Development of digital twins and optimization of resource-efficient steelmaking technologies

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Abstract. In this study, mathematical models, algorithms and software for dynamic simulating of processing technologies in a ladle furnace and vacuum degassers were developed, and a new method for optimizing ladle processing technologies for various steel grades was created. Physicochemical models were developed based on the laws of conservation of mass and energy, as well as the principles of non-equilibrium thermodynamics. The developed software allows us to calculate the basic characteristics of steel refining processes, such as temperature and chemical composition of slag and steel melts, kinetics of refining processes, economic indicators, energy and resource efficiency of technologies. To validate the software, the results of industrial hits and the results of the control of metal and slag were used. Nonmetallic inclusion analysis procedures have been developed using the fractional gas analysis method to control of steel cleanness and to detect and adjust the sources of inclusions formation at all stages of ladle furnace steel processing. For various steel grades, it was shown that it is possible to successfully optimize technologies using a combination of developed modeling software and fractional gas analysis. A mathematical model for the interaction of a high chromium iron base melt with a low temperature plasma was developed. Comparison of the experimental results in DC arc furnace with calculating data is in a good agreement.

1. Introduction

Over the 18 years of the 21-st century, global steel production has doubled from 800 million tons up to 1 billion 803 million tons, (by 2020, annual iron and steel production can reach up to 2 billion tons). A huge amount of by-products, such as slags, fluxes (more than 540 million tons / year) is produced. Annually, 300 kg of blast furnace slag per 1 ton of pig iron and 100 kg per 1 ton of steel are generated in the world. Steelmaking slags cannot be fully utilized due to the content of hazardous elements in it, such as heavy metals and fluorine.

The most important problem for Iron and Steel Industry in the 21-st century is the need to reduce the consumption of raw materials, energy, water, reduce CO2 emissions and waste slags at the global level.

It is known that the high quality of modern steel grades is based on a finely dispersed microstructure, which can be obtained in the processes of thermo-mechanical processing. The technology for the production of these steels is based on achieving narrow ranges of alloying element concentrations, reducing the concentration of impurity elements and the content of non-metallic inclusions. Achieving these parameters requires fine-tuning of refining technologies at each stage, taking into account changes in temperature and composition of slag and steel melt, as well as the introduction of additives. Modern metallurgical technologies of the 21st century provide various computer methods for controlling steelmaking technologies and optimizing the quality of steels. All industrial experiments on technology...
optimization are complex and very expensive. The best way is computer simulation of metallurgical technologies and operational monitoring of refining processes. Modeling metallurgical processes is a complex task requiring the development of physicochemical models and mathematical algorithms that adequately describe high-temperature processes in open nonequilibrium systems, which are metallurgical units. Most computer programs simulating real industrial metallurgical units are based on approximating and statistical models that require a huge amount of experimental data. This fact significantly limits the capabilities of the software, based on statistical models, which is not able to sufficiently respond to various disturbances and random processes in a wide range of parameter changes. The use of computational models that adequately model the refining processes of steel processing in a ladle allows one to calculate the optimal technology for the production of steel of a certain grade on a computer without carrying out a series of expensive industrial experiments. The combination of computer modeling with industrial experiments allows us to develop new steel production technologies and identify factors affecting product quality.

The quality of steels is determined not only by their structure and chemical composition, but also by the content of nitrogen and oxygen, which are distributed between the solid solution and various non-metallic inclusions, such as nitrides and oxides. It is known that non-metallic inclusions, which are largely present in the steel matrix, are the main sites of fatigue defects and crack nucleation during tensile strength. Therefore, to improve the quality of steel, it is important to develop new methods for controlling the quantitative and qualitative compositions of inclusions. It is important to choose the right method for monitoring the content of non-metallic inclusions in steel and develop criteria for assessing the quality of steel. The purity of steel according to non-metallic inclusions, estimated according to the data of fractional gas analysis (FGA), can be used to predict the durability of the steel products during their operation [1].

