

# Process Simulation of a Nanofiltration, Ion Exchange, and Electrodialysis Flowsheet for Lithium Production Using Fundamental Thermodynamic Modelling

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## **ABSTRACT**

As the world moves towards reducing reliance on fossil fuels via increased electrification, battery metals will play an increasingly important role in this initiative. Lithium is expected to play a key role in this transition.

Conventional processes involve evaporation in large ponds for the production of concentrated Li-bearing brines from salars. In recent years, there has been significant interest in membrane-based processes for preconcentration and purification of lithium brines. Furthermore, electrochemical processes such as electrodialysis have garnered attention as a means for direct production of lithium hydroxide from concentrated brines. In this work, a process model is presented which provides an evaluation of these technologies for lithium hydroxide production from brine feed. The presented process uses nanofiltration, ion exchange, and electrodialysis to produce lithium hydroxide brine from raw feed brine.

The models are based upon thermodynamic modelling for solution properties, along with published experimental data from the open literature. Using the models, the impact of operating parameters, brine feed chemistry, and other process variations are tested to understand their impact on the overall process.

In this work, AQSol is used within SysCAD via the Thermodynamic Calculation Engines interface. AQSol uses the extended UNIQUAC thermodynamic model for estimation of activity of solutes in salt solutions over a wide range of temperatures. Solubility of salt hydrates and double salts are calculated. AQSol calculations embedded in the overall process model allow prediction of solution properties, including osmotic pressure and conductivity, as well as scaling propensity.