SYSTEMATIC APPROACH TO DESCRIBING STEEL REFINING PROCESSES IN A LADLE FURNACE

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ABSTRACT

This work presents a systematic approach to describing the physicochemical processes occurring in the metal-slag system during steel refining in a ladle furnace. The aim of the study was to develop methods for predicting the distribution of main and impurity elements based on a comprehensive analysis of the initial and final melts of metal and slag. Industrial data on the chemical composition of SAE1006 grade steel and the corresponding slag were used as the input. Based on the methodological framework of the Directed Chemical Bonding Concept (DCBC) and mathematical processing of multivariate data, the applicability of interatomic interaction parameters and technological regime indicators as model parameters was substantiated. Complex indicators for the metal-slag and metal-additive systems were constructed using Harrington's desirability function, which enables integration of multidimensional parameters into a single generalized index. Analytical dependencies were developed for calculating the distribution coefficients of sulphur (S), silicon (Si), manganese (Mn), and aluminium (Al), considering both the composition of metallurgical phases and the smelting conditions. The proposed approach provides a quantitative assessment of the distribution coefficients of elements as variable quantities, which fundamentally distinguishes it from traditional methods. The results obtained form the basis for developing algorithms to predict the chemical composition of the final melt and for creating practical recommendations on the selection of optimal additives and slag-forming mixtures aimed at improving steel quality and reducing production costs.

Keywords: steel, ladle furnace, metal-slag system, metal-additive system, element distribution coefficients, interatomic interaction, Harrington's desirability function, chemical composition prediction.

INTRODUCTION

The problem of improving the quality of steel and the efficiency of its production technology remains one of the key challenges in modern metallurgy. The steel refining process in the ladle furnace (LF) is the final stage in achieving the required steel composition before its solidification. At this stage, the chemical composition of the metal is adjusted, harmful impurities are removed, and non-metallic inclusions are modified through directed, intensive interactions between the liquid metal and slag.

To achieve the target chemical composition and properties of steel, various alloying and fluxing additives are introduced, such as ferroalloys and slag-forming mixtures. Alloying is performed by adding elements such as chromium, nickel, or manganese to impart specific mechanical or corrosion-resistant properties to the steel. Slag-forming reagents create a slag layer that absorbs undesirable components (e.g., sulphur and phosphorus) and protects the metal from reoxidation. Deoxidizers (aluminium and silicon) are added to the steel to remove dissolved oxygen, resulting in the generated oxide inclusions being transferred to the slag. The process is controlled through intermediate chemical analysis of both the metallic and slag phases.

Achieving the required steel quality in the LF is the result of the synergistic interaction among multi-stage thermal, chemical, and mechanical processes. These include dissolution, deoxidation, oxidation-reduction reactions, and interphase mass transfer, making their prediction and control extremely complex tasks. Understanding the fundamental physicochemical mechanisms underlying these processes is crucial for improving process efficiency, reducing alloying element losses, minimizing energy and material consumption, and ensuring stable quality of the final product. This multifactor nature of the steel refining process in the LF necessitates the use of a systematic approach for comprehensive analysis and description of the physicochemical processes occurring in the metal-slag system. This approach must consider key influencing factors and enable the development of effective technological solutions.

Modern literature presents a series of studies investigating the metal-slag interaction in ladle furnaces using a systematic approach. Thus, A. Harada et al. developed kinetic and thermodynamic models that allow for the prediction of changes in the chemical composition of liquid steel, slag, and non-metallic inclusions during the steel refining process in the ladle [1]. These models consider multiple simultaneous reactions and mass transfer processes. D. Jochymczyk et al. conducted industrial research and presented the results of numerical simulation of the chemical homogenization process of liquid steel in a ladle furnace, which includes a description of gas flow hydrodynamics and alloying additions [2]. D. You and colleagues proposed a model for metal refining in the LF unit, which considers both steel mixing and multi-phase chemical reactions [3]. Several other models for ladle furnace treatment have been proposed, emphasizing that comprehensive modelling approaches are gaining importance, as they enable a deeper and more accurate analysis of the complex phenomena occurring in the LF.

To understand and optimize steel refining technology, publications pay significant attention to the physicochemical processes taking place at the liquid metal/slag interface [4-6]. These works emphasize the importance of slag composition in controlling oxygen activity in steel and how its physical and chemical properties influence refining processes. The study of interatomic interactions in metallic and slag melts is often conducted using methods of molecular dynamics and interatomic potentials, such as the Embedded Atom Method (EAM), pair potentials [7], Wagner interaction coefficients [8], and the Born-Mayer-Huggins potential [9]. These models account for attractive and repulsive forces between atoms as a function of interatomic distance. However, the development of universal methods capable of describing interactions in complex multicomponent systems across a wide range of compositions and temperatures remains a challenge. Moreover, traditional thermodynamic models for predicting the equilibrium distribution of elements in the metal-slag system lose their effectiveness under real industrial conditions, as true equilibrium is rarely achieved due to kinetic constraints.

In recent years, the Directed Chemical Bonding Concept (DCBC) has expanded the scope of its application to describe metal-slag interaction in metallurgical processes, including steel refining in the ladle furnace. The authors of this article have developed a new approach to evaluating the thermodynamic state of the metal-slag system based on interatomic interaction parameters [10]. G. Stovpchenko and co-authors established a correlation between the chemical composition of slag systems and the properties of their melts within the framework of DCBC and developed predictive models for calculating a complex of properties for slags and slag-forming mixtures in steelmaking production, such as viscosity, electrical conductivity, crystallization temperature, and density [11, 12]. This Concept has also been successfully applied in a different area of metallurgical production, specifically in pig iron smelting technology. In particular, the authors of this article developed a decision-making model for optimizing the blast furnace burden composition [13]. These studies confirm that the Directed Chemical Bonding Concept is becoming a valuable tool for deeper understanding of the fundamental nature of interactions in metallurgical systems, including the metal-slag system.