The purpose of this study was to develop mathematical models, algorithms and software for the dynamic simulating of steel refining processes in ladle metallurgy units and to create a new method for optimizing refining technologies using the developed software and the method of fractional gas analysis (FGA). The next goal of the work was the analysis and optimization of real technologies for refining of steel melts in real metallurgical units in order to improve the quality of steel, improve energy and resource efficiency and reduce the total amount of waste slag from steelmaking.

2. Methods and models
An original method for controlling the purity of steel for various steel grades using the method of fractional gas analysis (FGA) has been developed. Application of the FGA method allows us to determine the content of harmful oxide inclusions that affect the quality of steel and determine the sources of their origin in the processes of smelting, after furnace treatment and continuous casting of steel. The method of fractional gas analysis (FGA) is a modification of the method for oxygen and nitrogen determination by using of hot extraction in the carrier gas under non-isothermal conditions (constant heating rate of the test sample). This method involves the melting of samples in a double graphite crucible with a continuous increase in temperature up to 2500 K in a carrier gas helium stream. Oxygen and nitrogen are extracted from the melt and detected - oxygen in the form of CO2 in infrared (IR) cells and nitrogen in a thermo conductivity cell (TCC). Fractional gas analysis (PHA) is based on the difference in the thermodynamic stability of oxides and nitrides in the processes of dissociation and carbothermic reduction in carbon-saturated melts. The process of analysis of oxides and nitrides in a carbon-saturated analytical melt is carried out using smooth heating of a graphite crucible with a sample at a given rate in a pulse furnace of a gas analyzer to a temperature of 2500 C. The original OxSeP software for processing the analysis results [2-4] was developed and implemented on modern gas analyzer TC-600 LECO.

The "OxSeP" software developed calculates identification parameters - the temperature of the oxide reduction start - Ts, temperature of peak maximum – Tmax - to define certain kind of supposed oxide inclusions in the steel grade. As a final result of the real experimental data treatment by "OxSeP", one
can obtain the total oxygen and sample surface oxygen content, oxygen content in oxides as a sum of oxygen corresponding to oxides peaks and oxygen content for each peak.

The goal of the work was to build the method for analyzing and optimizing of real steel ladle technologies. The mathematical models, algorithms, and software for dynamic simulating of steel refining in ladle technologies and inclusions formation were developed and a new method for optimizing refining processing using developed software and fractional gas analysis (FGA) was built.

On the basis of physicochemical models and thermodynamics, original software was developed for modeling the processing of steel in a ladle furnace and a vacuum degasser [5-6]. The purpose of this software was to dynamically simulate changes in temperature and chemical composition of slag and steel melts during refining in a specific metallurgical unit (ladle furnace, vacuum degasser). Physical and chemical models based on the law of conservation of mass and energy and the principles of nonequilibrium thermodynamics are used. All stages of the refining processes (zones) were taken into account in this software. It was assumed that metallurgical systems do not reach equilibrium and are in non-equilibrium stationary states.

To calculate the reaction rates of interactions between components of slag-metal system was developed by an iterative algorithm. Model defines a direction of chemical reactions for metal-slag system witch presented as a matrix of k reactions and takes into consideration mass and energy balance equations. 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). The software includes: - a thermodynamic database, thermal, physical and chemical databases for added additives and inert gas and production database (for statistics). It was demonstrated that the software works stably even after making changes to the technological schemes of refining units.

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;
Calculations of heat of metal and slag melts, alloying elements and fluxes;
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 ;
- Calculations of nonmetallic inclusions formation and removal.

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

For testing of RH software and validation of the models, the results of ladle treatment of 5 real heats of low carbon steel in 350 t ladle of RH degasser of Magnitogorsk Metallurgical plant and sampling control results were used.

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

3. Results and discussion
The methods of quantitative metallography, X ray microprobe and fractional gas analysis (FGA) were applied for the non-metallic inclusion characterization and quantification. The chemical compositions of the steels were determined on GDS-850 LECO glow-discharge atomic emission spectrometer. Metallographic examination was performed on an Olympus PME-3 optical microscope and scanning
electron microscopes. The total oxygen in these steel samples and oxygen content in different oxide inclusions was determined using the TC-600 LECO analyzer and the original OxSeP software. The FGA results were compared with data obtained by Image analysis on IA-32 LECO Analyzer and X-ray microprobe analysis. The results obtained showed the high reproducibility of the oxide characterization procedure. The volume fraction of inclusions obtained by FGA method clearly illustrates the contamination of steel.

