Modelling viscosity of molten oxides (HotVeGas PartII)

Guixuan Wu[1], Elena Yazhenskikh[1], Klaus Hack[2], Michael Müller[1]
g.wu@fz-juelich.de

[1]IEK-2, Forschungszentrum Jülich GmbH, Jülich, Germany
[2]GTT Technologies, Herzogenrath, Germany

Viscosity as a function of temperature and composition is of practical importance for the description of slag flow behavior in entrained flow gasifiers. The viscosity essentially depends on the structure, a comprehensive description of structural dependence is therefore required for the development of a new viscosity model. In the framework of the HotVeGas project, a structure based model recently developed for the fully liquid system SiO_2-Al_2O_3-CaO-MgO-Na_2O-K_2O-FeO-Fe_2O_3 is further extended to describe the viscosity of the P_2O_5-containing systems in the Newtonian range. The structural treatment of P_2O_5 in multicomponent oxide systems is discussed. The preliminary results for the systems P_2O_5, P_2O_5-CaO, P_2O_5-Na_2O, P_2O_5-CaO-FeO, and P_2O_5-SiO_2-Al_2O_3-Na_2O are presented. Due to insufficient reliable experimental data for the assessment of model parameters, large deviations occur in some systems such as the quaternary system P_2O_5-SiO_2-Al_2O_3-Na_2O. Further assessment of the model parameters is necessary. Besides, the model parameters for FeO_x-containing systems need to be further modified for better description of the local viscosity maximum around the fayalite composition in the binary system SiO_2-FeO_x, which is analyzed in conjunction with the structrual information obtained from molecular dynamics simulations. The shift of viscosity maximum with repect to SiO_2 content in the ternary system SiO_2-Al_2O_3-Na_2O is also discussed using the different tricluster species calculated from molecular dynamics simulations.

Keywords:
viscosity, associate species, thermodynamic modelling, structure, molten slags, gasification