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MATHEMATICAL MODEL OF CHEMICAL PROCESSES OCCURRING IN ELECTRIC ARC FURNACES

The article provides a mathematical model of chemical processes occurring in electric arc furnace (EAF). The authors of the article are the first to build up a new algorithm of calculating the main characteristics of chemical processes taking place in EAF. This algorithm is notable for its simplicity and convenience of execution and helps to calculate the mass of substances entering into a chemical reaction and its products, the quantity of heat emitted or absorbed. So, it would be reasonable to use the algorithm described in this article while creating complex models of EAF, in particular, while studying the thermal and chemical processes occurring in the furnace and looking for their correlation, while constructing energy and material balance of EAF. Besides, due to the high level of calculations that are performed with the help of this algorithm, it is convenient to use it while formulating the laws of optimal management of EAF. Its adequacy is proved by comparison of the calculations to the experimental data.

Keywords: Electric Arc Furnace (EAF), Mathematical Model, Chemical Processes, Model Adequacy, Control Algorithm

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МАТЕМАТИЧНА МОДЕЛЬ ХІМІЧНИХ ПРОЦЕСІВ, ЩО ВІДБУВАЮТЬСЯ У ДУГОВИХ СТАЛЕПЛАВИЛЬНИХ ПЕЧАХ

У роботі представлена математична модель хімічних процесів, що відбуваються у дугових сталеплавильних печах (ДСП). Моделювання здійснене за допомогою розгляду основних хімічних реакцій, які мають місце у ДСП: реакції відновлення заліза і шлакоутворення, реакцій, що відповідають за формування пічної атмосфери. Дана модель у кожен момент часу надає інформацію про основні характеристики хімічних процесів, які протікають у ДСП, а саме: теплові коефіцієнти реакції та їх швидкість; масу речовин, що приймають участь у хімічній реакції та її продуктів; кількість теплоти, що виділяється або поглинається у результаті тієї чи іншої реакції. Запропонований авторами алгоритм розрахунку відрізняється простотою та зручністю використання. Цей алгоритм дозволяє уникнути побудови складних фізико-хімічних моделей, які включають елементи гідродинаміки ванни і потребують великої кількості початкової інформації.

З метою підтвердження адекватності створеної моделі розглянуті отримані залежності швидкостей хімічних реакції від температури. При цьому одержані результати збігаються з результатами проведених раніше експериментів. Крім того, авторами наведені дані про вміст розглянутих хімічних елементів у шлаку та розплаві згідно з протоколами виплавки та розрахунками, зробленими з використанням описаного алгоритму. Аналіз цих даних дозволяє підтвердити, що запропонований алгоритм, відображає реальну поведінку процесу. Розбіжність між реальними та розрахунковими даними не перевищує 20%, тобто, знаходиться у допустимих межах. Програмна реалізації наведеної моделі здійснена за допомогою мови програмування C++, з використанням відкритої бібліотеки OpenGL.

Розроблена авторами модель інтегрована в єдиний синергетичний комплекс, що забезпечує надання адекватної інформації про перебіг електричних, теплових та хімічних процесів, що відбуваються у дугових сталеплавильних печах, з урахуванням їх взаємного впливу та взаємозв'язку. Даний комплекс, у свою чергу, є підґрунтям для знаходження оптимального значення активної потужності, що подається у піч у кожен момент часу, та створення автоматизованої системи керування процесом виплавки сталі у дуговій печі.

Ключові слова: дугова сталеплавильна піч, математична модель, хімічні процеси, адекватність моделі, алгоритм керування

Introduction

Today, solving the energy problem of electric arc steelmaking is relevant. This problem lies in the energy intensity of steel production in arc furnaces along with a constant increase in energy prices. At the same time, it is expedient to use modern automated control systems (ACS) for electric arc furnaces (EAF). Numerous studies have proved the efficiency of automated systems based on mathematical models of processes (electrical, thermal, and chemical) that occur in the working chamber of the furnace during the melting period. However, despite a large number of adequate models, the efficiency of which is confirmed by numerous experiments, describing thermal and electrical processes, chemical processes have not been sufficiently studied. In addition, there is no complex synergetic model that describes the nature of electrical, thermal, and chemical processes in an EAF, taking into account their mutual influence and interrelation.

