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 (with addition of sulphates/carbonates of alkali and earth-alkali oxides and metal sulphides CaS, CrS, FeS, MgS, MnS) 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 on phase diagrams and thermodynamic properties. Self-consistent datasets have been obtained covering experimental information on all binary, ternary, and quaternary subsystems. 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 has been presented in form of a simple G(T) function. The solid solutions have been described using the sublattice approach.

The vanadium and titanium oxides have already been integrated into the core system CaO-MgO-Al_2O_3-FeO_x-Cr_2O_3-MnO_x-SiO_2 as presented earlier [2, 3]. The actual task implies the addition of alkali oxides into the database. The binary systems Alk_2O-V_2O_5 and Alk_2O-TiO_2 (Alk=Na, K) which are characterised by a large number of binary stoichiometric compounds were assessed taking into account the experimental information on thermodynamic properties and phase diagram. The current dataset allows a sufficient description of the phase equilibria. The ternary phase diagrams Na_2O-K_2O-V_2O_5 (TiO_2) were proposed.

Further development of the thermodynamic database concerns the addition of the ceramic relevant oxides in order to enable proper description of the interactions between materials and environments. The complete database including all relevant phases (gas, stoichiometric compounds, solid solutions and liquid slag) is required for calculations and predictions of equilibria under varying conditions (temperature, compositions, pressure). In the framework of the HotVeGas project the experimental study on different membrane materials for gas separation is carried out in terms of their chemical and thermal stability. The corresponding ceramic relevant systems are thermodynamically being assessed using Calphad approach. Thermodynamics and phase equilibria information on the systems BaO-ZrO_2, La_2O_3-WO_3 are critically analysed in order to generate the Gibbs energy dataset compatible with the core slag relevant oxide database. In summary, the recent updates of the HotVeGas database including NiO-containing systems will be discussed.

[1] T.M. Besmann, K.E. Spear, Thermodynamic modelling of oxide glasses, J. Am. Ceram. Soc. 85 (12) (2002) 2887-2894;
[2] T. Jantzen, K. Hack, Addition of Titanium oxides to the GTOX oxide database, GTT Annual Workshop, 2017;
[3] T. Jantzen, K. Hack, Addition of Vanadium oxides to the GTOX oxide database, GTT Annual Workshop, 2018.