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THE MODELING OF VACUUM STEEL REFINING IN THE RH DEGASSING UNIT BASED ON THERMODYNAMIC ANALYSIS OF THE SYSTEM

MODELOWANIE PROCESU PRÓŻNIOWEJ RAFINACJI STALI W URZĄDZENIU RH W OPARCIU O ANALIZĘ TERMODYNAMICZNĄ

Determining the state of equilibrium in steel refining processes plays an important role in view of process intensification possibilities, fuller process control and the related economic effects. The main objective of this paper is to analyze the states of equilibrium in heterogeneous systems for vacuum degassing of steel in the RH degassing unit. The kinetic model of the RH process was based on a metal bath mixing model in which account is taken of the gas-metal equilibrium of the boundary layer of the metal bath in the vacuum chamber. This objective can be attained by using a software package containing suitable thermodynamic data bases and computing software integrated with it. The computer applications used to solve the problem include *FactSage* and *ChemSheet*. This paper will contribute to explaining some of the processes taking place during steel refining in the RH degassing unit.

Keywords: steel refining, heterogeneous systems, states of equilibrium, RH process, *FactSage*

Określenie stanu równowagi w procesach pozapiecowej rafinacji stali odgrywa istotną rolę, ze względu na możliwość intensyfikacji procesu, jego pełniejszą kontrolę oraz związane z tym efekty ekonomiczne. Podstawowym celem pracy jest analiza stanów równowagi w układach wielofazowych dotyczących procesu próżniowego odgazowania stali w urządzeniu RH. Kinetyczny model procesu RH został oparty o model mieszania kąpieli metalowej, w którym uwzględniony jest fakt osiągnięcia stanu równowagi gaz-metal dla granicznej warstwy kąpieli metalowej w komorze. Realizacja celu pracy jest możliwa dzięki zastosowaniu pakietu komputerowego zawierającego odpowiednie bazy danych termodynamicznych oraz zintegrowane z nimi komputerowe programy obliczeniowe. Programem komputerowym zastosowanym jako narzędzie do rozwiązania postawionego problemu jest FactSage™ i ChemSheet. Praca stanowi wkład w wyjaśnienie niektórych procesów zachodzących podczas rafinacji stali w urządzeniu RH.

1. Introduction

The course of vacuum steel refining processes is characterized by high intensity [1]. It can be assumed that at any moment during the process a specific boundary layer of the metal bath in the vacuum chamber reaches the state of equilibrium with the gaseous phase. The time following which the metal portion reaches the state of equilibrium in the vacuum chamber is so short, and the capacity of the vacuum pumps so high, that the change in the chemical composition of the metal bath and of the gas phase due to degassing of the lifted portion does not lead to a change in the temperature of the system and pressure in the vacuum chamber. Therefore it can be assumed that at any specific moment the process runs under isothermal and isobaric conditions. This serves as a basis for the assumptions adopted for the thermodynamic calculations made for the systems investigated in this paper. One of the most important goals of vacuum degassing is to reduce nitrogen content in the metal bath [2]. The reduction degree depends on many factors. These include the temperature of the system, pressure in the vacuum chamber and chemical composition of the bath. The aim of modeling vacuum steel refining processes based on thermodynamic analysis is to examine the impact of these factors on the solubility of nitrogen in liquid iron.

2. Assumptions for the model

The mathematical model of vacuum degassing in the RH vessel was formulated based on the Tank Model

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theory [3] and the minimization of the Gibbs energy using the *FactSage*™ [4] and *ChemSheet* [5, 6] software packages, which permit thermodynamic calculations in the Microsoft Excel environment (thermodynamic model). For the Tank Model assumptions, the reactor used for the RH process was divided into three elementary tanks – Figure 1. The circulation of bath in the RH degasser is presented in Figure 2.
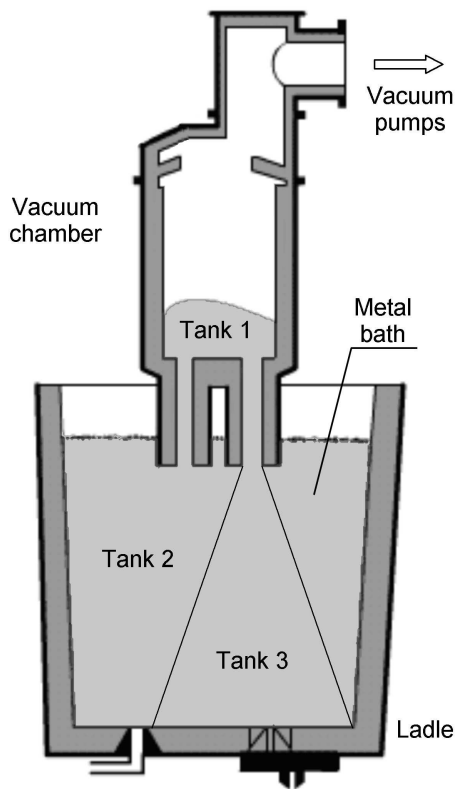