Related work

The works [1 - 3] are devoted to solving the energy problem of electric arc steelmaking. At the same time, the efficiency of using automated furnace control systems has been proven by the authors of the studies [1, 2, 4, 5]. The studies of the use of mathematical modeling apparatus in the development of ACS for EAF are described in scientific works [1 – 3, 6, 7]. Thereat, the expediency of applying this scientific approach is reasonably proven. Thus, let's move on to considering mathematical models of the processes occurring in the working chamber of an electric arc furnace during steel smelting.

To date, there are several models of electrical processes occurring in an EAF, which are characterized by low accuracy or a complex and inconvenient interface [8 - 11]. However, the authors of the studies [12, 13] have developed a number of computer models for studying the electrical processes of an electric arc furnace. Such models are adequate and efficient to use.

The works [14 - 17] are devoted to the modeling of thermal processes occurring in an EAF. These works are aimed at detailed consideration of the complex heat exchange in the EAF working chamber: heat exchange by radiation between the surfaces of electrodes, charge, walls, roof, and bottom of the furnace; convective heat exchange between solid charge, melt, slag, furnace gas, and lining; heat transfer inside solid, liquid, gaseous phases.

Despite a number of shortcomings (consideration at the initial stage of the furnace operation of one common well, which forms in the charge as a result of the operation of three electrodes; construction of models in a two-dimensional formulation; lack of description of methods for calculating the heat absorbed or released in the working chamber of the furnace due to chemical reactions; lack of taking into account the composition of solid charge, melt, furnace atmosphere when calculating their thermo-physical characteristics; simplification of the furnace shape), the models described in works [14 - 17] are inherent to a sufficient level of adequacy.

The works [18, 19] are devoted to the modeling of some chemical processes occurring in electric arc furnaces. The authors of the considered works propose to model chemical processes based on the consideration of reactions that describe them. This requires information about weight and temperature, Gibbs energy and heat of formation of substances included in the reactions, velocity constant and equilibrium constant of the reactions under consideration. This approach allows avoiding the construction of complex physical and chemical models that include elements of bath hydrodynamics that require a large amount of initial information. However, in the above-mentioned studies, the reactions of iron reduction and slag formation are not fully considered - the main reactions occurring in the working chamber of an EAF.

Thus, to date, there is no mathematical model of chemical processes occurring in electric arc furnaces and no complex synergetic model that describes the nature of electrical, thermal, and chemical processes in the working chamber of an EAF, taking into account their mutual influence and interrelation.

Purpose

The purpose of the study is the following: development of a mathematical model of chemical processes occurring in electric arc furnaces; integration of the developed model into a single synergetic complex describing energy exchange during steel smelting in an EAF; development of appropriate software.

Proposed technique

Let's consider the smelting of steel in electric arc furnace with the usage of "heel". In this case, the charge contains: steel scrap, pig iron, pellets, and coke. Lime, limestone, and fluorspar are used as slag-forming materials. Charge materials have chemical composition shown in Table 1.

Since admixtures make up less than 0,2%, their influence will not be analyzed in the further study of chemical processes taking place in electric arc furnace.

During the period of smelting in the working space of EAF numerous chemical reactions take place. The main of them can be divided into three groups:

- reactions of iron recovery;
- reactions of slag formation;
- reactions taking place in the atmosphere of the furnace.