The aim of this study is to develop a new systematic approach to describing the physicochemical interaction processes in the metal-slag system during steel refining in the ladle furnace. This approach is based on the Directed Chemical Bonding Concept (DCBC), which makes it possible to describe the structural-energy

state of metallurgical melts at the micro-level, and to account for the influence of interatomic interactions on the macroscopic properties of the system.

EXPERIMENTAL

Research methods

This study presents a systematic approach to describing and evaluating the physicochemical processes that occur in the complex heterogeneous metal-slag system during steel refining in a ladle furnace. The developed methodology is based on the synergistic combination of the mathematical framework of the Directed Chemical Bonding Concept and modern methods of multifactor data processing.

Directed Chemical Bonding Concept (DCBC)

Understanding ion-exchange processes at the level of interatomic interactions in the metal-slag system is fundamental to optimizing iron and steel smelting processes. A basic tenet of the Directed Chemical Bonding Concept is the notion of the variability of the charge state of the atoms of metallic and slag melt components, depending on their specific environment. The model of pairwise interatomic interaction in melts and the methodological basis of the theory of physicochemical modelling, considering the determining role of the directionality of interatomic interaction, are described in detail in work [10]. The new structure model for metallurgical melts, developed by E. Prikhodko, considers them as chemically unified systems whose compositional change affects all their properties through a change in the parameters of their electronic structure [10]. The metal-slag interaction is described as a cooperative ion-exchange process, in which each component of the melt interacts not with isolated counterparts, but with the entire system.

To predict the physicochemical properties of melts, integral indicators of metal and slag are used. These parameters describe their chemical and structural states, incorporating interatomic interaction parameters among the components of the melts.

The physicochemical model of the electronic structure of metallic melts is characterized by two groups of parameters. The main parameters include the effective charges of components (Zi), which are determined both for each pair of reactants ($Zi_{j\text{-}j}$), and for the entire system through their weighted average value (Zi_{avg}). The integral characteristics include the chemical equivalent (Z^Y), which summarizes information about the charges of the components considering the probabilities of forming bonds of various types, the structural parameter (d) that characterizes the mean interatomic distance, and the parameter (tgα), which represents the change in ionic radius as a function of charge.

The main integral parameters of the slag melt model are: the stoichiometry index ρ, defined as the ratio of the number of cations (K) (Fe, Cr, Al, Si, Mn,...) to the number of anions (A) (O, S, F,...); the parameter Δe, which characterizes the cation-anion bond interaction; the average interatomic distance d; the index of individuality of the cationic sublattice of the melt tgα; the weighted average charges and radii of the cations in the K sub-system, of the anions in the A sub-system, and in the direction of the K-A and A-K bonds.

The parameter De is calculated as the weighted average number of electrons localized in the cation-anion bond direction for the slag melt, represented in the form Me_rO. From a physical point of view, the integral parameter Z^Y for the metallic phase is analogous to parameter De and is defined as the weighted average number of electrons participating in the interaction between ions Me_i и Me_j. The calculation of integral characteristics of the metal and slag is performed based on their initial chemical composition using the computerized modelling systems “Metal” and “Slag.”

Harrington’s desirability function

A powerful tool for integrated assessment and optimization of multivariable processes is Harrington’s desirability function, which allows several parameters with different measurement scales and optimization goals to be combined into a single dimensionless index [14]. This approach, which provides a more comprehensive and objective evaluation of process efficiency compared to analyzing individual parameters, was applied to the assessment of physicochemical processes during ladle refining of steel. According to Harrington’s methodology, the key factors determining the chemical composition of finished steel can be transformed into individual desirability functions based on their quality ranges or target values.

The mathematical apparatus for calculating the Harrington desirability function transforms all potential parameters that determine the final process indicators into a single value scale ranging from 0 to 1 using an empirical function f = exp(-(exp(-y)). In this function, y is the transformed value of a specific indicator to the range of [- 1.5; 3.5], considering quality categories such as: "very good", "good", "satisfactory", "bad", and "very bad" (Fig. 1). Establishing the relationship between the response value *y* and the corresponding *f* value according to quality categories is inherently subjective, reflecting the researcher's perception of the importance of individual factors. The generalized desirability function (F) is obtained by aggregating the partial desirability functions f_i as their geometric mean:

$$F = \prod_{i=1}^{n} f_i^{\beta}$$

where Π - the product of partial desirability functions, f_i are individual desirability indices, n is the number of parameters, and b denotes the significance weight of each f_i in the overall evaluation.

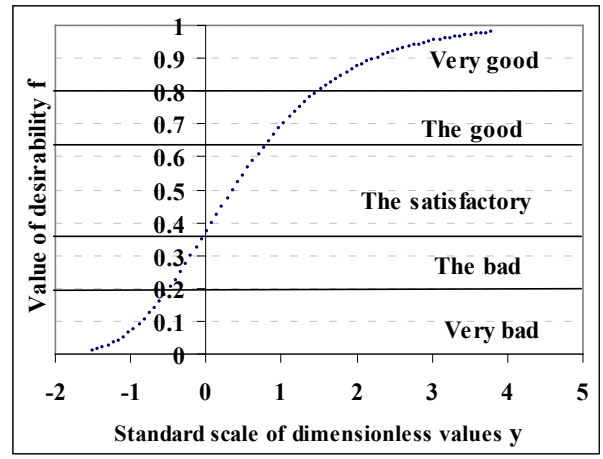

Fig. 1. Graph of the desirability function f = exp(-(exp(-y)).

RESULTS AND DISCUSSION

Modelling of physicochemical interaction processes in the metal-slag system during ladle refining

Prediction and modelling of informative indicators of the steelmaking process, based on reliable data concerning the properties of all participants in interphase interactions (metal, slag, additives, and slag-forming mixtures), significantly contribute to the rationalization of additive use, the enhancement of alloy element recovery, and the improvement of special steel characteristics.