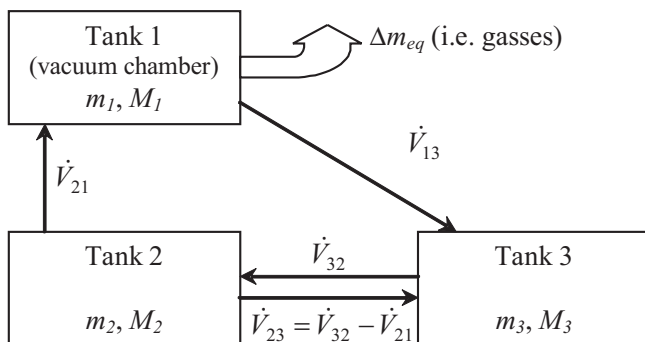Fig. 1. Diagram depicting the division of the bath in the RH degasser into tanks

Fig. 2. Diagram showing bath circulation in the RH degassing model (symbols are consistent with those adopted for the system of equations (1)

The tank which is used as the basic unit for the mixing model formulated is attributed the following properties:

- at any moment of the time t there is no gradient of the reactive substances concentrations in the tank (ideal mixing),
- the mass streams entering and leaving the tank are defined,
- changes in the concentrations of the reactants are made by steps, at a frequency reflecting the time steps adopted for the calculations.

As far as the bath circulation in the unit is concerned, it is assumed that the kinetic energy of the bath leaving the downleg snorkel is sufficient for the bath to reach the bottom of the ladle. Using the symbols in Figure 2 the following system of equations describing the flow of mass in the model adopted can be formulated:

$$dm_1 = -\frac{m_1}{M_1}\dot{V}_{13}dt + \frac{m_2}{M_2}\dot{V}_{21}dt$$

$$dm_2 = \frac{m_3}{M_3}\dot{V}_{32}dt - \frac{m_2}{M_2}\dot{V}_{23}dt - \frac{m_2}{M_2}\dot{V}_{21}dt$$

$$dm_3 = \frac{m_1}{M_1}\dot{V}_{13}dt + \frac{m_2}{M_2}\dot{V}_{23}dt - \frac{m_3}{M_3}\dot{V}_{32}dt \quad (1)$$

$$\dot{V}_{23} = \dot{V}_{32} - \dot{V}_{21}$$

$$\dot{V}_{21} = \dot{V}_{13}$$

where: m_i – mass of the reactants in tank i, [Mg], M_i – mass of tank i, [Mg], $\dot{V}_{ij}$ – intensity of the bath stream between tanks i and j, [Mg/min], t – time, [min]. It was assumed in the above equation – according to the applicable principle – that the mass stream leaving the tank has a negative value, while the inflowing stream has a positive value.

Based on the melting data of the actual RH vacuum degassing process, the following mean values of the process parameters were adopted. The total mass of the bath amounts to 330 Mg. The mass of the first tank is equal to the bath mass lifted to the vacuum chamber, i.e. 3% of the total bath mass. The mass of tank 1 $M_1 = 9.9$ Mg. The remaining bath mass is that which remains in the ladle. The ladle was divided into two tanks. In the above system of equations the masses of particular tanks of the ladle are unknown physical quantities, which can, however, be established through suitable verification methods. In the light of existing research in the field of modeling metal bath mixing processes in metallurgical reactors, it was assumed that the mass of tank M_3 constitutes 40.3% of the bath mass remaining in the ladle (mass M_2 is a variable and amounts to 59.7% of the bath mass remaining in the ladle) [3]. As a consequence, the bath mass in tank 2 is $M_2 = 191.1$ Mg, while that in tank 3 $M_3 = 129.0$ Mg.

