Modelling Viscosity of Molten Oxides (HotVeGas)

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ABSTRACT

Coal is the world's most abundant and widely distributed fossil fuel, which maintains around 41% of the power generation in the world. Coal-fired power plants using integrated gasification combined cycle (IGCC) technology in combination with carbon capture allow a cleaner and more efficient utilization of coal. The core of an IGCC power plant is the gasifier, in which slag viscosity as a function of temperature and composition plays a significant role in determining the optimum operating conditions. However, most of the early viscosity models are only applicable in a limited range of temperatures and compositions resulting from the lack of an effective description of the structural dependence of the viscosity.

In the framework of the HotVeGas project, a structure based model has been developed for the fully liquid system SiO_2-Al_2O_3-CaO-MgO-Na_2O-K_2O-FeO-Fe_2O_3 and its subsystems in the Newtonian range, based on the thermodynamic modified associate species model. To obtain an effective structural dependence of the viscosity, it is linked to the associate species distribution and the connectivity of associate species. With this principle, both the temperature- and composition-induced structural changes of oxide melts can be described with a set of monomeric associate species in combination with the critical clusters induced by the self- and inter-polymerizations. The new model is self-consistent and gives a reliable prediction over the whole range of compositions and a broad range of temperatures using only one set of model parameters, which all have a clear physico-chemical meaning. With the new model, the viscosity behavior when substituting one network modifier for another at constant SiO_2 contents is well described. The Al_2O_3-induced viscosity maximum is also well described, in which the position and magnitude of the viscosity maximum as a function of composition and temperature (charge compensation effect) are properly predicted. Another viscosity maximum when replacing Al_2O_3 with SiO_2 for constant contents of the network modifiers is presented. The Al_2O_3-induced charge compensation effect is more pronounced than that induced by Fe_2O_3. In addition, the iso-viscosity lines and 3-dimensional viscosity surfaces are generated and further applied to determine the coal ash fluxing and blending.