On the Thermochemical Modelling of Viscosities of Liquid Oxide Mixtures

A. Kondratiev

GTT-Technologies, Germany

Abstract

Two different approaches to the modelling of the physicochemical properties of liquid oxide mixtures have been applied to describe the viscosity of oxide systems relevant to coal ash slags. The first approach made use of such a mathematical tool as neural networks, while in the second one a physically based model was employed.

The application of neural networks to calculation of the viscosity of mould fluxes has recently been reported by the group of Prof Tanaka, Osaka University, Japan. On the basis of this work, a computer program called "SlagVis" has been developed in the Research Centre of Computational Mechanics (RCCM), Japan. This program enables the neural network model to be trained with different datasets and be applied to a multi-component system.

Using the SlagVis program, the model was tested with large viscosity-temperature-composition datasets (>1000 experimental points) relevant to the coal ash slags. These tests showed that interpolative and extrapolative capabilities of the model are reasonable, but depend on the "quality" of the dataset, i.e. compositional and temperature ranges covered, and a number of points used for training.

A viscosity model based on the Avramov equation, which links the viscosity to the average jump frequency of structural units, is currently being developed for liquid melts of the Al_2O_3-K_2O-Na_2O-SiO_2 system and sub-systems. The model is coupled with the associate species thermodynamic model and employs the associate species as structural units of flow. The concentrations of the associate species are obtained from assessment of the available thermodynamic and structural (e.g. spectroscopic) information. Both thermodynamic and viscosity descriptions of a given system are achieved using the same assemblage and concentrations of the associate species.

During preliminary model evaluation, it was found that the model can describe the viscosity-composition dependence in binary silicate systems with fewer parameters and better accuracy than a conventional viscosity model (e.g. based on the Eyring or Urbain equations). It was also found that the model cannot readily be applied to describe the viscosity-temperature dependence over a wide range of temperatures, including temperatures close to the glass transition; the latter might confirm different mechanisms of flow at these temperatures suggested by other researchers.