The main thermodynamic parameters that allow the assessment of the degree of completion of alloying and refining processes in the ladle are the interphase distribution coefficients of diffusing elements. Describing the distribution coefficients of elements as variable quantities that depend on specific raw material and technological conditions makes it possible to predict the final indicators of the technological process, as well as to solve the inverse problem of finding the optimal solution for obtaining metal of the required quality [13]. For example, a higher distribution coefficient of sulphur between metal and slag indicates a greater ability of the slag to absorb sulphur, and therefore, for sulphur, the desirability function corresponds to the rule "the greater, the better".

The present study utilizes current industrial data on the chemical composition of SAE1006 steel and corresponding slag before and after steel refining in the ladle-furnace unit at Private Joint-Stock Company "KAMET-STEEL" in Kamianske, Ukraine (Tables 1 and 2).

Based on the final chemical compositions of the steel and slag, the distribution coefficients of sulphur, silicon, manganese, phosphorus, and aluminium between the metallic and slag phases were evaluated. It was established that the efficiency of interphase redistribution of these elements is determined by a combination of factors, among which the physicochemical interaction between components in the metal-slag system plays the dominant role. To quantify this interaction, integral parameters were used - the chemical equivalent of the metal composition Z^y, the Δe, parameter for slag, and the stoichiometric index ρ of the slag phase (Table 3). The influence of deoxidation, alloying, and refining processes on the final content of elements in steel was evaluated considering the physicochemical characteristics of ferroalloys and slag-forming mixtures used, as well as technological parameters of the refining operation.

Special attention was given to calculating the temperature factor, characterizing the molten state in the ladle in relation to the melting temperature of ferroalloys (ferrosilicon and ferromanganese)

Table 1. Indicators of the chemical composition of SAE1006 steel before and after LF.

	Steel chemical composition, % ($\frac{\text{before}}{\text{after}}$E) *											
	C	Mn	Si	S	P	Cr	Ni	Cu	Al	V	As	Ca
	0.049 0.058	0.38 0.41	0.078 0.130	0.064 0.008	0.017 0.017	0.021 0.021	0.017 0.023	0.028 0.029	0.003 0.003	0.0050 0.0017	0.0050 0.0020	0.00001 0.0017
2	0.051 0.067	0.26 0.30	0.015 0.036	0.022 0.003	0.010 0.009	0.046 0.049	0.031 0.032	0.053 0.055	0.006 0.004	0.0050 0.0011	0.0050 0.0027	0.00001 0.0034
3	0.060 0.077	0.27 0.38	0.081 0.111	0.053 0.008	0.014 0.015	0.022 0.030	0.026 0.027	0.037 0.040	0.009 0.003	0.0050 0.0011	0.0050 0.0019	0.00001 0.0016

** Contents (before/after LF), % : Zr - (0.005/0.005); Ti - (0.005/0.001); Mo - (0.01/0.01); Nb - (0.01/0.001).*

Table 2. Indicators of the chemical composition of slag before and after LF.

Melting No	Slag chemical composition, % ($\frac{\text{before}}{\text{after}}$E) *									Basicity CaO / SiO_2
	CaO	SiO_2	MgO	FeO	Al_2O_3	P_2O_5	Fe_2O_3	MnO	S	
1	46.2 57.8	15.7 25.0	9.0 9.8	8.0 0.9	12.3 2.9	0.53 0.10	3.40 0.05	1.71 0.32	0.90 1.05	2.94 2.31
2	43.5 56.2	16.3 22.4	6.0 7.9	10.0 1.0	14.4 7.0	0.42 0.10	4.28 0.11	2.55 1.72	0.15 1.09	2.67 2.51
3	43.9 61.9	11.7 22.5	9.3 9.0	5.6 1.0	24.3 2.3	0.26 0.10	2.23 0.09	1.82 0.28	0.43 0.98	3.75 2.75

Table 3. Integral indicators of the chemical composition of melts before and after ladle furnace treatment of SAE1006 steel (in accordance with Tables 1 and 2).

Melting No	Steel		Slag		Distribution coefficients of sulphur, silicon, manganese, phosphorus, and aluminium				
	Chemical equivalent of composition Z^Y, e	Interatomic distance, d. 10^{-1} nm	Chemical equivalent of composition Δe, e	Stoichiometry indicator ρ	Ls	Lsi	Lmn	Lp	Lal
1	1.1580 1.1592	2.8165 2.8136	- 2.327 - 1.979	0.808 0.801	14.02 131.2	201.2 192.3	4.43 0.77	31.1 5.8	4100 966
2	1.1523 1.1541	2.8183 2.8149	- 2.429 - 1.942	0.793 0.801	6.94 363.3	1086.6 622.22	9.48 5.70	44.2 11.1	2400 1760
3	1.1562 1.1598	2.8143 2.8109	- 2.033 - 1.820	0.801 0.818	8.05 122.5	144.44 202.70	6.55 0.72	18.0 6.6	2700 770

compared to the liquidus temperature of steel before LF treatment. The intensity of interaction in the metal-additive system increases as the difference between these temperatures decreases. Melting temperatures of steel and additives were calculated using the integral parameters of the metallic system Z^Y, d and tgα [15]. To account for the influence of fluxing additions on desulphurization, the basicity (CaO/SiO_2) of the slag-forming mixture (composed of limestone and fluorspar) was calculated. The efficiency of argon purging was

evaluated by the integrated purging intensity indicator (I_{purg}), defined as the ratio of the total argon flow rate to the purging time (Table 4).

The desulphurization process in the ladle represents a complex system of interrelated parameters whose efficiency depends on numerous factors. These include slag composition regulation, properties of desulphurizing additives, steel temperature, mixing intensity, and the interaction within the metal-slag system.

