Thermodynamic Databases and Their Applications for Sulfur Control in Steelmaking

Youn-Bae Kang[1], Arthur Pelton[2].
1. *Graduate Institute of Ferrous Technology, POSTECH, Pohang, Korea.*
2. *Centre for Research in Computational Thermochemistry, Ecole Polytechnique de Montreal, Canada.*

ABSTRACT

A new thermodynamic model and database for sulfur dissolution in molten oxide slags composed of SiO_2-Al_2O_3-CaO-Fe_tO-MgO-MnO-SiO_2-TiO_x has been developed using the Modified Quasichemical Model in the Quadruplet Approximation and has been incorporated into the FactSage thermochemical software. In this model, both first-nearest-neighbor (FNN) and second-nearest-neighbor (SNN) short-range-ordering (SRO) are explicitly taken into account. The model predicts the dissolution behavior of sulfur with good accuracy. With the model and database, sulfide capacities ($C_S = (\%S)_{slag} \times (P_{O2}/P_{S2})^{1/2}$) in steelmaking slags are calculated within experimental error limits for all available experimental data in the SiO_2-Al_2O_3-CaO-Fe_tO-MgO-MnO-SiO_2-TiO_x system. Moreover, the model extends to high sulfur contents (up to pure molten sulfide). Solid sulfide solutions composed of CaS-MnS-MgS-FeS have also been thermodynamically modeled using a random mixing model with polynomial expansions for the excess Gibbs energies, and a thermodynamic database has been developed to allow the calculation of phase diagrams involving oxysulfide inclusions. By combining these models and databases with our database for molten steel, the sulfur distribution ratio between molten slag and steel ($L_S = (\%S)_{slag}/[\%S]_{steel}$) can be calculated. Various examples of applications to sulfur control in steelmaking processes are presented such as iso-C_S lines of slags, sulfide saturation limits of slags, the sulfur distribution ratio between slag and steel, the evolution of sulfide inclusions in steel, *etc*.