

SIMULATING MASS AND CHEMISTRY BALANCE IN A DIRECT LITHIUM EXTRACTION PROCESS

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ABSTRACT

We use rigorous electrolyte thermodynamics, DLE media database with reaction kinetics, and a steady state process simulator to predict the mass, energy, and chemistry balance in lithium extraction from geological fluids. The electrolyte thermodynamic model is used to predict the brine properties at each step in the process. The DLE media database and reaction kinetics are used to predict lithium uptake by the adsorbent materials. The process simulator is used to predict the mass, energy, and chemistry balance in the overall process.

The electrolyte model contains the thermochemical data of key elements like Li, Na, K, Ca, Sr, Fe, Cl, CO₃, SO₄, H, OH, and B. It is used to calculate pH, density, buffer capacity, vapor pressure, activity coefficients, solids saturation and precipitation formation, and chemical demand. It is needed to predict the equilibrium state of the brines as it flows in and out of each process unit in the extraction and regeneration process. It is the most critical of the three tools.

We then created a DLE database using experimental data from media providers to quantify lithium (and other ion) uptake as a function of contact time, pH, temperature, and brine chemistry. We back-calculate the media's formula using the moles of exchangeable sites available per gram of media. We also created a rate expression and a set of rate coefficients to calculate ion uptake as a function of temperature, pH and time. We have not developed a media degradation parameter that could be used to optimize plant costs.

We used the electrolyte model and DLE database in a steady-state process simulator to predict lithium extraction efficiency, contaminant ion uptake, solids deposition, chemical requirements, and LiCl extractant composition. We developed full-plant simulation for several extraction plant designs and present the essential parts of these designs in this paper. Although we cannot present actual plant information due to the proprietary nature of the operations, we present a hypothetical plant design of a geological fluid and describe the sections of the extraction plant that are and are not simulated accurately at this time. The limitations we describe are mostly mass-transport-based, such as solids settling rates, media fouling, incomplete mixing, and membrane and ion exchange performance.

In summary, we have used the above three capabilities to design, with a fair amount of accuracy, geological fluid extraction processes. This includes simulating critical unit operations like ion extraction and media regeneration, separation processes like ion exchange and membranes, predicting the formation of unwanted solids, and predicting the chemical and water demand under different process conditions.

Keywords: Direct Lithium Extraction, Lithium, process simulation