Analysis of the influence of physicochemical and technological parameters on the sulphur distribution coefficient after ladle refining revealed a series of dependencies. The most significant influence on desulphurization efficiency is exerted by the integral indicators of the initial chemical compositions of metal and slag, introduced into the ladle prior to refining. Furthermore, the key parameters include the temperature state of the metal-additive system, which determines the kinetics and thermodynamics of the inter-phase interactions, as well as the basicity of the slag-forming mixture, which directly influences the activity of oxygen-containing and sulphur-containing compounds (Fig. 2). It was also found that the final sulphur content in steel after refining largely depends on its initial content at the beginning of argon purging. This factor must be considered when constructing mathematical models and predictive algorithms for the interphase sulphur distribution coefficient. In practice, to improve desulphurization efficiency, fluxes enriched with calcium oxide (CaO) are intentionally added, increasing the basicity ratio (CaO/SiO_2). This approach allows for active control over the activity of sulphur in the slag and, consequently, the directionality and rate of its removal from the metallic phase. Furthermore, the specific composition of the fluxes is generally selected based on the initial sulphur content in the steel. Further analysis revealed that a statistically significant correlation exists between the traditional desulphurization index - the fraction of sulphur removed - and the final interphase distribution coefficient of sulphur (Fig. 2). This confirms that intensive ion-exchange processes occur within the metal-slag system, where sulphur is replaced by oxygen, predominantly from calcium and magnesium oxides. Thus, the chemical activity of slag components and their ion-exchange capacity with dissolved sulphur in metal play a decisive role in desulphurization efficiency.

The intensity of argon purging during ladle refining significantly affects the homogenization of both the chemical composition and the temperature field of the melt. Higher argon flow rates promote more efficient mixing, intensify mass transfer processes, and consequently accelerate reactions between the melt and slag, leading to reduced impurity content and a more stable final chemical composition of steel. Industrial data analysis revealed the quantitative contribution of the technological regime indicator - namely, purging intensity (I_{purg}) to the final sulphur distribution coefficient between refined steel and slag (Fig. 2).

The combined effect of the three main groups of factors on steel desulphurization is represented by the analytical dependence of the sulphur distribution coefficient between final ladle refining products $L_s = f(F_{ms}, F_{md}, F_t)$, where F_{ms}, F_{md}, F_t are the complex indicators of the metal-slag, metal-additive, and technological regime systems, respectively. We generated the structure of the complex indices by applying the mathematical apparatus of Harrington's

Table 4. Indicators of additives used in the ladle furnace treatment of steel.

Melting No	Consumption, t				T_{mFeSi}/T_{mSt}	T_{mFeMn}/T_{mSt}	Basicity of SFM CaO/SiO_2	Argon purging intensity L m^{-1}
	FeSi65	FeMn	fluorspar	limestone				
1	0.453	0.128	0.63	2.7	1.99	0.55	13.22	1031
2	0.039	-	0.25	1.1	0.16	0.00	12.96	1004
3	0.197	0.276	0.36	1.4	0.93	1.28	12.14	980

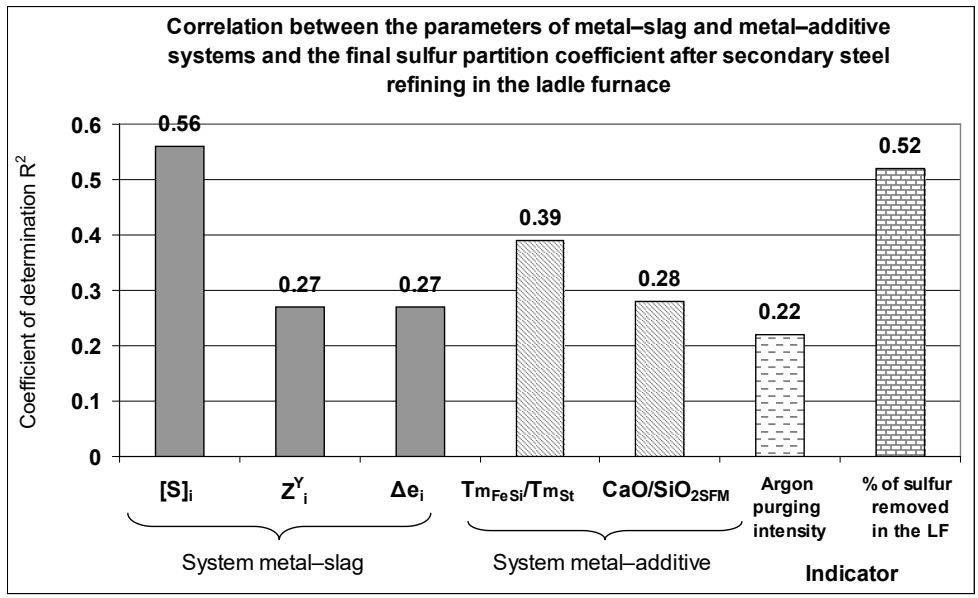

Fig. 2. The influence of physicochemical and technological parameters of ladle refining on the final sulphur distribution coefficient between metal and slag for SAE1006 ($[S]_i$ - initial sulphur content, Z^Y_i и Δe_i - integral parameters of initial metal and slag, T_{mFeSi}/T_{mSt} - ratio of melting temperatures of FeSi65 additive and steel, CaO/SiO_{2SFM} - basicity of the slag-forming mixture composed of lime and fluorspar).

generalized desirability function, accounting for the identified factors and their relative influence on the final interfacial sulphur distribution coefficient. For this purpose, the most preferable values for individual parameters were identified (Table 5). Based on these, we calculated the standard values on the ordinate axis y_i, the partial desirability indices f_i in dimensionless units for each component. The values of the complex indicators of the metal-slag, metal-additive, and technological regime systems for each melt are calculated using Eq. (1 - 3) (Table 6):

$$F_{ms} = [S]_i^{0.5} \cdot Z^Y{}_i^{0.25} \cdot \Delta e_i^{0.25} \quad (1)$$

$$F_{md} = (T_{mFeSi}/T_{mSt})^{0.6} \cdot (CaO/SiO_{2SFM})^{0.4} \quad (2)$$

$$F_t = I_{purg} \quad (3)$$

where $[S]_i$ is the initial sulphur content in steel, Z^Y_i and Δe_i are integral parameters of the initial metal and slag compositions, T_{mFeSi}/T_{mSt} is the ratio of melting temperatures of the FeSi65 additive and steel, CaO/SiO_{2SFM} is the basicity of the slag-forming mixture, I_{purg} is the intensity of argon purging.

