Database Development for the HotVeGas Project: Ternary Systems (K_2O, Na_2O)-(CaO, MgO)-P_2O_5

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ABSTRACT

Complex oxide systems containing phosphorus along with silica, alumina, alkali-earth and alkali oxides are important in many scientific and industrial fields. Thermodynamic properties of such systems for which the measurements are experimentally difficult can be described and predicted by thermodynamic modelling on the basis of reliable experimental data and appropriate Gibbs energy models for various phases.

In the framework of the *HotVeGas* project the oxide database containing SiO_2, Al_2O_3, alkali, earth-alkali, CrO_x, FeO_x, MnO_x with addition of sulphates of alkali and earth-alkali oxides and metal sulphides has been created.

The corresponding oxide systems have been thermodynamically assessed using all available experimental data on phase diagram and thermodynamic properties. Self-consistent datasets have been obtained covering experimental information on all binary, ternary, and quaternary subsystems.

The aim of the present work is the expansion of the database by addition of P_2O_5 as the next component for the modelling of a complete coal ash (slag) system. The binary systems with P_2O_5 have been already added into the database. The present work covers the ternary systems Alk_2O-EAlkO-P_2O_5 (Alk=Na, K; EAlk=Ca, Mg).

These systems are characterised by a large number of ternary stoichiometric compounds and by solubility between the corresponding alkali orthophosphates Alk_3PO_4 and ternary compounds with the general formula $(Alk_2O)_3$ (EAlkO) (P_2O_5) and $(Alk_2O)_2$ (EAlkO) $(P_2O_5)_2$.

The Gibbs energy of the stoichiometric compounds have been generated from those of the corresponding oxides and presented in form of a simple G(T) function.

The solid solutions have been treated using the sublattice approach according to the formula $(Alk_2O)_2(P_2O_5)(Alk_2O, EAlkO, Alk_2EAlkO_2)$ and the corresponding solid solution parameters have been found to obtain adequate representations of the available experimental data.

The Gibbs energy of the liquid phase has been modelled using a non-ideal associate solution approach. The current dataset allows the 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.

Generally, the thermodynamic assessment of the systems with P_2O_5 is continued, and the multi-component systems with both alkalis along with addition of further oxides (Al_2O_3, FeO_x) have to be taken into the assessment process.