Table 1

Charge composition

Chemical compounds (elements)	**Content, %**
Fe	48,91
Fe_2O_3	44,7975
C	2,724
Si	0,2375
CaO	1,2375
SiO_2	1,9305
Other admixtures	Remainder

$$3Fe_2O_3 + C \rightarrow 2Fe_3O_4 + CO - 121{,}8\,\frac{kJ}{mol}, \qquad (1)$$

$$Fe_3O_4 + C \rightarrow 3FeO + CO - 208\,\frac{kJ}{mol}, \qquad (2)$$

$$FeO + C \rightarrow Fe + CO - 115{,}5\,\frac{kJ}{mol}, \qquad (3)$$

$$3Fe_2O_3 + CO \rightarrow 2Fe_3O_4 + CO_2 - 129\,\frac{kJ}{mol}, \qquad (4)$$

$$Fe_3O_4 + CO \Leftrightarrow 3FeO + CO_2 - 36\,\frac{kJ}{mol}, \qquad (5)$$

$$FeO + CO \Leftrightarrow Fe + CO_2 + 57\,\frac{kJ}{mol}, \qquad (6)$$

$$2C + SiO_2 \rightarrow Si + 2CO + 1080\frac{kJ}{mol}, \quad (7)$$

$$SiO_2 + CaO \Leftrightarrow CaSiO_3 + 72{,}2\frac{kJ}{mol}, \quad (8)$$

$$2Fe + SiO_2 \Leftrightarrow 2FeO + Si + 1391\frac{kJ}{mol}, \quad (9)$$

$$CO_2 + C \Leftrightarrow 2CO + 172{,}5\frac{kJ}{mol}, \quad (10)$$

Heat coefficients of these reactions at a temperature of 298 K degrees are calculated according to the Hess's Law using the data about the heat of formation of substances entering into reactions and their products.

The algorithm of calculation of the chemical processes based on the reactions describing them is suggested in the works [18, 19]. This algorithm allows to avoid building complex physical and chemical models that include elements of tub hydrodynamic and need a lot of initial information. That is why for monitoring the quality of steelmaking in EAF it is reasonable to apply the algorithm proposed by the authors of the works [18, 19] for the calculation of characteristics of chemical interactions described with reactions (1) – (10).

Suppose t_{melt} - is a time of charge melting, τ - is a time step, than $t = 0, \tau, \ldots, t_{melt}$ are moments of time when the heat absorbed or emitted as a result of each reaction, the masses of substances entering into reactions, and the masses of obtained substances are calculated. To make these calculations, at every moment of time the information about the speed of reactions (1) – (10) and their temperature coefficients is needed. It is most expedient to find the speed of reactions occurring in EAF using the theory of active collisions and the experimental data given in the literary sources (6 – 7).

For the calculation of temperature coefficients of reactions, it is expedient to use the Kirchhoff's equation. Suppose that in every moment of time the charge and melt temperature is known, as well as the heat emitted or absorbed by the charge and "heel" as a result of heating with electric arcs, heat exchange with the walls, roof and bottom of the furnace, and the furnace atmosphere.

Let's consider the principle of modelling on the example of the following reaction

$$3Fe_2O_3 + C \rightarrow 2Fe_3O_4 + CO - 121{,}8\frac{kJ}{mol}.$$

The reaction rate is found by the formula:

$$w = \frac{n_{Fe_2O_3} n_C {\sigma_{12}}^2 \left[8\pi kT\left(\frac{1}{\mu_{Fe_2O_3}} + \frac{1}{\mu_C}\right)\right]^{\frac{1}{2}} e^{-\frac{E_A}{RT}}}{N_A}$$

where $n_{Fe_2O_3}$ - is the number of molecules Fe_2O_3 in 1 m^2 surface of interaction $(\frac{1}{m^2})$,

n_C- is the number of molecules Fe_2O_3 in 1 m^3 volume of interaction $(\frac{1}{m^3})$,

σ_{12}- is the average effective diameter at collision of molecules (m),

k- is the Stefan-Boltzmann constant $(\frac{J}{K})$,

T- is the temperature of reagents (K),

$\mu_{Fe_2O_3}$- is the mass of molecules Fe_2O_3 (kg),

μ_C- is the mass of molecules C (kg),

E_A- is the energy of activation of reagents $(\frac{J}{mol})$,

R- is the universal gas constant $(\frac{J}{mol \cdot K})$,

N_A- is the Avogadro constant $(\frac{1}{mol})$.