Based on the relationships between Fms, Fmd, and Ft and the sulphur distribution coefficient, the following analytical dependence was developed for predicting the final Ls value after ladle refining - Eq. (4) (R^2 is the coefficient of determination of the relationship, A_1 is the equation coefficient determined for a specific steel grade):

$$Ls = A_1 \cdot F_{ms}^{0.5} \cdot F_{md}^{0.3} \cdot F_t^{0.2}, \qquad R^2 = 0.75 \quad (4)$$

The exponents characterize the relative weights of partial indicators and are determined from prior expert assessments reflecting factor loadings on the general indicator.

The distribution of silicon, manganese, and aluminium between the metallic and slag phases during ladle refining is determined by a complex of thermodynamic and kinetic factors and therefore represents a multifactor function. The key parameters affecting the interphase equilibrium of these elements, like sulphur, include slag composition and basicity, process temperature, component activity in metal, and conditions of gas-slag-metal interaction. For efficient

Table 5. Desirability scale of partial indicators for the metal-slag and metal-additive systems that have a significant influence on the sulphur distribution coefficient between the final products of the melt.

Quality category	Sulphur content in steel $[S]_i$, %	Integral parameters of steel, Z^Y_i, e	Integral parameters of slag Δe_i, e	Basicity of SFM CaO / SiO_2	T_{mFeSi} / T_{mSt}	Argon purging intensity, l/m
Very good	0.006 - 0.012	1.150 - 1.156	(- 1.58) - (- 1.2)	15.2 - 18	0.10 - 0.58	1400 - 1700
Good	0.012 - 0.02	1.156 - 1.162	(- 1.96) - (- 1.58)	12.4 - 15.2	0.58 - 1.07	1100 - 1400
Satisfactory	0.02 - 0.03	1.162 - 1.168	(- 2.34) - (- 1.96)	9.6 - 12.4	1.07 - 1.56	800 - 1100
Bad	0.03 - 0.05	1.168 - 1.174	(-2.72) - (- 2.34)	6.8 - 9.6	1.56 - 2.04	500 - 800
Very bad	0.05 - 0.07	1.174 - 1.180	(- 3.1) - (-2.72)	4 - 6.8	2.04 - 2.52	300 - 500

Table 6. Calculated values of dimensionless partial indicators, desirability functions. and the integral desirability function for the complex indicators of the metal-slag (Fms) and metal-additive (Fmd) systems.

Melting No	Dimensionless partial indicators, partial desirability functions						Complex indicator	
	$[S]_i$	Z^Y_i	Δe_i	CaO / SiO_2	T_{mFeSi} / T_{mSt}	I_{purg}	Fms	Fmd
1	1.030 0.061	1.283 0.758	0.028 0.378	1.040 0.702	- 0.448 0.333	0.519 0.552	0.167	0.449
2	- 0.094 0.545	2.425 0.915	0.918 0.671	0.980 0.687	2.807 0.941	1.354 0.772	0.646	0.830
3	- 1.470 0.013	1.478 0.796	0.686 0.604	0.771 0.630	1.038 0.702	0.364 0.499	0.081	0.672

refining, slag composition optimization is required. Increased basicity is not always beneficial for all refining objectives. There exists an optimal range in which basicity effectively reduces the activity of SiO_2 and thus enhances silicon retention in metal, while maintaining sufficient oxidizing potential for other impurity removal mechanisms (e.g., dephosphorization). Optimal basicity also promotes manganese retention and phosphorus removal, but it must be balanced to prevent adverse effects on other processes. Silicon is also instrumental in shielding aluminium from being consumed unnecessarily during silica reduction, which in turn improves the effectiveness of deoxidation and desulphurization.

The content of FeO and MnO oxides in slag during ladle refining has a dual role: on one hand, they consume deoxidizers and promote inclusion formation; on the other, their controlled amount moderates magnesium transfer to steel and prevents the formation of solid spinel inclusions. Consequently, these components stabilize the redox environment, prevent abrupt fluctuations, and help control inclusion composition and properties.

The introduction of deoxidizers such as aluminium strongly affects the behaviour of all three elements by modifying slag composition. Aluminium effectively reduces slag oxidizing potential, creating favourable conditions for retaining alloying elements (Si and Mn) in steel. Aluminium oxide (Al_2O_3) influences slag fluidity and reactivity, displaying amphoteric behaviour dependent on concentration. Excessive aluminium additions may increase costs and promote harmful inclusions; therefore, maintaining an optimal level is essential. Effective control of these elements requires a comprehensive, parameter-monitored approach.

Thus, during ladle refining, a complex interaction occurs between metal and slag, where silicon, manganese, and aluminium are actively redistributed, participating in deoxidation, desulphurization, and alloying. Slag composition and properties are key control parameters governing these processes to achieve the desired steel quality.

