Incorporation of MnO_x as Well as Sulphides to the HotVeGas Database

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ABSTRACT

Non-metallic inclusions such as the sulphides are essential components for steel processing and products but can also occur in slags and ashes from coal combustion and gasification. Manganese oxides such as MnO and Mn_2O_3 are important for ferrous process metallurgy and can play an important role in corrosion of heat exchange materials in power plans. 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 metal sulphides (CaS, FeS, MgS, MnS, K_2S and Na_2S) 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 and sulphide 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 metal sulphide systems particular attention was given to the phase Oldhamite which forms completely miscible solid solutions in the systems CaS-MnS and MgS-MnS. The Oldhamite in the system CaS-MgS was reassessed using the formula (Ca,Fe,Mg,Mn)S while the phase diagram should have the same behaviour as the other two systems. The experimentally determined very wide mutual solubility of MgS and MnS in the Troilite-HT phase based on iron sulphide could be reproduced well by the new Gibbs energy parameters. The stoichiometric phases $8MnO{\cdot}MnS{\cdot}3SiO_2$ and $25MnO{\cdot}MnS{\cdot}9SiO_2$ were incorporated using the experimental data about thermal stability and phase boundaries from the literature.

MnO and Mn_2O_3 have been integrated into the complete system CaO-Cr_2O_3-MgO-Al_2O_3-FeO-Fe_2O_3-P_2O_5-SiO_2. Manganese is introduced into the thermodynamic description of 11 solid solution phases such as MeO, Corundum, Spinel, Tetragonal Spinel, Bixbyte, Olivine, Rhodonite, Protopyroxene, Iron-Cordierite, α-Ca_2SiO_4 and α'-Ca_2SiO_4 using available experimental information. The thermodynamic descriptions of 9 ternary and 1 quaternary systems containing manganese oxides are presented compared with experimental data.