It was assumed that the degassing process time t_c will amount to 20 minutes. The rate of circulation (R) of

liquid steel through the vacuum chamber [7, 8], which informs about the multiplicity factor of the residence time of the elementary bath volume in the vacuum chamber in the model is $R = 4$. The rate of circulation is tightly connected with the parameter of the intensity of the metal bath flow through the vacuum chamber calculated according to the following formula:

$$R = \frac{\dot{V}_{21} \cdot t_c}{M_k},\qquad(2)$$

where: $\dot{V}_{21}$ – intensity of the metal flow through the vacuum chamber using the symbols adopted in Figure 2, [Mg/min], t_c – effective bath degassing time equal to 20 [min] as assumed in the model, M_k – total mass of the metal bath undergoing the degassing process equal to 330 [Mg], as assumed in the model.

Taking into account the above assumptions, it was calculated that the intensity of the metal bath flow through the vacuum chamber is $\dot{V}_{21} = 66$ Mg/min. Apart from the above physical quantity $\dot{V}_{21}$ the other values for the system of equations describing the mass flow in the model adopted include the intensities of the bath flow $\dot{V}_{ij}$ between tanks 2 and 3. As a result of the tests performed using the model it was established that the flow intensity $\dot{V}_{23}$ constitutes nearly 70% of the flow intensity $\dot{V}_{32}$ [3].

Knowledge of the intensity of the bath flow through the vacuum chamber allows another process parameter to be established, i.e. the residence time of the elementary metal bath volume in the vacuum chamber. This parameter depends on the bath flow intensity $\dot{V}_{21}$ and on the mass of the bath in the vacuum chamber M_1. This dependence is expressed through the following equation:

$$t_R = \frac{M_1}{\dot{V}_{21}},\qquad(3)$$

where: t_R – residence time, [min].

The problem of residence time in the vacuum chamber is directly related to the time required for the chemical composition of the degassed bath portion to reach the state of equilibrium. With the assumptions made, the residence time of the elementary metal bath volume in the vacuum chamber is $t_R = 9$ s.

A parameter which influences the quality of the result obtained after using the mixing model presented is the time step of calculations Δt. It is obvious that as the time step approaches zero, the numerical solution should approach the accurate solution. In the simulation of RH degassing by vacuum presented the 20-minute time of the process was divided into 1000 steps, as a result the time step is $\Delta t = 1.2$ s. Most often, the time step in bath flow simulations in metallurgical reactors ranges between 0.1 and 5 s [3].

The time step value Δt both impacts the accuracy of the result of the mixing model and has significant importance for the thermodynamic model. In the mixing model the change in the mass of the reactant in the tank i at a specific moment of time $t + \Delta t$ is calculated on the basis of the known mass of the reactant at t and the known $dm_i(t)$:

$$m_i(t + \Delta t) = m_i(t) + dm_i(t).\qquad(4)$$

Because in the vacuum chamber of the RH degassing unit the portion of the metal bath reaches the state of equilibrium under reduced pressure, thus changing its chemical composition, a thermodynamic model has been developed taking into account the changes in the masses of the different components of the metal bath in tank 1. The thermodynamic model functions on the basis of the minimization of the Gibbs energy using the *FactSage* and *ChemSheet* software packages. As a consequence, the mixing model presented – taking into account the thermodynamic model – forces a change of the reactant mass in tank 1 at $t + \Delta t$, whose value is calculated based on the known mass of the reactant at t, the known $dm_1(t)$ and the know change of the mass of the reactant in the vacuum chamber once the state of equilibrium is reached $\Delta m_{eq}(t)$. In practice, the value of $\Delta m_{eq}(t)$ refers to the mass of the reactants which leaves the metal bath and is pumped away by the vacuum pumps in the RH unit.

$$m_1(t + \Delta t) = m_1(t) + dm_1(t) + \Delta m_{eq}(t)\qquad(5)$$

$$\Delta m_{eq}(t) = m_{eq}(t) - \alpha \cdot m_1(t),\qquad(6)$$

where: $dm_1(t)$ – change in the mass of the reactant in the vacuum chamber as a result of the mixing model, [Mg], $\Delta m_{eq}(t)$ – change in the mass of the reactant in the vacuum chamber during degassing, [Mg], $m_1(t)$ – mass of the reactants in the vacuum chamber prior to degassing, [Mg], $m_{eq}(t)$ – equilibrium mass of the reactants in the degassed bath layer, [Mg], α – bath degassing coefficient in the vacuum chamber, [–].