Industrial data analysis confirmed that the efficiency of interphase redistribution of these elements is primarily determined by physicochemical interactions in the metal-slag system. To quantify these interactions, integral parameters of "convolution" of the steel and slag chemical composition were used. Specifically, for SAE1006 steel, a relationship was established between the silicon distribution coefficient (Lsi) and the integral parameter of interatomic interaction - the chemical equivalent of the steel composition before its treatment in the LF (Z^Y). The relationship has two zones - a stable zone (Zone 1) and an unstable zone (Zone 2), in which silicon more actively transitions into the slag phase (for $Z^Y < 1.158$, Fig. 3a). The second zone corresponds to an increased average interatomic distance (for $d > 2.815$, Fig. 3b), which promotes silicon transfer into slag. A similar inverse relationship was identified between Z^Y_i and the manganese distribution coefficient (Lmn), confirming the key influence of the integral chemical composition indicator of the metal on interphase distribution behaviour.

Adequate description of the interactions between slag components and their influence on silicon, manganese, and aluminium distribution coefficients is achieved using the integral slag parameters - chemical equivalent Δe and stoichiometric index ρ. The combined influence of metal and slag composition before LF on the redistribution of Si, Mn, and Al is incorporated into the complex indicator of metal-slag Fms (Table 7).

Temperature factor also has a substantial influence, represented by the ratio of ferroalloy melting temperatures (ferrosilicon and ferromanganese) to steel's liquidus temperature. The closer these values, the more efficient the dissolution and assimilation of additives and the transfer of elements into slag. Fig. 4a shows the dependence of the manganese distribution coefficient (Lmn) on the ratio (T_{mFeMn} / T_{mSt}). Increased purging intensity enhances metal-slag mixing, intensifies interphase reactions, and thus increases element transfer to slag (Fig. 4b).

The aluminium distribution coefficient (Lal) between the steel and the slag is determined by the amount of the element introduced, the slag composition, the temperature regime, and the oxidizing potential of the system. During ladle refining aluminium is introduced in stages: as pigs (or blocks) at the steel pre-treatment unit and as granules at the LF unit, which determines the differences in its dissolution and redistribution.

Despite its high deoxidizing capacity, excessive aluminium increases cost and promotes inclusion formation. Its interaction with FeO and MnO reduces their concentrations and decreases slag's oxidation potential, facilitating oxygen removal from metal.

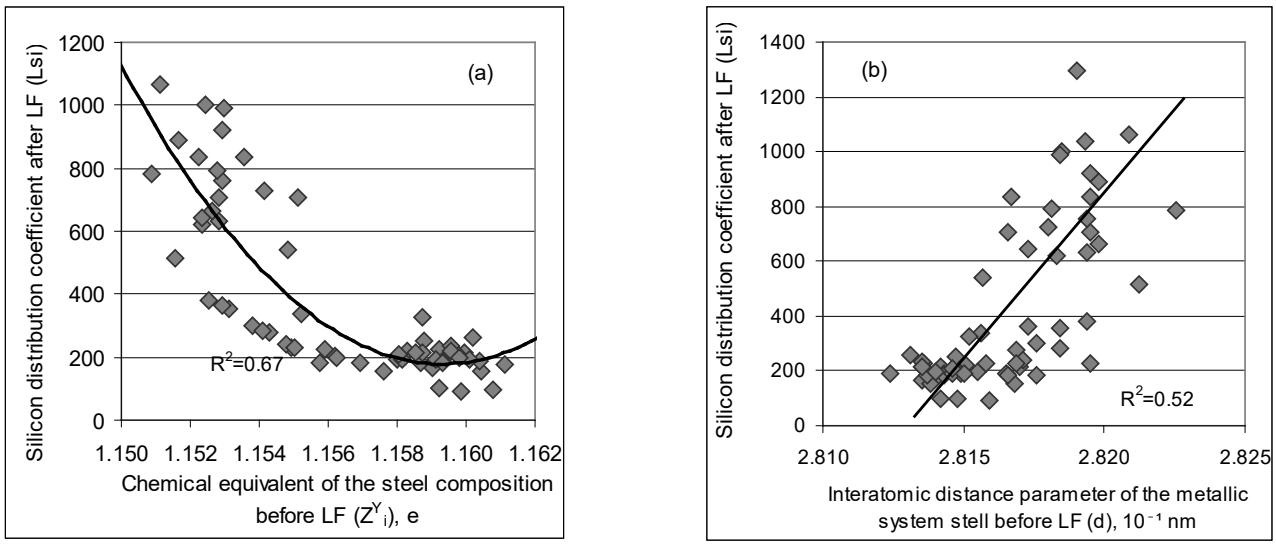

Fig. 3. Dependence of the interphase silicon distribution coefficient after ladle furnace refining of steel on the integral indicators of the steel's chemical composition before treatment.

