Database development for the HotVeGas project

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In the framework of the HotVeGas project the oxide database containing CaO-MgO-Al_2O_3-CrO_x-FeO_x-K_2O-Na_2O-MnO_x-NiO-ZnO-P_2O_5-SiO_2-TiO_x-VO_x (with addition of sulphates/carbonates of alkali and earth-alkali oxides and metal sulphides MeS, Me=Ca, Cr, Fe, Mg, Mn, Ni, Zn) relevant for coal/biomass combustion and gasification, metallurgical slag applications, glass processing as well as the development and production of refractory materials has been thermodynamically assessed using all available experimental data. Self-consistent datasets have been obtained covering experimental information. The Gibbs energy of the liquid phase has been modelled using a non-ideal associate solution approach in which 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 [1]. The Gibbs energy of the stoichiometric compounds as well as the constituents of the various solution phases has been presented in form of a simple G(T) function. The solid solutions have been described using the sublattice approach.

The binary systems containing alkali oxides with vanadium, phosphorous and titanium oxides have already been integrated into the database. The corresponding ternary systems Alk_2O-V_2O_5(TiO_2)-MeO_x (Alk=Na,K; Me=Al,Ca,Mg,Zn) were assessed considering the experimental information on phase diagrams/equilibria.

Regarding the P_2O_5-containing systems, in the framework of the HotVeGas project the experimental study on the NiO-P_2O_5 system was carried out in terms of thermodynamic properties and phase equilibria. The information obtained was used for the assessment of this binary system. Moreover, the ternary phase diagrams NiO-P_2O_5-Alk_2O (Alk=Na, K) were proposed.

Further development of the thermodynamic database concerns the addition of a new component (Li_2O). Lithium oxide has so far been integrated into the reduced core system CaO-MgO-Al_2O_3-FeO_x-Cr_2O_3-MnO_x-Na_2O-NiO-SiO_2-P_2O_5-ZnO. Lithium was introduced into the thermodynamic description of solid solution phases such as MeO, Spinel, Ca_2SiO_4-α, Ca_2SiO_4-α‘ using available experimental information. In the Li_2O-containing systems particular attention was given to the phase Spinel which forms the wide completely miscible solid solution range Fe_3O_4-$LiFe_5O_8$-$LiAl_5O_8$-$MgAl_2O_4$. The cations $Al_{0.5}Li_{0.5}^{+2}$ and $Fe_{0.5}Li_{0.5}^{+2}$ were introduced on the first sublattice of the present description of the Spinel phase $(Al^{+3},Fe^{+2},Fe^{+3},Mg^{+2},Al_{0.5}Li_{0.5}^{+2},Fe_{0.5}Li_{0.5}^{+2})(Al^{+3},Fe^{+2},Fe^{+3},Mg^{+2},Va)_2(Mg^{+2},Va)_2(O^{-2})_4$ with additional Gibbs energies where the missing values could be estimated using reciprocal equations.

[1] T.M. Besmann, K.E. Spear, Thermodynamic modelling of oxide glasses, J. Am. Ceram. Soc. 85 (12) (2002) 2887-2894