The bath degassing coefficient in the vacuum chamber refers to the actual mass of the bath which is degassed and reaches the state of equilibrium. The value of coefficient α is a result of the number of calculation steps in time t_R. Assuming 100% degassing of the metal portion lifted to the vacuum chamber during the residence time of the bath in the vacuum chamber t_R, the α coefficient is as follows:

$$\alpha = \frac{\Delta t}{t_R}.\qquad(7)$$

Apart from the knowledge of the initial masses of particular components of the metal bath – taking into account the division into tanks – the thermodynamic model requires knowledge of the other parameters of the system. It was assumed that the initial temperature of the melt is 1600°C. Besides a uniform temperature decrease by 50°C during the whole process was taken into account. The decisive parameter influencing the state of thermodynamic equilibrium is the value of the pressure in the vacuum chamber. The pressure value adopted as the standard pressure in the vacuum chamber was $p = 3$ kPa.

3. RH process simulation

The vacuum degassing process in the RH unit was computer-simulated using the mixing and thermodynamic models developed. For this purpose a file was prepared in the *FactSage* software comprising thermodynamic data of the Fe-N-C-O system. The masses of particular components and process temperature and pressure were the same as the initial values for calculating local states of equilibrium at particular time steps. The values of the parameters were given in the descriptions of each type of simulation. It was assumed that a gaseous phase, liquid metal and slag phase can be expected as the products of the states of equilibrium. However, the simulations carried out rule out the possibility of slag phase formation as the system reaches the state of equilibrium under the process conditions assumed. At each time step of the calculations the system reached local state of equilibrium in isothermal and isobaric conditions. The values that changed were the masses of the gaseous and liquid metal phases and their chemical compositions.

The RH process model based on the concept presented above was verified for a unit with the ladle capacity of 330 Mg. The accuracy of the model used to calculate the final N content was checked for a series of 40 melts. The results obtained are presented in Table 1.

TABLE 1

Distribution of the relative error of the final N content

Relative error [%]	5	10	15	20	25
% of heats	32	40	70	85	100

The verified model was subsequently used to carry out a series of simulations by means of virtual experiments. The experiments covered the following problems:
– determination of the time required for the RH unit to reach the near-equilibrium state,
– the level of degassing of the bath during residence in the vacuum chamber,

– influence of the initial oxygen content on the course of vacuum refining,
– influence of the vacuum chamber pressure on the course of refining.

3.1. Hypothetical 60-minute degassing of metal bath in the RH unit

Under industrial conditions the vacuum degassing process lasts approx. 20 minutes. The process simulation was carried out for the Fe-N-C-O system. The following concentrations of the different components were adopted as the standard initial composition: N = 0.015%, C = 0.2%, O = 0.01%. The remaining portion was iron. The division of the metal bath into tanks, the circulating streams values and the calculation steps were adopted as in the above description. The vacuum chamber pressure assumed was 3 kPa, while the initial temperature of the metal bath 1600°C, with a drop to the final value of 1550°C. The simulations were conducted for hypothetical metal bath degassing in the RH unit during 60 minutes. Figure 3 presents the resultant change in nitrogen content in the metal bath and particular tanks.
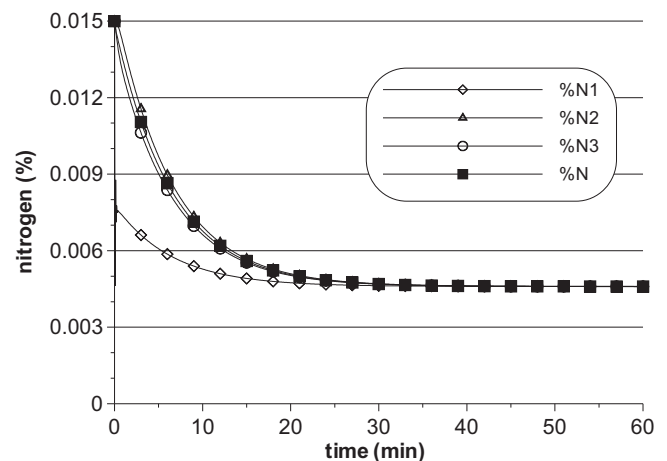

Fig. 3. Change in nitrogen content in the Fe-N-C-O system during degassing time $t_c = 60$ minutes (%N1 – nitrogen content in tank 1, %N2 – nitrogen content in tank 2, %N3 – nitrogen content in tank 3, %N – mean nitrogen content in the metal bath

The above diagram shows that after approx. 20 minutes the system reaches a state close to equilibrium. The metal bath is degassed to such a degree that although the process continues nitrogen content in the metal bath does not change.

