

modelling software in order to be able to accurately predict the eutectic temperature, eutectic composition, nucleation temperatures of ice and salt components, ice and salt recoveries and order of crystallization for crystal products.¹⁶

The following software packages have potential to be used in this application:

- Aspen Plus V10
- FactSage V7.2
- HSC Chemistry ® 5.1
- MINTEQA2
- OLI Stream Analyzer 9.5
- PHREEQC

In order to assess whether the software is appropriate for modelling hyper-saline streams, it needs to be able to fulfil the following criteria:

- i. Ability to model solid–liquid equilibria for multi-component, mixed-salt electrolytes
- ii. Robust concentration range
- iii. Robust temperature range
- iv. Ability to reconcile electro-neutrality of aqueous streams
- v. Comprehensive databank
- vi. Ability to be used as a predictive tool for:
 - Eutectic temperatures and compositions
 - Nucleation temperatures
 - Salt/ice recoveries
 - Order of salt/ice crystallization
- vii. Convergence
- viii. User friendly interface and debugger
- ix. Ease of input

14.2.1 ASPEN Plus V10

Aspen Plus allows the building and running of process simulations in order to predict the behavior of processes by using basic engineering relationships, such as mass and energy balances and chemical and phase equilibria. Aspen Plus calculates liquid phase properties from the Electrolyte-NRTL activity coefficient model. The model also incorporates the Henry's Law parameters for the calculation of partial pressures and the Meissner equation for the calculation of the water activities. The vapor phase properties are calculated from the Redlich–Kwong Equation of State. Aspen Plus also has a built-in model that includes ice formation at temperatures down to -263 °C. However, there are limitations to the database, especially when