The amount of substance and mass Fe_2O_3 involved in the reaction (1) for some time τ, are found using the formulas:

$$\nu_{Fe_2O_3} = wS\tau,$$

$$m_{Fe_2O_3} = \nu_{Fe_2O_3} M_{Fe_2O_3},$$

where S- is the contacting area of Fe_2O_3 and C (m^2).

The mass of C, Fe_3O_4, CO involved in the reaction (2) and the amount of heat absorbed during its course, are found by the chemical equation:

$$\begin{array}{ccccccc} \nu_{Fe_2O_3} mol & & & & & & \\ m_{Fe_2O_3} kg & & m_C kg & & m_{Fe_3O_4} kg & m_{CO} kg & QJ \\ 3Fe_2O_3 & + & C & \to & 2Fe_3O_4 + & CO & +H\frac{J}{mol}, \\ 3mol & & 1mol & & 2mol & 1mol & \\ 0{,}48kg & & 0{,}012kg & & 0{,}464kg & 0{,}028kg, & \end{array}$$

where H- is the thermal coefficient of reaction at a given temperature, found by the Kirchhoff's law.

$$m_C = \frac{m_{Fe_2O_3} \cdot 0{,}012}{0{,}48},$$
$$m_{Fe_3O_4} = \frac{m_{Fe_2O_3} \cdot 0{,}464}{0{,}48},$$
$$m_{CO} = \frac{m_{Fe_2O_3} \cdot 0{,}028}{0{,}48},$$
$$Q = \nu_{Fe_2O_3} \cdot H.$$

Thus, the created comprehensive model provides reliable information on the main characteristics of the melting at any time.

Results

For the software implementation of the developed model, the programming language C++ was used. The graphical user interface is developed using the OpenGL open-source library.

To check the adequacy of the described algorithm, let's examine the smelting of charge, the composition of which is given in Table 1, in EAF with the capacity of 100 tones along with 20 tons of "heel". To set up the electric melting conditions, let's use the performance charts.

The dynamic of chemical processes taking place in EAF is most completely characterized by the temperature dependences of the speed of reactions describing these processes. These dependences obtained with the use of the considered algorithm are given in Fig. 1 -4:

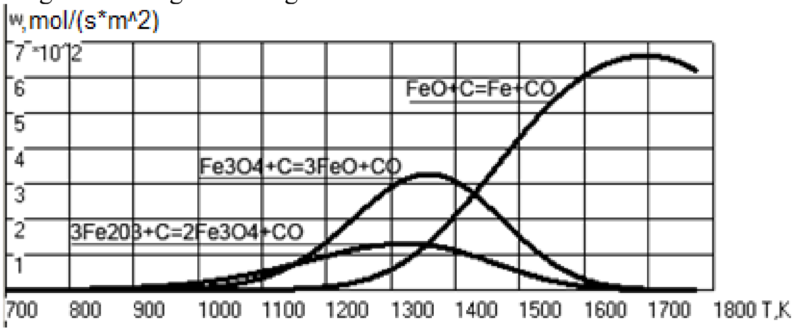

Fig.1.Temperature dependences of the speed of reactions (1) – (3)

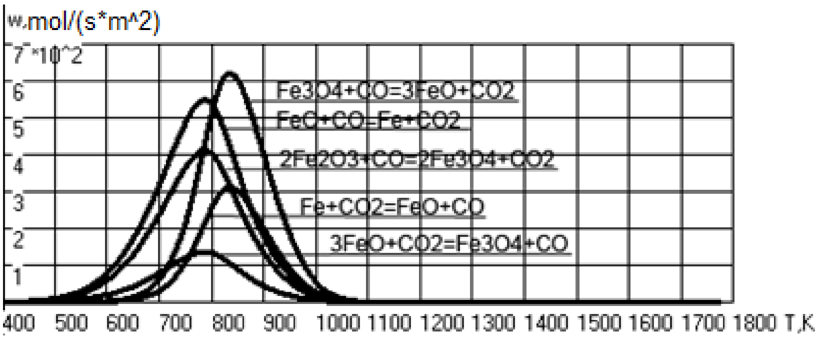

Fig. 2. Temperature dependences of the speed of reactions (4) – (6)

