

Development of models and databases for modelling of slag properties

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One of the major issues when operating entrained flow slagging gasifiers is to ensure the continuous drainage of the molten slag out of the reactor. Therefore, the necessary process temperature, which influences the efficiency of the process, is often determined by the properties of the slag. Reliable modelling tools with corresponding thermo-chemical and physical databases for calculation of chemical and physical (rheological) properties of oxide slags in dependence of slag and gas phase composition, temperature, and pressure enable optimization of the gasifier operation. Such tools also provide the necessary input data for development of slag sub-models needed in CFD simulations.

In recent years, the system $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-CaO-MgO-FeO}_x\text{-K}_2\text{O-Na}_2\text{O-P}_2\text{O}_5\text{-SO}_x$ relevant for the development and production of refractory materials as well as for slag applications has been thermodynamically assessed using all available experimental data on phase equilibria and thermodynamic properties. Self-consistent data sets have been established covering experimental information on all binary, ternary, and quaternary subsystems. The Gibbs energy of the liquid phase is modelled using a non-ideal associate solution description. Stoichiometric solids are treated with a simple $G(T)$ function, whereas the compound energy formalism (CEF) is used for solid solutions.

In addition to the thermochemical assessment, an Arrhenius-type model for the calculation of slag viscosities has been developed. The model is based on the same structural units, i.e. the associates, as the one for the Gibbs-energy of the melt. Thus, a two-step calculation approach is introduced. First, the equilibrium distribution of the associates in a melt with given overall composition is calculated, and then the resulting associate mole fractions are applied in a weighted sum of the logarithms of the associate viscosities taking into account the possibility of polymerisation of silica and silicates. For example, the charge compensation effect and the lubricant effect (near pure SiO_2) can be described well with the model.

Furthermore, the influence of crystallisation, which not only transforms the liquid into dispersion but also usually changes the composition of the residual liquid, on the viscosity is considered applying appropriate physical models. The equilibrium description can be extended by a kinetic description of the crystallisation process.