modelling solid species. Furthermore, many of the hydrated salts that are present at the sub-zero temperature ranges are not included in the database. It is only recently that Aspen Plus has started to further develop its electrolyte database. Aspen Plus is available with the more comprehensive OLI Stream Analyzer database, since we evaluated OLI Stream Analyzer on its own, Aspen Plus was not deemed suitable as a thermodynamic package for EFC systems.

14.2.2 FactSage V7.2

The FactSage software is the fusion of two well-known software packages in the field of computational thermo-chemistry: FACT-Win (formerly F*A*C*T) and ChemSage (formerly SOLGASMIX).[17] This software package allows for the calculation and manipulation of phase diagrams although FactSage's database is limited at the lower temperature ranges. It does have the facility to import databanks from the OLI Stream Analyzer, but unfortunately, this databank can only be exported to the equilibrium model of the FactSage software and not the phase diagram section. Therefore, FactSage was not further investigated.

14.2.3 HSC Chemistry V5.1

The HSC Chemistry software has been designed to model various chemical reactions as well as equilibria. It contains fourteen calculation modules, of which the equilibrium module is of interest for eutectic freeze crystallization. This enables the calculation of multi-component equilibrium compositions in heterogeneous systems. Calculations are based on the GIBBS or SOLGASMIX solvers which use the Gibbs energy minimization method.[18] HSC Chemistry uses Criss–Cobble extrapolation for the heat capacity of aqueous species at elevated temperature (>25 °C), up to 300 °C. The activity coefficients are calculated using the Raoultian activity scale.[18] A limitation of the software is that it is essential for the user to input all defined phases into the system. Since, in simulating EFC processes, it is a requirement that the model predicts the crystallization of salts, this software was found to be inapplicable for EFC simulation.

14.2.4 MINTEQ V3.1

MINTEQ is a chemical equilibrium model that has an extensive thermodynamic database that allows for the calculation of speciation, solubility, and equilibrium of solid and dissolved phases of minerals in an aqueous solution.[19] However, it is not able to model streams at temperatures less than 0 °C.[20] Therefore, this software package is not suitable for EFC processes.