Database development for the HotVeGas project

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In the framework of the HotVeGas project the oxide database containing SiO_2, Al_2O_3, alkali, earth-alkali, FeO_x, CrO_x, MnO_x with addition of sulphates/carbonates of alkali and earth-alkali oxides and metal sulphides has been created. The corresponding systems have 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 according to the successful method of Spear and Besmann. 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 actual task consists of re-assessment of the thermodynamic data on the P_2O_5-containing systems. Firstly, the binary systems Alk_2O-P_2O_5 (Alk=Na, K) have been re-optimised taking into account the new experimental information. Further, the corresponding ternary systems containing $AlkPO_x$ should be considered. The present work covers the ternary systems Alk_2O-Me_xO_y-P_2O_5 (Alk=Na, K; Me=Ca, Mg, Zn, Al). The binary and ternary sub-systems will be discussed.

The solubilities based on the corresponding crystallographic modifications of Na_3PO_4 and K_3PO_4 have been included into the dataset. The solid solutions have been treated using quasi-sublattice approaches according to the following formulae:

$(Na_2, K_2, Zn)_2\ (Na_2, Na_2CaO, Mg, Na_2MgO)_1\ (PO4)_2$ (1)

$(K_2)_2(P_2O_5)(K_2, Ca, K_2CaO, Na_2, Mg, K_2MgO, K_2AlPO_4)_1\ (PO_4)_2$ (2)

It should be noted that these models do not respect the crystallographic structure of the solutions; however, these formulae provide reasonable descriptions of the solubility ranges of the phases between binary and ternary constituents.

The solid solutions between Na_3PO_4 and K_3PO_4 have been calculated in the system Na_2O-K_2O-P_2O_5 along with the ternary compounds. The systems Alk_2O-MeO-P_2O_5 (Alk=Na, K; Me=Ca, Mg, Zn) are characterised by a large number of ternary stoichiometric compounds and by solubility between Alk_3PO_4 and ternary compounds with the general formula $(Alk_2O)_3(MeO)(P_2O_5)$ and $(Alk_2O)_2(MeO)(P_2O_5)_2$. The solid solutions have been treated using the sublattice approach according to the formulae (1-2). The ternary systems Alk_2O-Al_2O_3-P_2O_5 (Alk=Na, K) are presented including the phase equilibria on the quasi-binary sections and the ternary phase diagram. The solid solutions between Alk_3PO_4- and $AlPO_4$ have also been considered.

The current dataset allows a sufficient description of the phase equilibria. The pseudo-binary sections in the framework of all ternary systems are calculated as a first approximation. The ternary phase diagrams including sub-solidus equilibria are proposed.