Development of a Database for the Na_2O–K_2O–Al_2O_3–SiO_2 System

E. Yazhenskikh, K. Hack*, M. Mueller

IEF-2, Forschungszentrum Jülich
* GTT-Technologies, Herzogenrath

Abstract

Alkali release and behaviour of molten coal ashes (slags) are among the main problems in coal combustion and gasification processes. Therefore, the thermodynamic properties of complex oxide systems containing high amounts of silica and alumina as well as alkali, alkaline-earth, and iron oxides are important. The experimental measurements can be difficult for the complex and reactive systems such as slags at high temperature and often not feasible for the whole range of composition and temperature of technological interest, whereas thermodynamic modelling permits to generate results within shorter time and at less expense while allowing free variation of parameters such as temperature and chemical composition of the system. Moreover, the thermodynamic properties cannot only be calculated in the temperature and composition ranges of the experimental data on which the data assessment was based, but may be used for extrapolation into extended regions as well. Therefore, it is necessary to develop a new database for the modelling of the complete coal ash (slag) and gas system.

The associate species model was applied to the thermodynamic representation of the liquid and solid phases in the Na_2O–K_2O–Al_2O_3–SiO_2 system. The ternary K_2O–Na_2O–SiO_2, K_2O–Al_2O_3–SiO_2, Na_2O–Al_2O_3–SiO_2 systems were considered.

The available phase diagrams were collected and evaluated for the purpose of improving the solution database. These new data for the

liquid phase are compatible with data for the solid stoichiometric compounds from the FACT Pure Substance database.

The phase equilibria calculated using the new optimised solution data showed good agreement with the experimental points. In contrast to other databases the new dataset allows the description of the whole composition range including the alkali rich parts of the corresponding subsystems.

Moreover, the solid solution phases of mullite, nepheline, carnegieite and $KAlSiO_4$ were described as a first approximation in the framework of the associated species model as well. Solid solution components were selected and their thermodynamic data were assessed in order to get the best agreement with the experimental phase diagram data.