

Database development for the HotVeGas project

Elena Yazhenskikh¹, Tatjana Jantzen², Klaus Hack², Michael Müller¹

1: IEK-2, Forschungszentrum Jülich GmbH, Germany

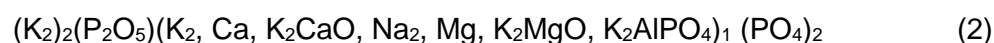
2: GTT-Technologies, Kaiserstr. 103, Herzogenrath, D-52134, Germany

In the framework of the HotVeGas project the oxide database containing SiO₂, Al₂O₃, 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 P₂O₅-containing systems. Firstly, the binary systems Alk₂O-P₂O₅ (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 Alk₂O-Me_xO_y-P₂O₅ (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 Na₃PO₄ and K₃PO₄ have been included into the dataset. The solid solutions have been treated using quasi-sublattice approaches according to the following formulae:



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 Na₃PO₄ and K₃PO₄ have been calculated in the system Na₂O-K₂O-P₂O₅ along with the ternary compounds. The systems Alk₂O-MeO-P₂O₅ (Alk=Na, K; Me=Ca, Mg, Zn) are characterised by a large number of ternary stoichiometric compounds and by solubility between Alk₃PO₄ and ternary compounds with the general formula (Alk₂O)₃(MeO)(P₂O₅) and (Alk₂O)₂(MeO)(P₂O₅)₂. The solid solutions have been treated using the sublattice approach according to the formulae (1-2). The ternary systems Alk₂O-Al₂O₃-P₂O₅ (Alk=Na, K) are presented including the phase equilibria on the quasi-binary sections and the ternary phase diagram. The solid solutions between Alk₃PO₄- and AlPO₄ 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.