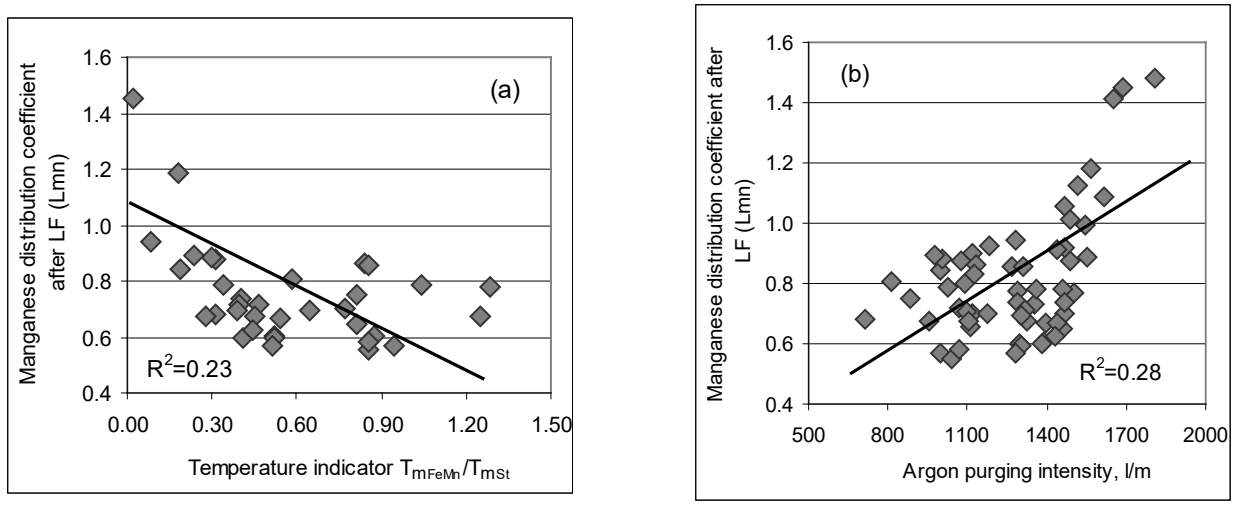

Fig. 4. Dependence of the final manganese distribution coefficient on the temperature parameter of the metal-additive system before ladle furnace treatment of steel and on the purging intensity.

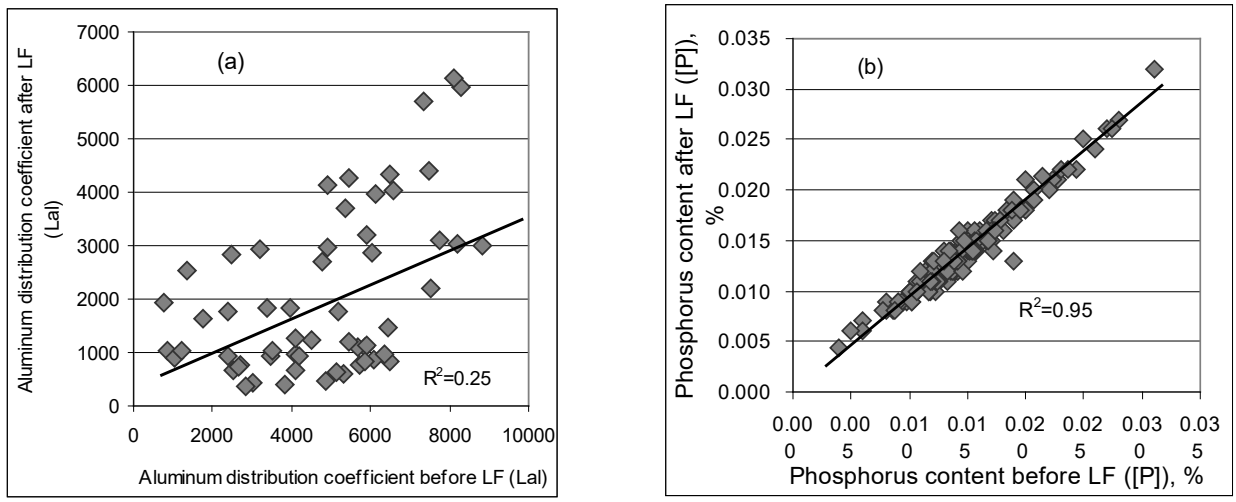

Fig. 5. Correlation between the final and initial values of the aluminium distribution coefficient (Lal) (a) and the phosphorus content (b) before and after ladle furnace refining of SAE1006 steel.

Optimal aluminium content balances effective deoxidation with minimized cost and inclusion formation. Quantitative assessment of its behaviour under ladle furnace conditions enables more efficient use and reduced aluminium losses.

The substantial correlation observed between the aluminium distribution coefficient (Lal) before and after the steel's refining in the LF (Fig. 5a) reflects the two - stage aluminium addition process used for deoxidizing of the metal. The influence of other key factors on the final aluminium content is expressed through their weighting coefficients within the complex indicators Fms, Fmd, and Ft (Table 7).

Analysis of phosphorus distribution between metal and slag (Fig. 5b) shows strong correlations between its initial and final values, indicating the absence of significant dephosphorization during ladle refining for this steel grade. This stability suggests that phosphorus removal occurs at earlier process stages and that ladle conditions do not favor its extraction.

Table 7. Structure of the complex indicators of the physicochemical state of the metal-slag and metal-additive systems, generated to assess their influence on interphase element distribution processes based on ladle furnace refining data for SAE1006 steel.

System	Complex indicators			
	Sulphur	Silicon	Manganese	Aluminium
metal-slag, F_{ms}	$[S]_i^{0,5} \cdot Z^{Y}{}_i^{0.25} \cdot \Delta e_i^{0.25}$	$Z^{Y}{}_i^{0.7} \cdot \Delta e_i^{0.3}$	$Z^{Y}{}_i^{0.55} \cdot \Delta e_i^{0.45}$	$Lal_i^{0.4} \cdot Z^{Y}{}_i^{0.3} \cdot \rho_i^{0.3}$
metal-additive, F_{md}	$(T_{mFeSi./} T_{mSt})^{0.6} \cdot (CaO/SiO_2)_{SFM}^{0.4}$	T_{mFeSi} / T_{mSt}	T_{mFeMn} / T_{mSt}	T_{mFeSi} / T_{mSt}

For describing the regularities of silicon, manganese, and aluminium redistribution between steel and slag, the structure of the complex indicator Fms was generated, incorporating the integral characteristics of the initial metal and slag compositions. Similarly, the structure of the complex metal-additive system indicator Fmd was constructed using Harrington's desirability methodology (Table 7).

