Osmotic Pressure Simulation

The osmotic pressure was simulated using a model developed by Nir et al.1 and modified to fit the hydrodynamic settings of the system taking the feed composition and operational conditions as input parameters. This simulation code written in Python programming language2 executes the membrane transport and mass balance equations required for the model. Simultaneously, osmotic coefficients, and solution densities are obtained from PHREEQC3. Data communication between these two coupled programs allows detailed and comprehensive chemical equilibrium modeling at each iterative step. Osmotic pressure computation for each numerical recovery segment is implemented using the solution-diffusion-film model.

= --------- (1)

= --------- (2)

= ---------- (3)

In Eq. 1 – Eq. 3, C is the concentration (mol/l), , transmembrane volumetric permeate flux (m/s), k, mass transfer coefficient (m/s), membrane salt permeability (m/s). Subscripts b, p, and m stand for bulk, permeate, and membrane respectively. PHI (, osmotic coefficient (unitless), T, temperature(K), and PI (∏) is the osmotic pressure (Bar).

**References**

1. Nir, O., Ophek, L. & Lahav, O. Acid–base dynamics in seawater reverse osmosis: experimental evaluation of a reactive transport algorithm. *Environ Sci (Camb)* **2**, 107–116 (2016).

2. Hernández, E. & Martín, M. *Python for Chemical Engineering*. (CRC Press, 2019).

3. Parkhurst D. L. & Appelo C. *User’s guide to PHREEQC (Version 2): A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations*. (1999) doi:10.3133/wri994259.