Thermodynamic Optimisation of the System Al_2O_3-K_2O-Na_2O-SiO_2

E. Yazhenskikh[1], K. Hack[2], M. Müller[1].
1. *Forschungszentrum Jülich, Germany.*
2. *GTT-Technologies, Germany.*

ABSTRACT

In the framework of our work on the creation of a new database for slag relevant oxides, the present study is devoted to the generation of thermodynamic data for the liquid and solid phases in the ternary systems K_2O-Al_2O_3-SiO_2 and Na_2O-Al_2O_3-SiO_2. The description and prediction of the thermodynamic properties of such complex systems remain actually, especially in cases when the measurements are experimentally difficult. The thermodynamic database has to be produced using appropriate models of the Gibbs energy for the phases and by optimisation of the required parameters taking into account the reliable experimental data. The available databases are not sufficient to model the complete ash (slag) and gas systems. Therefore, the development of a new database is necessary.
The liquid was described with the use of the modified associate species model, which is suitable for aluminosilicate melts. The following solid solutions were also introduced using the multi-sublattice model: $(AlkAl)_{1-x}Si_xO_2$ (with Alk=Na or K) and $(NaAl)_{1-x}Si_xO_4$ (for both modifications, low- and high-temperature phases, nepheline and carnegieite, correspondingly). The Gibbs energy data of the solution components and corresponding interaction parameters between them were obtained to represent the phase relationships in the systems under consideration.

For pure oxides, in liquid and solid states, the initial thermodynamic data were taken from the SGTE Pure Substances Database, which is, especially with respect to SiO_2, considered as more appropriate than other commercial available databases we used in earlier assessments. Because of these changes, it was necessary to perform the work in two stages. First, the Gibbs energy data for binary species and the respective interaction parameters were modified. In that way, the binary systems Alk_2O-SiO_2, Alk_2O-Al_2O_3 (Alk=Na, K), Al_2O_3-SiO_2 and the ternary system Na_2O-K_2O-SiO_2 have been successfully re-evaluated. These were then kept constant during the assessment of the ternary parameters.

The phase equilibria and activity data (if they are available) calculated using the new optimised solution data show good agreement with the experimental data. In contrast to other available databases the new dataset allows the predictive description of the whole composition range including the alkali rich parts of the corresponding subsystems with lack of the experimental data.