3.2. Degree of degassing of the lifted bath mass

The RH process simulation permits investigation as to what degree the changes in nitrogen content in the metal bath depend on the degree to which the metal bath lifted to vacuum chamber is degassed. According to the

findings at the model formulation stage, the thickness of the metal layer in the vacuum chamber which reaches the state of thermodynamic equilibrium depends on the time during which the vacuum acts. If the residence time of the elementary bath volume in the vacuum chamber is adopted as the reference point (t_R), it is possible to verify the hypothetical influence of the layer thickness on the degassing process of the whole melt. It can be expected that the reduction in the height of the degassed layer of the lifted portion will extend the time required for the state of equilibrium to be reached. A simulation was carried out for the Fe-N-C-O system in which the initial concentrations of the components and the process conditions were equal to the values adopted as base values, i.e. N = 0.015%, C = 0.2%, O = 0.01%, T = 1600°C, with a fall by 50°C, p = 3 kPa. The equilibrium nitrogen content in the metal bath was calculated after a hypothetical degassing was conducted during t = 20 minutes for situations taking into account various degrees of degassing of the portion lifted to the vacuum chamber. The simulation was performed for a system in which at t_R 100%, 50%, 37.50% and 25% of the bath lifted to the vacuum chamber is degassed respectively. Figure 4 presents the influence of the degree to which the lifted bath mass is degassed on nitrogen content changes in the system.
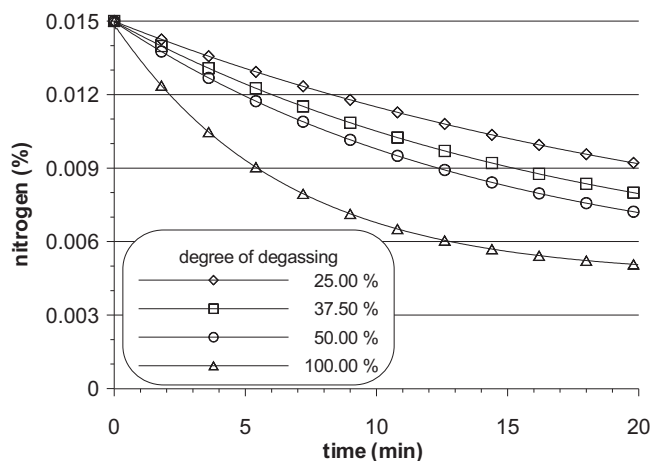

Fig. 4. Influence of the degree to which the lifted bath mass is degassed on the final nitrogen content in the system

Although the result of the simulation is purely hypothetical, it indicates that reduction in the thickness of the fully degassed part of the lifted portion significantly extends the time required for the nitrogen content equilibrium in the metal bath to be reached. In a real RH process the position of the vacuum chamber over the ladle should be controlled so as to ensure that at t_R a bath mass is degassed equal to the mass lifted to the vacuum chamber. This will permit shortening the degassing time

and ensure that a near-equilibrium nitrogen content is reached.

3.3. Initial oxygen content

Another series of simulations of the RH process addressed the impact of the initial content of oxygen in the metal bath on the final content of nitrogen in the liquid solution of iron. The initial conditions for the model were selected similarly to the example presented above. The oxygen contents for the successive simulations were 0.002%, 0.005%, 0.01%, 0.02%. Table 2 presents the influence of the initial oxygen content in the metal bath on the nitrogen content after RH degassing.

