14.2.5 PHREEQC V3

PHREEQC is a general geochemical program and is used extensively for hydro-geochemical environments. The software uses ion-association and Debye Hückel expressions to account for the non-ideality of aqueous solutions. However, it is not applicable at high ionic strengths and also suffers from lack of internal consistency of the data in the databases. The databases that are distributed with the code have different origins and no systematic attempt has been made to ensure that the databases are congruent. Therefore PHREEQC was not investigated as a software package for EFC processes.[21]

14.2.6 OLI Stream Analyzer 9.5

The OLI Stream Analyzer software uses a speciation-based model that employs both accepted equations of state and experimental data to predict thermodynamic properties of multi-electrolyte aqueous solutions over a wide range of concentrations, temperatures, and pressures.[22] In addition, the software has in-built aqueous models which it applies to electrolyte systems in water, organic or mixed solvents.[23] The thermodynamic framework has been designed by combining the excess Gibbs energy model with detailed speciation calculations. The excess Gibbs energy model consists of a long–range interaction contribution represented by the Pitzer–Debye–Hückel expression, a short-range term expressed by the UNIQUAC model and a second-virial-coefficient term for specific ion interactions. The Helgeson–Kirkham–Flowers equation of state is incorporated to predict the equilibrium constants. The built-in model also integrates the Bromley–Meissner, Pitzer, Helgeson and Bromley–Zematis equations for calculations of the activity coefficients.[24] OLI software also includes a mixed solvent electrolyte (MSE) database, which uses the Helgeson direct method, and has the capability of successfully modelling temperatures as low as −200 °C.

The parameters of the model are determined using thermodynamic data of various types including vapor–liquid equilibria, activity and osmotic coefficients, solubility of salts in water or other solvents, amongst others.[23] The ability of the model to reproduce solubilities in multi-component systems together with accurately predicting the correct solid phases in multi-component systems means that the software is applicable to EFC processes.

14.2.7 Summary of Thermodynamic Software Packages

Presented in Table 14.2 is a comparison of the criteria used to evaluate the various thermodynamic models. As can be seen, OLI Stream Analyzer fulfils all the criteria set out.