Optimisation of real ladle technology of 13ХФА steel of VMZ plant using original LF software developed and FGA method was done. The probes of steels were sampled (dual samples) from the ladle after tapping, ladle furnace, LD degasser and tundish during all steps the ladle treatment technology. Chemical composition of 13ХФА steel for a pipeline is presented in a Table 1.

Table 1. Chemical composition of 13ХФА steel grade for a pipeline, % mas.

|   | C   | Si  | Mn  | S   | P   | Cu  | Ni  | Cr  | V   | Al  | N   |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|   | 0.05-0.07 | 0.25-0.35 | 0.55-0.70 | 0.002 | 0.012 | 0.25 | 0.30 | 0.36-0.7 | 0.07-0.09 | 0.02-0.05 | 0.008 |

For testing of LF Software and validation of the model, the results of ladle treatment of real heats of 13ХФА steel grade and sampling control results were used. On the Fig. 1 presented results of calculated values obtained by the software and results of chemical composition control of metal melt during treatment at the ladle furnace.

For testing of LF Software and validation of the model, the results of ladle treatment of real heats of 13ХФА steel grade and sampling control results were used. On the Fig. 1 presented results of calculated values obtained by the software and results of chemical composition control of metal melt during treatment at the ladle furnace.

![Figure 1. LF Software interface. Calculating of changes in the chemical composition of steel melt in 150 t ladle furnace of VMZ plant during ladle treatment. Lines - is calculating results.](image)

Figure 1 shows the dynamic changes in temperature and chemical composition of the melt occurring during the treatment in the ladle furnace and reaction to the control effects. For example, after entering the materials containing calcium and aluminum, metal desulfurization occurs. Entering the alloying materials results in increased concentrations of the respective components in the metal, the including of electric heating increases the temperature of the bath. Shutting down the arcs led to decreasing of metal bath temperature that was connected with losses into the ladle lining, losses of heating of inert gas, and losses of heating of master alloys that was introduced into the ladle. The ladle treatment technology of steel grade for pipelines was optimized using software for dynamic simulation of ladle treatment processes and correction procedures. In this investigation was shown that original LF software allows us to perform the dynamic simulation, optimize of ladle treatment technology and to lead the process within an optimal way.

It was shown that original LF Software allows us to produce dynamic simulation and optimization of ladle treatment technology. It was established that the software to adequately describe the dynamic changes of the basic characteristics of the metal, slag and reaction of system on the process control feedback. The resulting standard deviations of the calculated and experimental data (Figure 2) is: [Mn] - 0.11%; [C] - 0.015%; [Si] - 0.02%; [P] - 0.0005%; [S] - 0.0026%; Temperature - 17°C.
Figure 2. Comparison of values calculated by the LF software and data of chemical analysis of probes that were sampled (dual samples).

For testing of the software and validation of the model, the results of ladle treatment of real heats and sampling control results were used. It was shown that original software allows us to make dynamic simulation of ladle treatment technology in real LD degasser.

The FGA results were compared with data obtained by Image analysis on IA-32 LECO Analyzer and X-ray microprobe analysis. The results obtained showed the high reproducibility of the oxide characterisation procedure. The volume fraction of inclusions obtained by FGA method clearly illustrates the contamination of steel. Figure 3 presents the FGA results: the mean values and standard deviation for probes that were sampled from the ladle furnace (LF) and the ladle vacuum degasser (LD) during the ladle and vacuum treatment of steel [7].

Figure 3. The total oxygen and nitrogen contents and content of different oxide inclusions in the steel melt.

All the peaks were divided into three groups according to the chemical composition of oxides identified using by the original OxSeP software. The first group of peaks with Tmax< 1750-1770 K was attributed to silica and manganese silicates. The second group of peaks was attributed according the calculations to alumina and complex spinel, which are more harmful for these steel grades. The third group of peaks was attributed to complex (Mg and Ca-rich) - silicates.

