Development of LF-software for modeling of refining processes in a ladle-furnace

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Abstract The modern production technology's of steel is based on the production of metal with narrow intervals of chemical composition, alloying elements and decreasing contents of non-metallic inclusions. Mathematical models help to carrying out the process along the optimal way with minimal energy and material costs, reducing emissions. That allows to optimize production technologies, to provide a reduction the cost of steel, high production stability. An original mathematical model for the dynamic simulating of steel treatment technology has been developed. Physical and chemical models based on the law of conservation of mass and energy, as well as the principles of non equilibrium thermodynamics were used. All the stages of the process (zones) were taken into consideration in this software. This software takes into account input data such as: ladle equipment facilities, initial temperatures of slag and metal mass and chemical compositions, input time and mass of additives, blowing, electrical and time regimes, thermodynamic database, thermal, physical and chemical databases for additives and inert gas, production database (for statistics). For validation of the software, the results of ladle treatment of real heats of steel and sampling control results were used.

1. Introduction

The production technology of modern steel grades is based on the production of metal with narrow intervals of chemical composition, alloying elements, modifiers, reducing the content of harmful impurities and non-metallic inclusions. Achieving these parameters requires fine-tuning of steel smelting technologies at each stage, taking into account changes in the temperature and composition of the melt of steel and slag and the mode of introduction of additives. Modern metallurgical technologies of the XXI century provide for various methods of ladle processing to control the quality of steels and alloys. All industrial experiments on technology optimization are complex and extensive. The best way is a computational modeling of metallurgical technologies. The modeling of metallurgical processes is a difficult problem which requires the development of physical - chemical models and mathematical algorithms, allowing adequate description high-temperature processes occurring in open non-equilibrium systems which represent aggregates of ladle treatment of steel. The majority of computer programs, modeling the work of real industrial metallurgical machines, are based on using approximating and statistical models demanding enormous numbers of experimental data. This fact essentially limits possibilities of the modeling programs, which aren’t capable to sufficiently react to various disturbance and random processes in a wide range of parameters change.
2. Methods and models

Based on the physical and chemical models and thermodynamics, the original software for modelling of steel treatment in a ladle furnace was developed. The target of this software was modelling and on-line control of steel temperature and chemical composition of slag and steel melt during steelmaking processes (ladle-furnace, vacuum degasser). Physical and chemical models based on mass and energy conservation law and principals of non-equilibrium thermodynamics were used. All process stages (zones) were taken into account in this software. It was assumed that the metallurgical systems do not reach equilibrium and are in non-equilibrium steady states.

All interaction zones are described by deterministic rather than statistical dependencies, models are stable over a wide range of variables and it is stable even after changes of technology. This software takes into consideration input data such as: temperature, slag and metal mass and compositions, input time and mass of additives, blowing, electrical and time regimes. Additional data which is to be used in calculations are ladle equipment facilities (ladle geometry, transformer parameters, electrode consumption, number of lances, type of refractory materials), thermodynamic database, thermal, physical and chemical databases for additives and inert gas, production database (for statistics). It was demonstrated that software is stable even after changes in technological scheme [1-4].

Mathematical model consists of the following blocks:
- Calculation the speed of interaction between the components in the slag-metal system;
- Calculating the amount of metal and slag in the interaction zone depending on the power of stirring of the bath;
- Calculation of the mass of metal and slag;
- Calculation of the chemical composition and temperature of the slag and metal bath.

Calculations of energy balance for metal-slag system and in all areas including arc heating and takes into consideration heats of chemical reactions;

Heat loss calculations through the lining by radiation, for heating the inert gas and the reacting components at the boundary of the slag - metal lining.

The slag contain of $n$ oxides as: (FeO), (MnO), (CaO), (SiO$_2$), (Cr$_x$O$_y$), etc. The metal contain of $k$ elements as: Fe, [Mn], [C], [Si], [Cr], [S], [P], [O], etc. The aim of this study was to develop a mathematical model of the interaction of components at the slag-metal interface and reaction zone. Physical and chemical models based on the law of conservation of mass and energy and the principles of nonequilibrium thermodynamics were used. It was assumed that metallurgical systems do not reach equilibrium and are in non-equilibrium stationary states.

All components in the interaction zone in the slag-metal system are under conditions of turbulent mass transfer. Therefore, it was assumed that the interaction surface area is the same for all components of the system. An iterative algorithm has been developed to calculate the reaction rates of interaction between the components of the slag-metal system. The model determines the direction of chemical reactions for the metal-slag system, represented in the form of a matrix of $k \cdot n$-reactions (table 1), and takes into account the balance equations of mass and energy [5].

Recalculation of the chemical composition of the metal and slag according to an iterative algorithm, occurs every second ($t = 1$ sec).

