Phase Field Modeling of Isothermal Slag Crystallization Using FACT Databases

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ABSTRACT

In this work, we present the use of FACT databases [1] for oxide systems in phase field simulations of isothermal crystallization of metallurgical slags. The considered systems are CaO-Al2O3-SiO2 and FeO-Fe2O3-SiO2. Both systems have a wide spread of applications in both ferrous and non-ferrous pyrometallurgical industries. In the phase field model, the oxides molecules (CaO, FeO, Fe2O3, …) are assumed to be the diffusing species and the components. The phase field model is constructed using the multiphase field approach from [2] and the multicomponent approach from [3]. The Gibbs energies of all phases and the chemical potentials of all components in all phases are retrieved from the thermodynamic database using ChemApp [4]. Stoichiometric phases are often present in slag systems and cannot be readily treated by the phase field method. An artificial parabolic Gibbs energy is constructed for such phases, based on the method used in [5]. The simulation results provide unique insight in the crystallization of minerals in a liquid slag. In the CaO-Al2O3-SiO2 system, elementary diffusion path simulations show the influence of the diffusion kinetics in the liquid on the selection of the tie-line in a two phase region (between liquid and stoichiometric solid). In the FeO-Fe2O3-SiO2 system, simulations illustrate how the diffusion of O2 (due to an open boundary with the atmosphere) influences the growth of spinel (FeO.Fe2O3) particles in the liquid.

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