3.168	0.747
8	39.19	40.36	10.28	0	0.43	1.02	8.69	0.68	2.871	2.528	0.741

Table 10. Composition and model parameters of pig iron according to Ref. [27].

No. of sample	Composition of pig iron, %						Integral indicators of pig iron	
	C	Mn	Si	S	P	Fe	d, 10^{-1} nm	Z^Y, e
1	4.45	0.14	0.94	0.048	0.042	94.3	2.344	1.403
2	4.42	0.15	0.78	0.035	0.043	94.5	2.348	1.397
3	4.42	0.15	0.60	0.038	0.043	94.7	2.349	1.392
4	4.49	0.16	1.06	0.037	0.046	94.2	2.341	1.407
5	4.46	0.16	0.99	0.026	0.047	94.3	2.343	1.405
6	4.44	0.16	0.93	0.031	0.045	94.4	2.345	1.402
7	4.52	0.16	1.30	0.024	0.046	93.9	2.338	1.415

Table 11. Composition and model parameters of slag corresponding to the composition of pig iron in Table 10.

No.	Composition of slag, %										Integral indicators of slag		
	MgO	Al_2O_3	SiO_2	CaS	CaO	MnO	FeO	K_2O	TiO_2	CaO/SiO_2	d, 10^{-1} nm	$-\Delta e$, e	ρ
1	4.77	7.81	36.4	1.69	50.2	0.078	0.35	0.34	0.5	1.38	2.787	2.172	0.726
2	4.86	7.66	38.5	1.67	49.6	0.103	0.32	0.37	0.58	1.29	2.8	2.244	0.719
3	5.01	7.48	39.9	1.58	47.8	0.129	0.29	0.39	0.65	1.20	2.814	2.325	0.712
4	5.47	7.38	39.4	1.71	48.1	0.129	0.4	0.35	1.6	1.22	2.842	2.374	0.713
5	5.52	7.2	39.0	1.7	47.8	0.129	0.32	0.35	1.67	1.23	2.844	2.377	0.714
6	5.65	6.97	38.6	1.58	46.7	0.155	0.3	0.36	1.88	1.21	2.856	2.411	0.713
7	5.67	4.06	40.6	1.48	44.5	0.309	0.26	0.62	1.41	1.10	2.883	2.55	0.707

of the chemical composition of smelting products indicate the actively occurring ion exchange processes of the interaction of elements in the ‘metal–slag’ system during the formation of the final compositions of pig iron and slag until the end of the production.

Further the actual data of pig iron output for modern conditions of blast furnaces DP-A, DP-B and DP-S have been analyzed. As a result, a similar regularity of the consistency of changes (regularity of coordinated changes) in the chemical compositions of pig iron and final slag has been established. In particular, an analytical dependence of the consistency condition for DP-B (533 pig iron output) is as follows:

$$Z^Y = 1.79 + 0.17 \cdot \Delta e + 0.1 \cdot \rho \quad (R = 0.670). \qquad (22)$$

Obviously, the relationship between the parameter of chemical composition of pig iron Z^Y and the parameters of slag Δe and ρ for this sample of pig iron outputs is less tight than the similar dependence (21), which was obtained from the data of several measurements of one output. However, for ‘good’ outputs of the data sample with high values of the degree of achievement of the equilibrium on sulfur ($E_S > 75\%$) a closer connection between the parameters of smelting products with the value of correlation coefficient $R = 0.83$ is established. For ‘bad’ outputs with the value of $E_S < 50\%$ the relationship was found to be weak ($R = 0.45$). Consequently, the relationship between the parameter of the chemical composition of pig iron Z^Y and the slag parameters Δe and ρ, expressed by the corresponding dependence, can be used as a criterion for assessing the degree of thermodynamic consistency of the melts of the ‘pig iron–slag’ system when it strives for equilibrium in the main elements of the interface. In practice, the condition of consistency of melts can be used to assess the efficiency of the slag regime in blast furnace smelting for the desulfurization of pig iron and the degree of achievement of the equilibrium in the ‘metal–slag’ system for sulfur.

5. Conclusions

The article presents the theoretical foundations and practical application of a new approach to modelling the interaction processes of melts during the smelting of pig iron and steel. The development of this approach is due to the lack of a unified methodological basis for describing the regularities of element distribution in the 'metal–slag' system, assessing its thermodynamic state, and deviations from the equilibrium under various charge and technological conditions. The thermodynamic apparatus traditionally used for these purposes has limited capabilities in describing real processes.

In this work, the interaction in the 'metal–slag' system is considered from the perspective of cooperative ion exchange processes using the model of the structure of metallurgical melts developed at the Iron and Steel Institute of the NAS of Ukraine, which describes the chemical and structural state of the system using interatomic interaction parameters.

Experimental data of the results of the process of reaching sulphur equilibrium in the 'pig iron–slag' system have been investigated. The dependence of the equilibrium coefficient of sulphur distribution and the content of the main elements in pig iron on the model parameters describing the chemical and structural state of metallic (Z^Y) and slag (Δe and ρ) systems was established. A criterion for assessing the degree of attainment of the equilibrium with respect to sulfur under real conditions of blast furnace smelting was proposed, which is equal to the ratio of the actual sulfur distribution coefficient L_S to the equilibrium L^0_S: $E_\mathrm{S} = L_\mathrm{S}/L^0{}_\mathrm{S} \cdot 100\%$.

As a criterion for the deviation of the system from the equilibrium under real conditions of domain melting, the use of the element 'recharging' parameter ΔZ_el is shown, which characterizes the change in the charge state of the element when transitioning from one phase to another. The ΔZ_el parameter is determined by the difference in the element charges in metal $[Z^\mathrm{el}_\mathrm{M}]$ and slag $(Z^\mathrm{el}_\mathrm{Sl})$: $\Delta Z_\mathrm{el} = [Z^\mathrm{el}_\mathrm{M}] - (Z^\mathrm{el}_\mathrm{Sl})$.

As a result of the analysis of production data on the compositions of reacting melts during the smelting of pig iron and steel, a regularity of the consistency formation of the compositions of metallic and slag melts was established, which is evidenced by a significant relationship between the chemical equivalent of the metal composition Z^Y and the slag Δe. Analytical dependences were obtained in the form of $Z^Y = f(\Delta e, \rho)$, which characterizes the thermodynamic condition of consistency of the composition formation of melts in the smelting of pig iron and steel.

The inconsistency of the 'metal–slag' system, namely the absence of an established relationship between the parameters of metal and slag, indicates a violation of the thermal regime of melting, a discrepancy between the blast regime and fuel and raw material conditions, a decrease in the consistency of all processes that determine the heat balance of melting.

The identified regularities, relationships and criteria can be integrated into automated process control systems to assess the thermodynamic state of the 'metal–slag' system and its deviation from the equilibrium when solving problems of controlling the slag regime to obtain pig iron and steel of the required quality.

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NAUJAS BŪDAS ĮVERTINTI LYDALŲ TERMODINAMINĘ DERMĘ METALO IR ŠLAKO SISTEMOJE, NAUDOJANT TARPATOMINĖS SĄVEIKOS PARAMETRUS

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