

4. FACTSage

FACTSage is a quasichemical thermodynamic modelling tool with copyright to Thermfact Ltd. and GTT Technologies. This software enables the user to perform a variety of tasks namely:

- Calculation of thermodynamical properties of species or chemical solutions
- Calculation and plotting of isothermal and nonisothermal predominance area diagrams
- Calculation and plotting of E-pH (Poubaix) diagrams
- Gibbs energy minimisation module featuring ChemSage for treating complex heterogeneous equilibrium
- Calculation and plotting of phase diagrams
- Optimisation of thermodynamic and phase diagram data.

For this thesis only the equilibrium calculation and phase diagram options were employed, to predict the equilibrium phases present in partially solidified ilmenite smelter slags and to draw phase diagrams of the $\text{FeO-Ti}_2\text{O}_3\text{-TiO}_2$ system. From these phase diagrams valuable predictions were obtained with regard to the solidification behaviour of these slags.

For these calculations, the slag composition was expressed in terms of FeO , TiO_2 and Ti_2O_3 . To aid with constructing these diagrams, the main components expected to be present in the partially solidified slag were identified namely metallic iron, ilmenite, M_3O_5 , TiO_2 and the liquid oxide phase. A temperature range between 1700 and 2000 K was used. From the results of the calculations, the molar amount of Ti, Fe and O in every phase was obtained. By adding the amount of Fe and Ti in all the phases, the total amount of cations in the slag was obtained. The mole fraction of phases present in the slag was calculated by expressing the total amount of Fe and Ti in a specific phase and as a fraction of the total amount of cations in the system. Calculations were done for the main components in the slag as mentioned earlier. The results were plotted as a function of temperature over the chosen range.