Thermodynamic Assessment of the Al_2O_3-K_2O-Na_2O-SiO_2-CaO-MgO System

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Abstract

The description and prediction of the thermodynamic properties of the complex systems with the slag relevant oxides remain actually, especially in cases when the measurements are experimentally difficult. 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 present study is devoted to the generation of thermodynamic data for the liquid and solid phases in the system Na_2O-K_2O-CaO-MgO-Al_2O_3-SiO_2. This work on the creation of a new database is carried out jointly with our partners in the framework of the HotVeGas project. 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 liquid was described with the use of the modified associate species model, which is suitable for aluminosilicate melts. Sublattice model was successfully applied for the solid solutions. 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 several stages. First, the Gibbs energy data for binary species and the respective interaction parameters were modified. Second, the corresponding ternary systems should be considered. In that way, the binary and ternary systems Alk_2O-SiO_2, Alk_2O-Al_2O_3, Al_2O_3-SiO_2 Na_2O-K_2O-SiO_2, Alk_2O-Al_2O_3-SiO_2 (Alk=Na, K) have been successfully re-evaluated. Further, earth alkali oxides are added to the basic systems Na_2O-K_2O-Al_2O_3-SiO_2. The thermodynamic description of the ternary system with one alkali and one earth-alkali oxides (K_2O-CaO-SiO_2 and K_2O-MgO-SiO_2) are here presented.

The phase equilibria 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.