The importance of computational thermodynamics in process modelling and control: The oxygen converter as an example (BOF DePhos)

Sabrine Khadhraoui

R&D/ Steelmaking Technology, SMS group GmbH

The experimental investigation of metal-slag-reactions, under conditions pertinent to steelmaking, has been subject of laboratory research since 1930. The aim was to quantify the equilibrium state of metal-slag reactions in form of simplified relations which can be used to model and control steelmaking processes. For this purpose, equilibrium relations based on intensive experimental investigations for a wide range of steelmaking slags in equilibrium with low alloy steels were established. However, the applicability of those relations is limited to the experimental ranges studied, which are relevant, in most cases, only for the end of blow state in the converter process.

In the scope of the European BOFdePhos project, funded by the Research Fund for Coal and Steel (RFCS), the metal-slag-equilibrium pertinent to the oxygen converting of steel, with the dephosphorization reaction being the main focus, was studied by means of computational thermodynamics. For this purpose, a thermochemical database, covering the oxide system CaO-FeO-SiO2-P2O5-MnO-MgO-Al2O3 has been developed. The objective was to develop thermodynamic relations covering temperature and composition ranges which are applicable for the total blowing time and can thus be used for dynamic modelling of the oxygen converter process.

The simulation results have shown that the formed slag during the oxidation process is heterogeneous for a large part of the blow and that the solid phases, depending on their type and amount, contribute either positively or negatively to the dephosphorization potential of the slag. Since most modeling approaches of P equilibrium in the literature considered the liquid slag part only, a new approach for modeling metal-slag-equilibrium with respect to dephosphorization in a heterogeneous slag was developed.