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SIMULATION OF METAL AND SLAG MELTS INTERACTION FOR OPTIMIZATION AND DEVELOPMENT OF TECHNOLOGICAL PROCESSES

Mikhail Zinigrad

Dept.of Welding Technology, Ural Polytechnic Institute,Russia

Synopsis: Physical-chemical and mathematical modeling of the interaction of metal and slag to predict composition of interacted phases have been studies. The mathematical model of technological process allowing diffusion of all the components in metal and slag, kinetic control of some reactions, the influence of temperature, hydrodynamics conditions initial composition of phases and peculiarities of technological process on formation of steel composition and properties has been developed to produce steel by the method of mixing

Key words: mathematical model, physical-chemical interaction, composition calculation,steel refining,optimize technological parameters

1. Introduction

The possibility to predict chemical composition of metallurgical products given some more ways to improve characteristics of technological process

The availability of prediction methods with physical-chemical and mathematical interaction modeling of phases in the base allows to optimize process already during design work. Thus it is possible to choose optimal technological parameters ensuring the required composition and properties of the produced material, to decrease spoilage, to improve productivity of agregates,to reduce energy and raw materials consumption,to improve labour conditions.It is impossible to develop mathematical models without knowledge of thermodynamic and kinetic constants, physical and physical chemical properties of the interactive phases. The necessity for deeper understanding of physical-chemical essence of the modeled processes was paid attention to in Ref [1].

The principles of such mathematical modeling will be illustrated by the example of steel refining under mashing treatment in the ladle.

2. Mathematical model development

The technological scheme runs as follows [2]: iron carbon melt (semi- product), refinery oxidic melt (synthetic slag) and alloying composition containing alloying elements and deoxidizers are smelted independently in tree different melting vessels. There are poured into the bottom of the ladle firstly, the synthetic slag, secondly, semi-product from the furnace and,thirdly,molten alloying composition from the intermediate ladle.

In general case, molten metal being pound out into a ladle containing synthetic slag their interaction takes place at the following boundaries of phases (Fig. 1) and surface area S_j (j=1,2...,6): metal jet - gas (surface area S^1 ,m^2), metal jet - slag (S^2), metal in the ladle - slag (S^3), metal drops - slag (S^4), slag drops - metal (S^5), slag - gas (S^6).

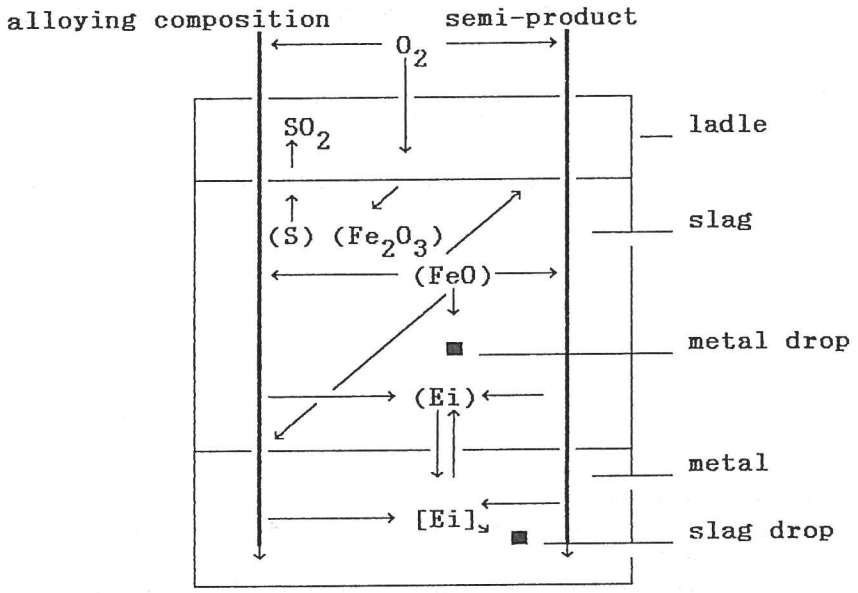

Fig.1 Phases interaction scheme

Additives are oxidized, metal is refined from sulphur, oxygen and non-metallic inclusions on these interfaces.On the slag - gas interface (S^{σ}) the low oxides (FeO, MnO) change into higher ones, sulphur is oxidized, moisture is absorbed,etc.

As long as melts of two different compositions are poured out into a ladle simultaneously,the concentration of elements in metal changes both due to chemical reactions and due to mixing of semi-product and alloying composition.