TABLE 2

Influence of initial oxygen content in the Fe-N-C-O system for final nitrogen content in the bath after degassing

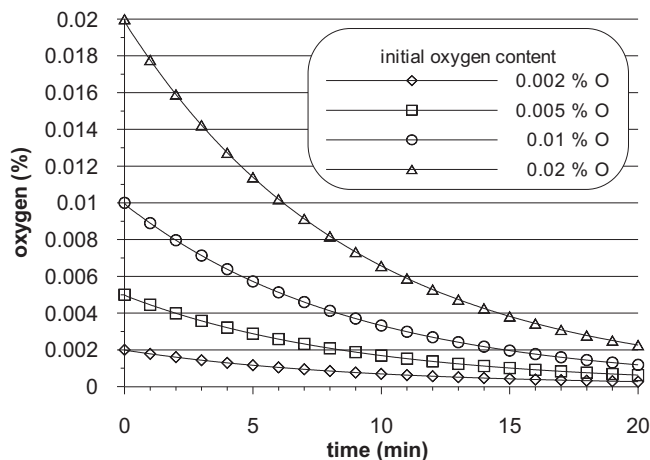| Initial oxygen content [%]	Final nitrogen content [%]
0.002	0.0072
0.005	0.0064
0.01	0.0057
0.02	0.0049

Fig. 5. Change in oxygen content during vacuum steel refining depending on initial oxygen content in the Fe-N-C-O system

Figure 5 presents the change in oxygen content during the vacuum steel refining process depending on its initial content in the system. During vacuum steel deoxidization not only oxygen but also carbon is removed. The increase in the deoxidization capacity of carbon in a very low vacuum is so huge that along with the deoxidization of steel by vacuum also the reduction of oxide inclusions by carbon can take place. Figure 6 presents the change in carbon content during vacuum steel refining depending on the initial oxygen content in the system. As expected, as the initial oxygen content in the liquid iron solution increases, the degree of decarburisation also increases.
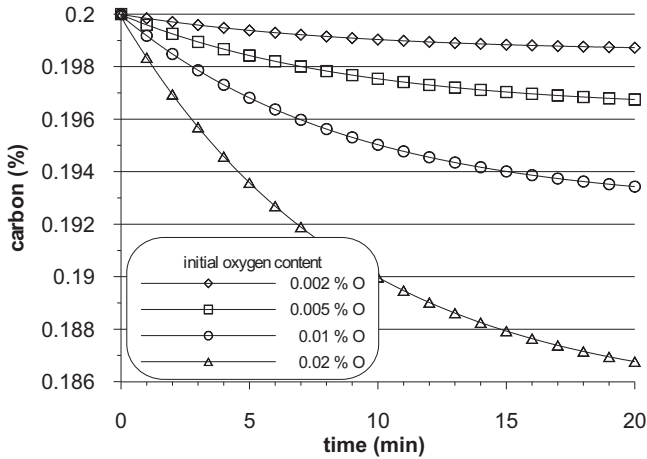
Fig. 6. Change in carbon content during vacuum steel refining depending on the initial oxygen content in the Fe-N-C-O system

3.4. Pressure in the vacuum chamber

RH process simulations were also carried out to investigate the influence of the vacuum chamber pressure on final nitrogen content in the Fe-N-C-O system. Taking into account the system composed of N = 0.015%, C = 0.2%, O = 0.01%, with the initial temperature of 1600°C, and a fall by 50°C, the system was subjected to vacuum at the following pressures: p = 1, 3, 5, 10, 20, 30 kPa. Table 3 presents the influence of pressure on the final content of nitrogen and the other components in the RH degassing process. Figure 7 presents the change in nitrogen content in the Fe-N-C-O system during vacuum degassing for the different pressures in the vacuum chamber. Figure 8 and Figure 9 present the changes in oxygen and carbon contents respectively for the same system.

TABLE 3

Influence of vacuum chamber pressure on the final contents of the components in the Fe-N-C-O system

p [kPa]	Final N content [%]	Final C content [%]	Final O content [%]
1	0.0023	0.1933	0.0010
3	0.0057	0.1934	0.0012
5	0.0067	0.1935	0.0013
10	0.0084	0.1937	0.0016
20	0.103	0.1942	0.0022
30	0.0115	0.1947	0.0028

