K1-MET

Competence Center for Excellent Technologies in Advanced Metallurgical and Environmental Process Development

Main Location	Linz, Upper Austria
Other Locations	Leoben, Styria
Key topic	K1-MET has its focus on the modeling and simulation of metallurgical processes, including metallurgical raw materials and refractories with the goal of an optimal process control with respect to product quality, zero waste and the minimization of energy and raw materials.

Title: Project 5.3: **Thermodynamic and Kinetic Modelling of Metallurgical Reactions**

Success Story short version

The objective of the project is the development of thermodynamic model for complex metallurgical systems on basis of available thermodynamic databases and under consideration of reaction kinetics. Development of thermodynamic and kinetic model is focused on the simulation of oxidation-reduction reactions for phosphorus, manganese and vanadium. Developed model allows to simulate not only end blow temperature, composition of steel and slag, but also behaviour of these parameters, as well as dissolution and melting of charge materials during the heat.

Success Story long version

Objectives

- Thermodynamic and kinetic investigation of the de-P and de-V processes during the converter steelmaking technology.
- Thermodynamic and kinetic investigation of the Mn distribution between slag and steel during the converter steelmaking process.
- Development of thermodynamic and kinetic model of the converter steelmaking technology

Approach

The model is based on the coupled reaction model, which includes combining of both thermodynamic and kinetic calculations. The thermodynamic part includes the calculations of: equilibrium constants of the oxidation reactions, the activity coefficients of hot metal and slag components. The kinetic part comprises the calculations of: the rate constant of the carbon monoxide gas generation, the total mixing energy and the mass transfer coefficients in the metal and slag phases. The mass transfer coefficient in the metal phase is defined by the technological parameters of the process and the specific geometry of the converter. The new BOF model was enhanced by such sub-models as: lime, scrap and other charge materials dissolution, the interfacial area, the post combustion and the dust formation. Developed lime dissolution sub-model includes the slag diagram calculation and the calculation of the mass transfer coefficient for the dissolution. The simplified model of the ternary slag diagram calculation was developed, which allows:

1. to take into account the slag temperature
2. to define the CaO saturation concentration
3. to define the amount of liquid fraction in considered slag.

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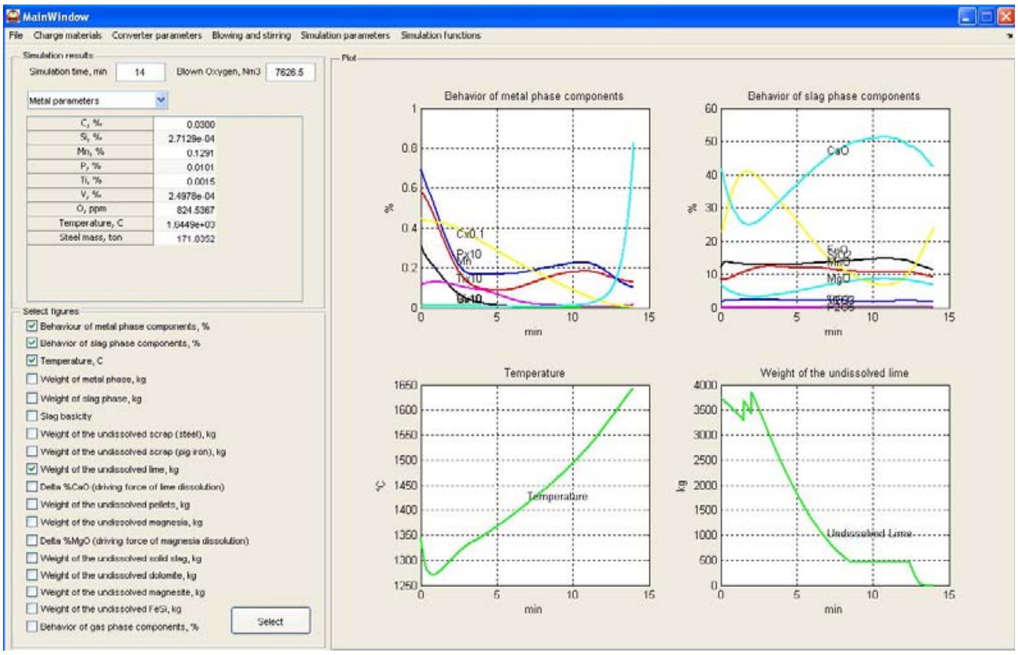
The heat balance includes the separate calculation for heating and dissolution of each charge material portion. Considered sub-models can be improved, replaced and tuned according to the technological features of a specific converter.

Results and Economic Impact

Developed BOF model allows to take into account such features of the converter steelmaking process as: the lance practice, the change of the oxygen blow rate and the flow rate of the bottom stirring gas during the blowing and the time of charge materials bringing into the converter. End blow parameters, such as temperature, composition of steel and slag can be accurately defined by the use of tuning parameters for each specific converter. The influence of technological parameters on the final chemical composition of steel can be investigated by the developed BOF model. Thereby the converter steelmaking process can be optimized by: the definition of the optimal lance practice; the economical use of lime, ferrosilicon, inert gas for the bottom stirring etc; the use of increased amount of the scrap. After the model validation and tuning, the BOF model can be implemented in industrial solution. The final version of the model was accomplished as software with the graphical user interface.



The graphical user interface of the BOF model

Next Steps

The second phase of project 5.3 includes testing and improvement of the developed BOF model. The first step will be the validation of developed model using the actual data of the BOF process in order to define the main technological parameters, which influence on the variation of tuning parameters. As a result of this step, statistical or semi-empirical models of considered tuning parameters should be improved or developed. Later, defined technological parameters can be used for the dynamic BOF process simulation and the accurate prediction of end blow parameters.

Contact:	Montanuniversitaet Leoben Yuriy Lytvynyuk Franz-Josef-Strasse 18, 8700 Leoben, Austria yuriy.lytvynyuk@unileoben.ac.at http://www.metallurgy.ac.at

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