Taking all this into account,the content of Ei - element in the metal by τ - time can be defined with the expression:

$$[Ei]=\frac{[Ei]_{ac}\int_0^{\tau}V_{ac}d\tau + [Ei]_{sp}\int_0^{\tau}V_{sp}d\tau + 100A_{Ei}\sum_{j=1}^{5}\int_0^{\tau}I_{Ei}^{j}S_j d\tau}{\int_0^{\tau}V_{ac}d\tau + \int_0^{\tau}V_{sp}d\tau} \qquad (1)$$

The concentration of the same element (being a component of Ei_nO_m-oxide) in slag is:

$$(Ei_nO_m)=(Ei_nO_m)_o - \frac{100\,M_{Ei_nO_m}}{m_{sl}\,n}\sum_{j=2}^{6}\int_0^{\tau}I_{Ei}^{j}\,S_j\,d\tau, \qquad (2)$$

where,$[Ei]_{ac}$,$[Ei]_{sp}$,$(Ei_nO_m)_o$-basic concentrations of the element in alloying composition,semi - product,slag,% by mass;V_{ac} and V_{sp} -rates of pouring out alloying composition and semi - product,kg/s;I_{Ei}^{j}- rate of transition of the element from slag into metal and gas on the surface S_j mol/sm^2 · s;m_{sl}- slag mass,kg; A_{Ei} and $M_{Ei_nO_m}$ - atomic and molecular masses, kg/mol.

Some additional alloying elements and oxidizers may be introduced into the ladle during operation. In this case the equations (1) and (2) can be completed with the corresponding items.

To define I^{Ei} - values let us use the method (that we've developed in collaboration with Boronenkov V.N. and Shanchurov S.M. [3]) of kinetic ana-

lysis of reaction between metallic and oxidic melts which take place simultaneously. This method takes account of the reactions mutual influence and the diffusion of all the reagents in metal and slag.

Ion oxide FeO being chosen the general reagent, the reactions for metal and slag interaction may be represented as follows:

$$\frac{n}{m}\,[Ei] + (FeO) = \frac{1}{m}\,(Ei_nO_m) + Fe,\ I_{Ei} \qquad (3)$$

where, [Ei] -element dissolved in metal; I_{Ei} -reaction rate (3),(mol/sm^2·s) for i-th element.

To reveal the character of composition change depending on time the process is divided into small time-segments ($\Delta\tau$) during which reactions rates can be considered constant.Then the element concentrations by the moment $k\cdot\Delta\tau$ are:

$$[Ei]^k = ([Ei]^{k-1} m^{k-1}_{Me} + [Ei]_{sp} V^k_{sp} \Delta\tau + [Ei]_{ac} V^k_{ac} \Delta\tau + [Ei]_{al} V^k_{al} \Delta\tau - 100\, A_{Ei}\, \Delta\tau \sum_{j=1}^{5} I^{j,k-1}_{Ei}\, S^{k-1}_j) 1/m^k_{Me} \qquad (4)$$

$$(Ei_nO_m)^k = [(Ei_nO_m)^{k-1} m^{k-1}_{sl} + (Ei_nO_m)_{sl} V^k_{sl}\, \Delta\tau + 100 \frac{M_{Ei_nO_m}}{n}\, \Delta\tau \sum_{j=2}^{6} I^{j,k-1}_{Ei}\, S^{k-1}_j] 1/m^k_{sl} \qquad (5)$$

These equations take account of concentration change, when deoxidizers, alloying composition of $[Ei]_{al}$ - concentration and V^k_{al} - rate are introduced into metal, and also the ingress of furnace slag of $(Ei_nO_m)_{sl}$- oxide concentration and V^k_{sl} - rate in the slag. It is apparent that the equations (4) and (5) can be supplemented with items taking account of other additives or changes of technological process.

In this case, the elements which are of interest for us may be represented as follows:

$C + FeO = CO + Fe$; $\quad 1/2\ Si + FeO = 1/2\ SiO_2 + Fe$;

$Mn + FeO = MnO + Fe$; $\quad 2/5\ P + FeO = 1/5\ P_2O_5 + Fe$;

$2/3\ Al + FeO = 1/3\ Al_2O_3 + Fe$; $\quad CaS + FeO = CaO + S + Fe$;

$FeO = O + Fe$; $\quad FeO = 1/3\ Fe_2O_3 + 1/3\ Fe$.