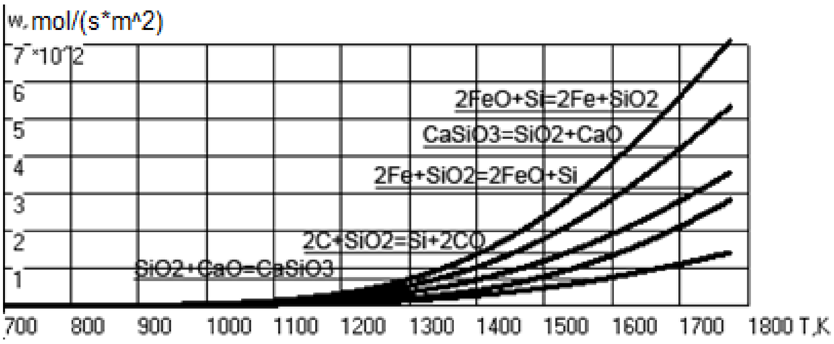

Fig. 3. Temperature dependences of the speed of reactions (7) – (9)

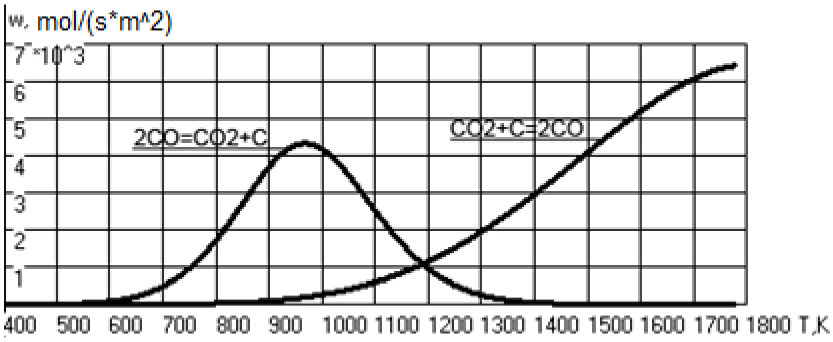

Fig. 4. Temperature dependences of the speed of reaction (10)

Fig. 1 shows that reactions of direct iron recovery proceed stepwise at temperatures higher than 1000K degrees, notably the most developed is the reaction (3). These results coincide with the experimental data and the information given in the sources [20].

Fig. 2 shows that indirect iron recovery takes place mostly at the zone of moderate temperatures, notably reactions (5) – (6) take place actively in both directions due to the correlation of the components of CO and CO_2 gas mixture that are close to equivalent.

Temperature dependences of the speed of reactions that have a strong effect on the composition of furnace atmosphere are shown in Fig. 4.

It is experimentally determined that the speed of the reaction $CO_2 + C \rightarrow 2CO$ begins to increase at a temperature of 1000 K degrees and higher, while the speed of the reverse reaction decreases at this range of temperatures [20]. Fig. 4 proves this fact.

For a more detailed study of the correlation of thermal and chemical taking place in EAF, let’s choose some control volume and show the charts of its temperature changes regardless of the energy of chemical reactions and taking into account the heat, emitted or absorbed as a result of chemical interactions proceeding within this volume (Fig. 5).