In the light of the simulation results presented, it can be concluded that the pressure value in the chamber has a crucial influence on nitrogen content in the bath. The differences between the final nitrogen contents for the extreme pressures adopted in the research is fivefold. The influence of the vacuum chamber pressure on the degree

of decarburisation and deoxidization is less pronounced. The carbon contents across the range of the pressures examined do not differ considerably. The difference in the oxygen contents is nearly threefold.
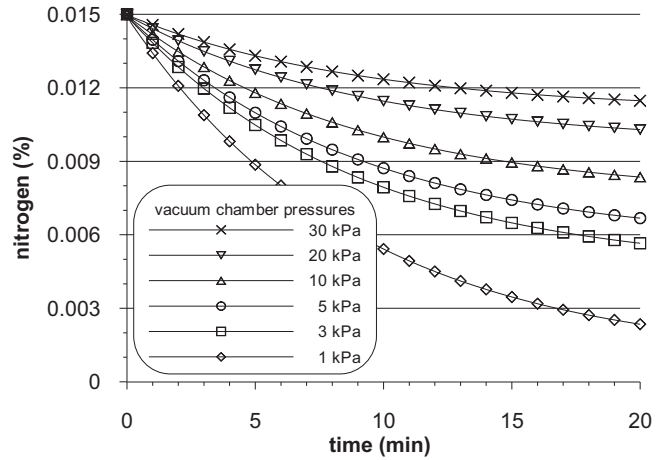

Fig. 7. Change in nitrogen content in the Fe-N-C-O system during vacuum degassing for the different vacuum chamber pressures
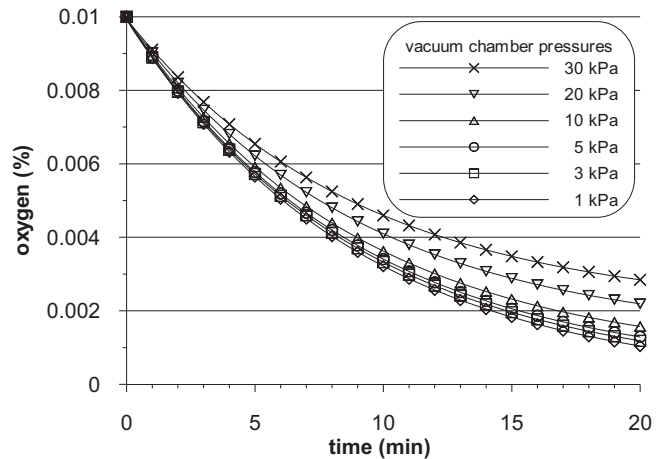

Fig. 8. Change in oxygen content in the Fe-N-C-O system during vacuum degassing for the different vacuum chamber pressures
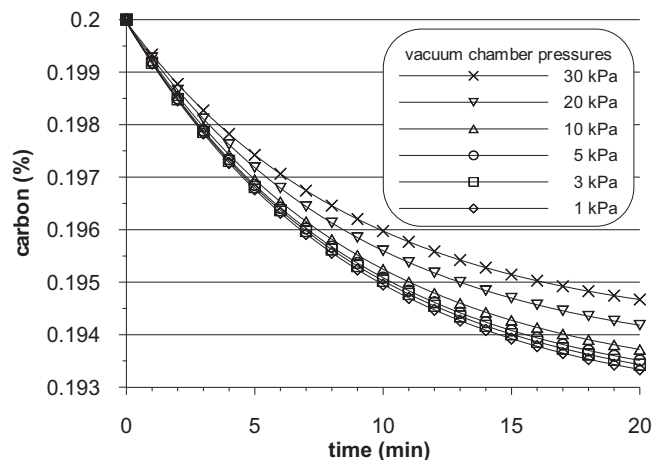

Fig. 9. Change in carbon content in the Fe-N-C-O system during vacuum degassing for the different vacuum chamber pressures

4. Summary

The results of the research confirm the usefulness of combining a metal bath mixing model with a thermodynamic model, taking into account that the boundary layer of bath in the vacuum chamber reaches the gas-metal equilibrium state. The acquired hybrid RH model comprising both the mixing and the thermodynamic model presented above enables complex calculations required to evaluate the effectiveness of steel refinement. The vacuum level in the system has the most significant influence on the equilibrium nitrogen content. It was demonstrated that the residence time of the elementary metal volume in the vacuum chamber t_R is sufficient to reach a near-equilibrium state. The observed deviations from this rule result mainly from the bath mixing process, which runs continuously. It is possible to limit considerably the error of the model application results by using for the calculations real values of the process-controlling parameters. The tool created may be adjusted in a simple way to simulate other vacuum refining processes and may be used to forecast the final nitrogen content in the bath under industrial conditions. It is possible to apply the model to control the process *on-line*. The accuracy of the model obtained allows it to be used to conduct virtual experiments supporting difficult and costly experimental research.

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