In accordance with [3] the rates of these reactions are

$$I_c = \beta \frac{x K_c [C] - P_{CO}}{\beta \frac{\sqrt{x K_c [C]}}{I^o_c} + \frac{x K_c\ 1200}{D^{0.5}_c\, d_{Me}}}, \qquad (6)$$

$$I_{Si} = \beta \frac{x^2 K^2_{Si} [Si] - (SiO_2)}{\frac{x^2 K^2_{Si}\ 2800}{D^{0.5}_{Si}\, d_{Me}} + \frac{6000}{D^{0.5}_{SiO_2} d_{Sl}}} \qquad (7)$$

$$I_{Mn} = \beta \frac{x\,K_{Mn}[Mn]-(MnO)}{\frac{x\,K_{Mn}\,5500}{D_{Mn}^{0.5}\,d_{Me}} + \frac{7100}{D_{MnO}^{0.5}\,d_{Sl}}} \tag{8}$$

$$I_p = \beta\, D_p^{0.5}\,\frac{d_{Me}}{3100}\left[[P] + \frac{D_p^{0.5}\,d_{Me}\,1.15}{D_{P_2O_5}^{0.5}\,d_{Sl}\,x^5\,K_p^5} - \sqrt{\left\{[P] + \frac{D_p^{0.5}\,d_{Me}\,1.11}{D_{P_2O_5}^{0.5}\,d_{Sl}\,x^5\,K_p^5}\right\} - [P]^2 + \frac{(P_2O_5)}{x^5\,K_p^5}}\right], \tag{9}$$

$$I_{Al} = \beta\,\frac{D_{Al}^{0.5}\,d_{Me}}{2700}\left[[Al] - \frac{(Al_2O_3)^{1/2}}{x^{3/2}\,K_{Al}^{3/2}}\right], \tag{10}$$

$$I_S = \beta\,\frac{x\,K_S(S)-[S]}{\frac{3200}{D_{[S]}^{0.5}\,d_{Me}} + \frac{x\,K_s\,3200}{D_{(S)}^{0.5}\,d_{Sl}}}, \tag{11}$$

$$I_o = \beta\,\frac{D_{[O]}^{0.5}\,d_{Me}}{1600}\,(x\,K_o-[O]), \tag{12}$$

$$I_{Fe_2O_3} = \beta\,\frac{D_{Fe_2O_3}^{0.5}\,d_{Sl}}{1600}\left[K_{Fe_2O_3}^3 X^3-(Fe_2O_3)\right], \tag{13}$$

$$I_{FeO} = \beta\,\frac{D_{FeO}^{0.5}\,d_{Sl}}{7200}\left[(FeO) - x\right], \tag{14}$$

In accordance with the equation for flow balance [2] one can write:

$$I_c + 2I_{Si} + I_{Mn} + \frac{5}{2}I_p + \frac{3}{2}I_{Al} + I_S + I_o + 3I_{Fe_2O_3} = I_{FeO} \tag{15}$$

For all these equations: x - FeO-concentration at metal-slag boundary; K^i - constant including equilibrium constant, coefficients of activity and recalculation of concentrates for % by mass; D^j - diffusion coefficient; d - metal or slag density; I^c - exchange rate for process of anodic oxidation of carbon; β - convection constant, the same for all the substances.

Deriving kinetic equations (6)-(14), the authors neglected the influence of Fe, Al_2O_3 and CaO - diffusion on the reactions rate due to their high concentration and allowed for kinetic control of the reaction C+FeO = CO+Fe using the methodology described in Ref.[4].

For a first approximation metal and slag interaction can be conventionally considered as a single - staged one taking place on a single interface S_{eff} with a definite effective value of ate constant K_{Ei}^{eff}. In this case, the additional alloying and the ingress of furnace slag in the ladle being neglected, the reagents concentrations are equal to:

$$[E_i]^k = \left([E_i]^{k-1} m_{Me}^{k-1} + [E_i]_{Sp} V_{Sp}^k \Delta\tau + [E_i]_{ac} V_{ac}^k \Delta\tau - \right.$$
$$\left. - 100\, A_{E_i} I_{E_i}^{k-1} \cdot S_{eff} \cdot \Delta\tau\right) \frac{1}{m_{Me}^k}, \qquad (16)$$

$$(E_{in}O_m)^k = (E_{in}O_m)^{k-1} + \frac{100 M_{E_{in}O_m} \cdot I_{E_i}^{k-1} S_{eff} \cdot \Delta\tau}{n \cdot m_{Sl}}, \qquad (17)$$

The calculation is run in a consecutive order : firstly,the rates for the initial compositions of phases are defined, and, secondly, the compositions and masses of phases by the beginning of the following interval are found. Then the calculation cycle is repeated.

The equations (6)-(17) are process mathematical model which allows to predict composition of metal when it interacts with slag in the ladle.

