Modelling viscosity of molten oxides (HotVeGas Part III)

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In the framework of the HotVeGas project, the structure based viscosity model recently developed for the fully liquid system SiO_2-Al_2O_3-CaO-MgO-Na_2O-K_2O-FeO_x-P_2O_5 is further improved. In terms of FeO_x-containing systems, a new associate species Fe_3O_4 referring to the charge compensation of Fe and Fe^{2+} is introduced to describe the local viscosity maximum around the fayalite composition in the binary system FeO_x-SiO_2. The position and magnitude of the local viscosity maximum as a function of temperature, composition and oxygen partial pressure can then be properly predicted. Some larger structural units due to self- or inter-polymerization are employed to describe the viscosity behavior of the systems FeO_x-SiO_2 and FeO_x-Na_2O. For P_2O_5-containing systems, two larger structural units due to self-polymerization of P_2O_5 are used, which are analogous to the silica critical clusters for SiO_2-based systems. The corresponding model parameters are reassessed in conjunction with the structural features of the associate species. The extrapolated viscosities in the ranges where no experimental data are available in literature are then more reasonable. To achieve better model performance, more experimental data are required for both FeO_x- and P_2O_5-containing systems.