14.13 Example of Thermodynamic Modelling of a Brine Stream Being Subjected to EFC

In order to establish the feasibility of EFC for treatment of a saline stream, the first step is to use a thermodynamic model to predict the nucleation temperatures and the salts that will be formed.

14.13.1 Modelling Using the OLI Stream Analyzer 9.5

The reverse osmosis concentrate stream specified in Table 14.6 is used as an example in thermodynamic modelling of a brine stream being subjected to EFC.

a. Creating a synthetic salt stream
   The first step involves carrying out a charge balance using OLI Systems Stream Analyzer.[61] Adjustment is also made for the pH by adding either an acid or a base, depending on the properties of the stream.
b. Prediction of salt crystallization at reduced temperatures
   Figure 14.14 shows the predictions of the successive crystallization of various salts as the temperature is lowered from ambient (from right to left on the *x* axis). Even at ambient temperatures, the RO retentate stream was supersaturated with $CaSO_4$, and this is reflected by the crystallization of $CaSO_4{\cdot}2H_2O$ across the entire temperature range. This would need to be taken into account in designing an appropriate EFC process.

Once the temperature reaches −1 °C, ice crystallizes out, followed by $Na_2SO_4{\cdot}10H_2O$ at −2 °C and $NaCl{\cdot}2H_2O$ at −23 °C. Trace quantities of CaF_2 and KNO_3 also crystallize out of the brine – these are species that will accumulate with increased brine volumes.

Table 14.6 Composition of stream to be modelled.

Species	Units	Concentration
Na^+	mg l^{-1}	5400
K^+	mg l^{-1}	300
Mg^{2+}	mg l^{-1}	41
Ca^{2+}	mg l^{-1}	390
Li^+	mg l^{-1}	0
NH_4^+	mg l^{-1}	0.5
Br^-	mg l^{-1}	<0.1
Cl^-	mg l^{-1}	4010
F^-	mg l^{-1}	13.86
NO_3^-	mg l^{-1}	29.6
SO_4^{2-}	mg l^{-1}	8690
pH		7.26
κ	mS cm^{-1}	>20
TDS	ppt	>10