Development of a New Thermodynamic Database for Slag Relevant Oxide Systems Containing P_2O_5

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ABSTRACT

Complex oxide systems containing silica, alumina, alkali-earth and alkali oxides are important in many scientific and industrial fields, e.g. in coal combustion and gasification processes where alkali release and behaviour of slags are among the main problems.

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.

The oxide system SiO_2-Al_2O_3-Na_2O-K_2O-CaO-MgO has already been thermodynamically assessed using all available experimental data on phase equilibria and thermodynamic properties. Self-consistent datasets have been obtained covering experimental information on all binary, ternary, and quaternary subsystems. P_2O_5 is considered as the next important slag component to be added into the database, because phosphates are essential components for biomass ashes and metallurgical slags.

The aim of the present work is the development of a database for the slag relevant oxide system containing P_2O_5 for the modelling of a complete coal ash (slag) and gas system.

The Gibbs energy of the liquid phase has been modelled using a non-ideal associate solution approach. The compositions of the pure liquid oxide species have been chosen to have two moles of cations per associate thus keeping 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. In the binary system SiO_2-P_2O_5, the experimental information on the phase diagram is contradictory.

The current dataset allows the adequate description the phase equilibria. In the system Al_2O_3-SiO_2-P_2O_5, a reciprocal solid solubility between $AlPO_4$ and SiO_2 is included in the dataset. The corresponding solid solutions based on SiO_2 and $AlPO_4$ are described using the sub-lattice model according to the formula $(Al^{3+},Si^{4+})(P^{5+},Si^{4+})(O^{2-})4$. The ternary system MgO-SiO_2-P_2O_5 was evaluated including the quasi-binary sections. The agreement with experimental information is most satisfactory.

Generally, the thermodynamic assessment of the further systems with P_2O_5 is continued, and alkali oxides have to be taken into account. Simultaneously, an accompanying experimental study is carried out in our group in order to cover the lacking composition ranges using the DTA and KEMS methods.