Addition of ZnO to the HotVeGas Oxide Database

TATJANA JANTZEN, KLAUS HACK

GTT-Technologies, Herzogenrath, Germany

ABSTRACT

Zinc oxide is important for ferrous process metallurgy as potential material for hot metal desulfurization but also in corrosion of heat exchanger materials in power plans. The high melting Spinel and Zincite phases form extensive solid solutions and are stable over a wide range of compositions, temperatures and oxygen partial pressures.

Knowledge of the equilibrium relations between ZnO and the other components of the slag is therefore necessary to understand the behaviour of the slag during pyrometallurgical processes as well as formation of slags and ashes in coal combustion and gasification processes.

The oxide system CaO-MgO-Al_2O_3-CrO_x-MnO_x-FeO_x-K_2O-Na_2O-SiO_2-P_2O_5 with addition of ZnO has been thermodynamically assessed using all available experimental data on phase equilibria and thermodynamic properties.

The Gibbs energy of the liquid phase has been modelled using a non-ideal associate solution model. The compositions of the pure liquid oxide species as well as the associates have been chosen to have two moles of cations per associate thus keeping the successful method of Spear and Besmann.

In the zinc oxide containing systems particular attention was given to the phase Spinel which forms the wide completely miscible solid solution Fe_3O_4-$ZnFe_2O_4$. The cation Zn^{+2} was introduced on the first sublattice into the present description of the Spinel phase with the additional forty Gibbs energies where the missing values were estimated using reciprocal equations.

The experimentally determined solubility of Zn in Olivine is described using the formula: $(\underline{Ca}^{+2},\underline{Fe}^{+2},\underline{Mg}^{+2},\underline{Mn}^{+2},Zn^{+2})(\underline{Ca}^{+2},\underline{Fe}^{+2},\underline{Mg}^{+2},\underline{Mn}^{+2})(Si^{+4})(O^{-2})_4$.

Zinc is introduced into the thermodynamic description of 8 solid solution phases such as MeO, ZnO, Spinel, Tetragonal Spinel, Olivine, Protopyroxene, Willemite (Zn_2SiO_4) and α'-Ca_2SiO_4 using available experimental information.

The thermodynamic descriptions of 8 binary and 5 ternary systems containing zinc oxide are presented compared with experimental data.