Software for Calculating Viscosities of Molten Oxides

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ABSTRACT

Software for calculating viscosities of molten oxides is presented. At the current stage of the development, slag viscosity is calculated using “compositional” viscosity models, which makes the software independent of the thermodynamic solution model used for a slag phase. Calculations can be performed for a range of parameter values with a specified step. Graphic capabilities of the software allow flexible plotting of the calculated values. Generated plots can be printed out or saved in different formats.

Being developed in the course of “HotVeGas” project, the software allows calculating phase equilibrium for an arbitrary blend of three coal ashes at specified temperature and oxygen partial pressure. The software also allows calculating liquidus and solidus temperature as well as solidus slag composition. Two Urbain-type viscosity models (Kalmanovitch & Frank and Kondratiev & Jak) can be used for calculating slag viscosity. When the equilibrium phase assemblage contains slag and solid phases, the viscosity of slurry is calculated according to the Roscoe equation. All phase equilibrium related calculations in the software are performed using GTT's own Programmer's Library ChemApp.

Directions for further development of the software, such as an implementation of Avramov-type viscosity models and expanding graphic capabilities towards ternary diagrams, are discussed