3. Computer results

Let us calculate smelting of 115ton-product at temperature 1823 K. The following available constants were used for calculation: $K_S = \frac{[S]}{(FeO)(S)} = 0.0027$ [5]; $K_O = \frac{[O]}{(FeO)} = 0.0025$ [6]; $K_{Ei} = \frac{(Ei_nO_m)^{1/m}}{(FeO)[Ei]^{n/m}} = 97.6$; 17.5; 3.7;2.13; 1360 for carbon, silicon, manganese, phosphorus [6] and aluminium [5], accordingly; $K_{Fe_2O_3} = \frac{(Fe_2O_3)^{1/3}}{(FeO)} = 0.11$ [7]. Coefficients of elements diffusion in metal $D_{[Ei]} \cdot 10^9 = 20.0$; 4.0; 4.4; 1.9; 11.4; 8.7; 4,5 m^2/s for carbon, silicon, manganese, phosphorus, oxigen [7], sulphur and aluminium [5], accordingly. Coefficients of elements diffusion in slag are assumed: $1 \cdot 10^{-9}$ m^2/s; $d_{Me} = 7.1 \cdot 10^3$ kg/m^3; $d_{Sl} = 2.8 \cdot 10^3$ kg/m^3 [4,5]; $I_C^o = 2.04 \cdot 10^{-3}[C]^{1/2}$,mol/$m^2$·s [8]; V_{sp}=18 ton/min, V_{ac}=75 ton/min; m_{sl}=3,74 ton; the initial mass of metal in the ladle m_{me}=0.3 ton. Value $\beta = 3.3\, S^{-1/2}$ [5].

The computer results are shown in Table 1. The calculated metal composition agrees with experimental one obtained in working conditions .

Table 1. Concentrations (% by mass) and rates ($I_{Ei} 10^2$,mol/m^2·s) of reactions

τ ,s	0	15*)	35**)	300	300 experimental smelting
[C]	0.35	0.334	2.47	0.992	1.0
[Si]	0	0.0024	1.088	0.324	0.33
[Mn]	0.125	0.079	0.927	0.375	0.39
[P]	0.001	0.006	0.016	0.012	0.019
[Al]	0	0.0001	0.0013	0.0015	0.0014
[S]	0.038	0.0088	0.0076	0.0088	0.007
[O]	0.031	0.0073	0.0033	0.0054	0.006
x	1.84	1.07	0.102	0.20	-
I_C	0.95	0.69	1.58	0.88	-
I_{Si}	-0.11	-0.04	0.879	0.14	-
I_{Mn}	1.57	0.36	-0.12	-0.006	-
I_P	0.1	0.06	-0.09	-7 10	-
I_{Al}	-0.004	-0.002	-0.21	-4 10	-
I_S	-1.82	-0.42	-0.37	-0.41	-
I_O	-3.92	-0.68	-0.45	-0.73	-

*) and **)- the beginning and the end of pouring out alloying composition, accordingly.

I_{Ei}- values allow to estimate the contribution of individual reactions and their direction during process. So, sulphur and oxygen are intensively withdrawn from metal (I_O and I_S are negative) event at the beginning when FeO - concentration at the metal-slag boundary (x) approaches 1-2 % by mass. It is

due to the fact that the semi-product composition including the elements of Table 1 was being formed in open-hearth furnace where (FeO) = 10 - 20 % by mass. Therefore, slag enrichment with ferrooxides does not practically reduce rates of desulphurization and metal deoxidation.

Phosphorus behaviour is more complex. According to strong I_P - dependence on x (equation 7) before pouring alloying composition out, when x = 1-2 % by mass, phosphorus oxidizes ($I_P > 0$). And after beginning pouring alloying composition out, when x < 0.2 % by mass, phosphorus is reduced from slag ($I_P < 0$). As a result, the final P-content in metal appears to be higher than that of initial one (see Table 1). The calculation also predicts the significant aluminium reduction ($I^{Al} < 0$). In the same way the behaviour of all the elements of interest can be analyzed.

4. Conclusion

The results shown are indicative not only of possibility of quantitative prediction of composition of metal when it interacts with slag but also of possibility of more detailed and meaningful understanding of the technological process.

The developed mathematical model allows to simulate on a computer different technology versions, thus optimizing them before test - operation. "Technological games" performed on the base of here offered mathematical modelling of the interaction of metal and slag allows to solve definite practical problems: to optimize technological parameters of the operational process; to choose optimal composition of charge materials; to produce steels and alloys of present composition and properties, etc. The creation of training complexes for detailed studying of the current technological processes and developing new ones can be planned on the basis of these models.

Besides the model described in this paper, the mathematical models for electroslag remelting [9], oxygen-jet melting of copper concentrates [5], technological process of welding and hard surfacing [10] have been developed.

The expansion of work on computer modeling is delayed, in particular, for lack of necessary physical-chemical constants, physical and technological parameters and, in some cases, for lack of information about their reliability and field of application.

When organizing such works one must have in the base detailed analysis of information available; correctness estimation of constants used and metallurgical melts; their applicability in different conditions.

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