Based on these complex indicators, predictive models were developed to calculate the distribution coefficients for silicon, manganese, and aluminum, the values of which are determined by Eq. (5) - (7) (R^2 is the coefficient of determination of the relationship):

$$Lsi = A_2 \cdot F_{ms}^{0.57} \cdot F_{md}^{0.2} \cdot F_t^{0.23}, \; R^2 = 0.77 \quad (5)$$

$$Lmn = A_3 \cdot F_{ms}^{0.4} \cdot F_{md}^{0.3} \cdot F_t^{0.3}, \; R^2 = 0.62 \quad (6)$$

$$Lal = A_4 \cdot F_{ms}^{0.45} \cdot F_{md}^{0.35} \cdot F_t^{0.2}, \; R^2 = 0.58 \quad (7)$$

where Fms, Fmd, and Ft are the complex indicators of the metal-slag, metal-additive, and technological regime systems, respectively, and A_2 - A_4 are coefficients determined for the specific steel grade.

The main difference of the obtained integral indicators and dependencies for calculating the distribution coefficients of the analyzed elements lies in the values of the corresponding exponents, which reflect the weighted influence of each partial indicator on the overall indicator. Furthermore, the content of elements in the finished steel is largely determined by the interaction processes between the metallic and slag phases before the steel refining stage in the ladle furnace unit, which is confirmed by the relatively small difference in the exponents within the complex indicator Fms. The thermal state of the metal-additive system also significantly affects final element distribution: the closer the melting temperatures of steel and ferroalloy,

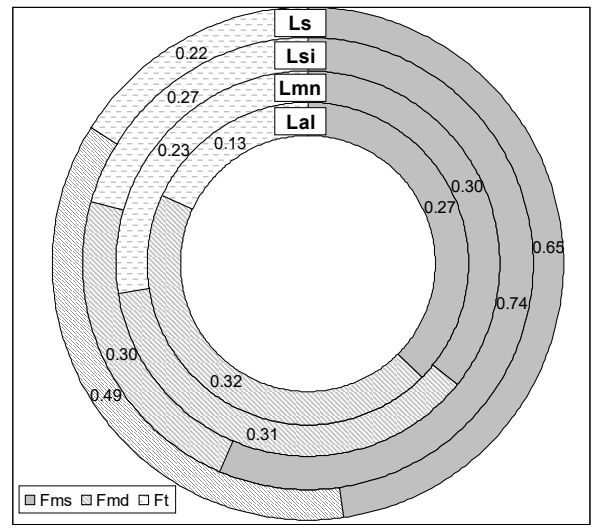

Fig. 6. Comparative characteristic of the degree of influence of the complex indicators of the metal-slag, metal-additive and technological regime systems on the interphase distribution coefficients of sulphur, silicon, manganese, and aluminium between the refined steel and slag after ladle furnace treatment, based on the coefficient of determination (R^2) for SAE1006 steel.

the more intense the redistribution processes and the higher the element assimilation by steel (Fig. 6).

The identified regularities and obtained analytical dependencies enable quantitative evaluation of element distribution coefficients between metallic and slag phases during ladle refining. They form the scientific foundation for constructing predictive algorithms for the final chemical composition of refined steel. The developed systematic approach allows not only the description of current redistribution processes of S, Si, Mn, and Al, but also prediction of their behaviour depending on slag composition, oxidation degree, and temperature-technological parameters.

CONCLUSIONS

A systematic approach has been developed for describing the physicochemical processes occurring in the metal-slag system during steel refining in a ladle furnace, based on the methodological framework of the Directed Chemical Bonding Concept (DCBC) and mathematical methods for processing multifactor data.

Current industrial data on the chemical composition of SAE1006 steel and the corresponding slag before and after ladle furnace refining were used as the informational basis of the study. An analytical apparatus for finding interconnections between the initial and final parameters of the distribution processes of the main steel elements in the metal-slag system before and after its treatment with appropriate additives (ferroalloys, deoxidizers, slag-forming mixtures) is described.

The use of interatomic interaction parameters in melts, which characterize the chemical composition of steel, slag, and additives, as well as technological regime indicators, is substantiated as model parameters for predictive models to calculate the distribution coefficients of elements (sulphur, silicon, manganese, and aluminium) during the secondary treatment of steel.

The structure of composite indicators for the metal-slag and metal-additive systems was generated, considering their chemical composition and physicochemical properties, using the mathematical apparatus of Harrington's generalized desirability function. This function enables multidimensional indicators to be integrated into a single generalized index and serves as an effective optimization tool for improving steel quality and reducing production costs.

The study identified patterns and developed analytical dependencies for calculating the distribution coefficients of sulphur, silicon, manganese, and aluminium between metallic and slag phases in the following generalized form: $L_{el} = A \cdot F_{ms}^{\alpha_1} \cdot F_{md}^{\alpha_2} \cdot F_t^{\alpha_3}$ where Fms, Fmd, and Ft represent the composite indicators of the metal-slag, metal-additive, and technological regime systems, respectively; A, α_1, α_2, and α_3 are equation coefficients determined through expert evaluation for a specific steel grade.

The developed systematic approach to describing the physicochemical processes within the metal-slag system during ladle furnace refining makes it possible to account for the totality of metallurgical factors and to predict system behaviour under various technological conditions. The quantitative evaluation of element distribution coefficients between final products in the metal-slag system as variable quantities distinguishes this approach from traditional methods, which treat them as constants.

The results obtained lay the groundwork for developing an algorithm for the prediction and targeted formation of the final melts' chemical composition, considering the initial composition of the metal and slag, alloying and fluxing additives. The implementation of these results as an Expert System software to evaluate the efficiency of steel refining processes at the ladle treatment unit will provide scientifically based recommendations for selecting optimal alloying and deoxidizing additives, as well as for adjusting the technological parameters of ladle treatment. This will make it possible to minimize the loss of valuable elements to the slag, reduce the process cost, and ensure the stable production of steel with the required chemical composition and quality.

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Authors' contributions

D.T.: Conceptualization, Methodology, Supervision, Editing, A.B.: Writing, Investigation, Methodology and Study Design, D.S.: Project Supervision, Review,

Formal Analysis, Resources.

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