Thermochemical Assessments for Alkali-containing Oxide Systems with Silica and Alumina

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Abstract

The thermodynamic properties of complex oxide systems containing high amounts of silica and alumina 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 molten coal ashes (slags) are among the main problems. Thermodynamic modelling is considered to be a powerful tool for the description and prediction of thermodynamic properties, especially in cases where measurements in such complex slag system are experimentally difficult. Moreover, experimental investigations are often not feasible for the whole range of composition and temperature of technological interest, whereas thermodynamic modelling permits to obtain results within shorter time and at less expense allowing free variation of parameters such as temperature and chemical composition of the system. Therefore, it is necessary to develop a database for the modelling of the complete coal ash (slag) and gas system.

In continuation of our work on a database for the slag relevant oxide system Na_2O-K_2O-Al_2O_3-SiO_2 the two ternary systems Na_2O-K_2O-SiO_2 and K_2O-Al_2O_3-SiO_2 are considered. The binary systems Alk_2O-SiO_2, Alk_2O-Al_2O_3 (Alk=Na, K) and Al_2O_3-SiO_2 have already been successfully evaluated. The phase equilibria calculated using the new optimised solution data show good agreement with the experimental points. In contrast to other available databases the new dataset allows the description of the whole composition range including the alkali rich parts of the corresponding subsystems. These new data for the liquid and solid phases are compatible with data for the solid stoichiometric compounds from the FACT Pure Substance database.

The associate species model is applied for the description of the liquid and solid phases in the Na_2O-K_2O-SiO_2 and K_2O-Al_2O_3-SiO_2 systems. The available phase diagrams were collected and evaluated for the purpose of improving the solution database. Data on the solution components and interaction parameters are optimised to represent the phase relationships in the system under consideration. The mullite phase is described using the associated species model and the modified four-sublattice model. The solution based on the potassium aluminate $KAlO_2$ is described in the framework of the associated species model. Solid solution components were selected and their thermodynamic data were assessed in order to obtain the best agreement with the experimental data.