The chemical composition of the metal was calculated by the equation:

$$[i]_t = \frac{m_t^{[i]}}{m_t^{met}} \times 100\%$$

where $i$ - the number of the metal element in the reaction matrix; $t$ is time, sec; $m_t^{met}$ is mass of metal at the $t$ time moment, kg; $m_t^{[i]}$ is mass of the $[i]$ element of metal at the $t$ time moment, kg.

$$m_t^{[i]} = \frac{[i]_{t-1}^{met}_{t-1} M_i}{100\%} - V_t^{[i]}$$

where $V_t^{[i]}$ is oxidation rate of the $[i]$ element of metal, kmol/s; $M_i$ is molar mass of $i$ element of metal, kg/ kmol
### Table 1 Matrix reactions system Metal-Slag [10]

|   | 1          | 2          | 3          | ... | n          |
|---|------------|------------|------------|-----|------------|
|   | (FeO)      | (MnO)      | (SiO₂)     |     | (CrₓOᵧ)    |
| 1 | [Fe]       | [Fe]⁺(MnO)=| [Fe]⁺0.5(SiO₂)=|     | a[Fe]+b(CrₓOᵧ)=|
|   |            | =(FeO)+[Mn]| =(FeO)+0.5[Si]|     | =c(FeO)+d[Cr] |
| 2 | [Mn]       | [Mn]⁺(FeO)=| [Mn]⁺0.5(SiO₂)=|     | a[Mn]+b(CrₓOᵧ)=|
|   |            | =(MnO)+[Fe]| =(MnO)+0.5[Si]|     | =c(MnO)+d[Cr] |
| 3 | [Si]       | [Si]⁺2(FeO)=| [Si]⁺2(MnO)=|     | a[Si]+b(CrₓOᵧ)=|
|   |            | =(SiO₂)+2[Fe]| =(SiO₂)+2[Mn]|     | =c(SiO₂)+d[Cr] |
| 4 | [C]        | [C]⁺(FeO)=| [C]⁺(MnO)=|     | a[C]+b(CrₓOᵧ)=|
|   |            | ={CO}+[Fe]| ={CO}+[Mn]|     | =c{CO}+d[Cr] |
| ...| ...        | ...        | ...        | ... | ...        |
| k | [A]        | [A]⁺a (FeO)=| [A]⁺a (MnO)=|     | a[A]+b(CrₓOᵧ)=|
|   |            | =c(AₓOₓ)+a[Fe]| =c(AₓOₓ)+a[Mn]|     | =c(AₓOₓ)+d[Cr] |

On the basis of the Onsager principles, the rates of oxidation and reduction processes between all components of the slag-metal melt were described by the following equation:

$$V_t = -SL\frac{1}{\delta}RTln\frac{K_{ac}}{K_{eq}}$$

where $V_t$ is the rate of formation of the oxidation product for bath component $K$, kmol/s;

$S$ is the area of the reaction surface, m²;

$\delta$ is the boundary-layer thickness, m;

$R$ is the universal gas constant ($R = 8.31$ kJ/kmol K);

$T$ is the temperature, K;

$K_{ac}$ is the actual reaction constant of the oxidation process;

$K_{eq}$ is the equilibrium constant of the reaction, determined as a function of the temperature.

Material balance of metal is calculated by the equation:

$$m_t^{met} = m_{t-1}^{met} - \sum_{i=1}^{k} M_i V_t^{[i]}$$

where $t$- time, sec;

$m_{t-1}^{met}$ is mass of metal at the $t-1$ time moment, kg.

Material balance of slag was calculated by the equation:

$$m_t^{slag} = m_{t-1}^{slag} + \sum_{j=1}^{n} M_j V_t^{[j]}$$

where $j$ is the number of the metal element in the reaction matrix;

$m_{t-1}^{slag}$ is mass of slag at the $t$ time moment, kg;

$m_t^{slag}$ is mass of slag at the $t-1$ time moment, kg;

$M_j$ is molar mass of $j$ element of slag, kg/ kmol;

$V_t^{[j]}$ is slag $j$ component formation rate, kmol/s.
3. Results and discussion

Validation of mathematical model and checking the adequacy of the software was performed on the ladle treatment data industrial heats of steels for pipe lines of metallurgical steel plant.

It was shown that the software designed allows us to proceed with dynamic simulation and optimization of ladle treatment technologies.

This is the interface of calculations of the chemical composition of the metal during ladle treatment. Circles show the results of the chemical composition of the metal during ladle treatment, lines are the result of calculation (Figure 1).

![Figure 1. The interface of calculations of chemical composition metal during ladle treatment](image1)

![Figure 2. Results of validation of the model](image2)
It was shown that Software designed allows us to proceed of dynamic simulation and optimization of ladle treatment technologies. For validation of LF software the results of ladle treatment of real heats of steel and sampling control results were used (Figure 2).

The comparison shows that the experimental results are in good agreement with the calculations for the proposed model.

4. Conclusions
A mathematical model for simulation of ladle treatment procedure has been developed. Physical and chemical models based on the law of conservation of mass and energy, as well as the principles of nonequilibrium thermodynamics, were used. All stages of the process (zone) were taken into account in this model. The comparison shows that the calculated data of the model and the experimental results are in good agreement. This software allows us to calculate the main characteristics of the ladle treatment such as temperatures and chemical composition of slag and the steel melts. This software can be used in online calculations and control of process parameters during ladle treatment, modeling and optimization of ladle treatment technology, teaching and training of steelmaking staff.

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