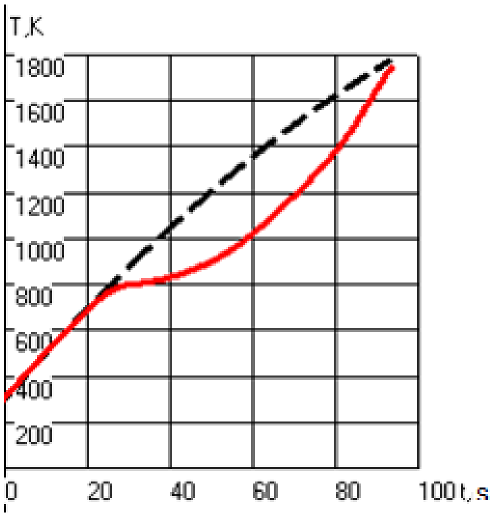

Fig.5. Changes of the charge temperature (- - - regardless of the energy of chemical reactions, -- with regard to the energy of chemical reactions)

At a charge temperature of lower than 700 K degrees, the speeds of chemical reactions are close to 0, respectively, the energy of reactions is insignificant, that’s why the charts of charge temperature increase regardless of and with regard to the chemical interaction coincide (Fig. 5). At the range of temperatures from 700 K to 1100 K degrees, the reactions of direct and indirect iron recovery characterized by the heat absorption proceed actively. The charge temperature with regard to the chemical interaction increases slower than the charge temperature regardless of the heat given for proceeding of chemical reactions (Fig. 5).

However, at a temperature higher than 1100 K degrees, slag-formation reactions with sudden outburst of energy start to proceed, whereby their speed is increasing, and thus the quantity of emitted heat is increasing, too.

The charge temperature with regard to the chemical interaction is rapidly increasing (Fig.5). Thus, the chart of the charge temperature change with regard to the heat of chemical reactions corresponds the real behavior of the process. Moreover, the time of charge melting down regardless of and with regard to the chemical interaction nearly coincide. This fact can explain a rather high level of adequacy of earlier studies of the thermal processes taking place in EAF without exact calculation of the energy of chemical reactions.

Tables 2 - 3 contain the data on the contents of considered chemical elements in slag and melt according to the smelting protocols and calculations made with the use of the described algorithm. The analysis of this data allows to confirm that the proposed algorithm reflects the real behavior of the process, the divergence between real and calculated data is within permissible limits.

Table 2

Content of Fe, C, Si in melt

Chemical compounds (elements)	Content, % (smelting protocols)			Content, % (calculation)		
	1	2	3	1	2	3
Fe	97,2	97,4	96,43	96,25	97,69	95,42
C	2,25	2,21	3,007	3,64	2,09	4,45
Si	0,15	0,123	0,09	0,11	0,22	0,13

Table 3

Content FeO, CaO, SiO of in slag

Chemical compounds (elements)	Content, % (smelting protocols)			Content, % (calculation)		
	1	2	3	1	2	3
FeO	12,79	13,76	10,16	9,12	11,22	8,45
CaO	43,25	40,7	41,17	45,01	37,89	34,12
SiO_2	24,05	22,18	23,58	20,18	25,003	18,37

Conclusions

Thus, the study carried out by the authors allows to draw the following conclusions:

1. Electric furnace steelmaking is a rapidly developing branch of modern metallurgy, which has a tendency to occupy a leading position in the world steel market. At the same time, electric arc furnace remains one of the most energy-intensive units used in ferrous metallurgy. It is economically expedient to upgrade electric arc furnaces on the basis of the use of a modern control system, which ensures the reduction of energy costs of the unit while maintaining the quality of the obtained production.

2. The authors have built a model describing the chemical processes occurring in electric arc furnaces, which allowed to calculate the characteristics of the main chemical processes occurring in EAF (mass of substances entering into any chemical reaction and its products; quantity of heat emitted or absorbed).

3. It is reasonable to use the algorithm described in this article while creating complex models of EAF, in particular, while studying the thermal and chemical processes occurring in the furnace and looking for their correlation, while constructing energy and material balance of EAF.

4. The adequacy of the model is proved by comparison of the calculations to the experimental data.

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