Using the FGA data, we can rapidly determine the volume fraction of oxide and nitride inclusions in the steels. This parameter characterizing the cleanness of steel, is estimated by quantitative metallography, and is controlled by a number of documents such as DIN 50602, method K; ASTM-E45,
method D. Since FGA can quantitatively determine the oxygen content in each type of inclusions, we can easily show that the volume fractions of oxide inclusions \( V_{\text{oxides}} \) can be calculated to a higher accuracy as compared to that providing by metallographic methods using formula:

\[
V_{\text{oxides}} = \frac{\rho_{\text{steel}}}{\rho_{\text{OX}}} \sum_{i=1}^{n} \frac{O_{\text{OX}} M_{\text{OX}}}{\rho_{\text{OX}} y M_{O}}
\]

where \( \rho_{\text{steel}} \) and \( \rho_{\text{OX}} \) are the density of steel and oxides of a given composition, respectively; \( M_{O} \) is the atomic mass of oxygen; \( M_{\text{OX}} \) is the oxide molecular mass; \( y \) is the stoichiometric coefficient outside oxygen atom in oxide and \( O_{\text{OX}} \) is the FGA determined content of oxygen (wt %) fixed in the oxide of this type of inclusions [6]. Figure 1 allows us to estimate the influence of ferroalloys and deoxidizers added during each step ladle treatment on the total oxygen and nitrogen contents as well as the amount and content of different oxide inclusions in the steel melt.

It has been shown that the use of the software developed for the dynamic simulation of ladle treatment of steel and fractional gas analysis method allows optimizing the secondary treatment technology. This software can be used in online calculations and control of process parameters during ladle treatment, modelling and optimization of ladle treatment technology, teaching and training of steelmaking staff.

The processes of decarburization of iron-based melts with a high content of Cr and Ni with oxidizing plasma were experimentally studied. It was found that it is possible to carry out plasma decarburization of melts with a high content of chromium and nickel to low carbon concentrations without loss of alloying elements [8]. Semi-industrial experiments were carried out in 100 kg of a constant current furnace. A mathematical model for the interaction of a melt with a low-temperature plasma was developed [9]. For experiments on the decarburization of stainless steel, an experimental 100 kg DC arc furnace was used. Purging the metal with a gas through a hollow steel tube inserted into a hollow graphite electrode began after the charge was melted. Then the first metal sample was taken and the temperature of the melt was measured. In the course of the decarburization, metal samples were taken, the temperature was measured and the argon metal was purged with an oxygen – oxygen mixture (Table 2).

| Step | Time, min | \( O_2 \), l/min | \( Ar \), l/min | T, C | [C], % | [Cr], % |
|------|----------|-----------------|----------------|-----|-------|--------|
| 1    | 0-5      | 5               | 44             | 1620| 0.198 | 26.54  |
| 2    | 5-10     | 5               | 50             | 1634| 0.159 | 26.35  |
| 3    | 10-14    | 3               | 42.75          | 1641| 0.119 | 25.64  |
| 4    | 14-17    | 3               | 41.25          | 1646| 0.099 | 25.45  |
| 5    | 17-20    | 2               | 41.25          | 1653| 0.085 | 25.34  |

Calculations and analysis of the samples taken during the process showed that it was possible to obtain a deep decarburization of stainless melt by oxygen content plasma with a relatively small loss of chromium in slag. The experimental data of the hits were compared with the results of calculations based on the developed model and are presented in Figure 4.
Figure 4. Comparison of calculation results using software (lines) with the results of sampling and control of the chemical composition of the metal (dots)

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

4. Conclusions

The real ladle treatment technology of steels using combination of original software for dynamic simulation and FGA method were optimized. It was shown that software designed allows us to proceed the dynamic simulation of ladle treatment technology and to lead the process within an optimal way. It was shown that the FGA application allowed us to find a quantity of harmful oxide inclusions, identified as non-deformable and to detect sources of their origin during the ladle treatment process. Fractional gas analysis allows us to provide the favourable composition of oxide inclusions in melt and to increase the steels quality. It results in reduction of energy, additives and costs and steel quality increasing. 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. A mathematical model for the interaction of a melt with a low temperature plasma was developed. Comparison of the experimental results in DC arc furnace with calculating data are in a good agreement.

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