SIMULATING MASS AND CHEMSITRY BALANCE IN A DIRECT LITHIUM EXTRACTION PROCESS

By

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ABSTRACT

We use rigorous electrolyte thermodynamics, direct lithium extraction (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. A 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, precipitation formation, and chemical demand. The electrolyte model 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 created a DLE media database with two approaches, empirical and rigorous, 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 media degradation parameters that could be used to optimize plant costs.

We used a steady-state process simulator with the electrolyte model and DLE media database to predict lithium extraction efficiency, contaminant ion uptake, solids deposition, chemical requirements, and LiCl extractant composition. We developed a full-plant simulation for several extraction plant designs, the essential parts of the plant are presented 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 relative 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

INTRODUCTION

Geologic fluids produced in geothermal and oil/gas production contain lithium at low concentrations compared to conventional sources of lithium like salars and ore. These low concentrations make the use of conventional extraction techniques such as evaporation or membrane technologies impractical. Many entrepreneurial startups and established mining companies have developed materials that selectively extract lithium directly from the brine, without taking up the other solutes (e.g., Na, Cl, Ca, Mg. etc.). The material, generally termed DLE media, is comprised of a porous magnesium oxide (MgOx) or titanium oxide (TiOx) matrix containing positive-charge deficiencies. These materials are manufactured in ways that allow Li^+ and H^+ to diffuse and attach to sites in the media, but larger ions like Na^+, K^+, Ca^{+2}, to largely remain in the bulk fluid.

In DLE, lithium-containing brine contacts the protonated form of the media, allowing the ion-exchange reaction between Li^+ and H^+ to occur, the media is then separated from the brine and washed with acid to reverse the exchange, extracting lithium from the media. The resulting solution is an acid-containing pregnant liquor with lithium concentrations in the several thousands of mg/l.

With these new DLE processes, there is a strong demand to develop mass, chemistry, and energy balances around these techniques enabling designs of pilot and full-scale extraction plants. The challenge is that no predictive software tool exists to simulate the extraction process in any mechanistic way. This is in part because the extraction media vary by manufacturer, and therefore uptake rates, adsorption capacity, ion selectivity, and degradation rates vary.

OLI addresses these limitations by developing a semi-empirical thermodynamic and kinetic database that simulates direct lithium extraction and the larger process design. We use one of two approaches to simulate ion uptake, a kinetic-based uptake reaction (empirical) and an ion-exchange reaction with fixed selectivity coefficients (rigorous). We present our development of the kinetic database, and test it using the electrolyte model coupled with a process simulator to analyze a complete DLE plant.

APPROACH TO MODELING CATION ADSORPTION IN DLE MEDIA

We developed a private database containing two types of extraction mechanisms. The first uses a rate-based expression where adsorption is defined using a set of kinetic reactions (empirical). The equation below is the expression for Lithium uptake and release. Similar rate expressions are used for Na^+, K^+, Ca^{+2}, and Mg^{+2}. This approach does not use an equilibrium constant, although one can be back-calculated. We fixed the enthalpy of formation for each adsorption species so that there is negligible temperature change when the reaction proceeds.

$$HMedia + LiCl \leftrightarrow LiMedia + HCl$$

$$Rate\left(\frac{dLi^+}{dt}\right) = \left(\left[A_f * e^{B_f/T(K)} * (HIX^a * Li^b * H2O^c)\right] - \left[A_r * e^{B_r/T(K)} * (H3O^d * LiIX^e)\right]\right) * V_{liq}$$

The strength of the empirical approach is that adsorption and desorption extent is fit to measured data. The rate expression can be expressed to include the temperature, pH, and composition effects.

The second approach uses an equilibrium ion exchange reaction (rigorous). The papers we reviewed define the media as having two exchange sites per mole of central metal, e.g., H_2TiO_3. We evaluated four possible exchange reactions, an exchange of one mole M^{+1} per mole of media or an exchange of 0.5 mole M^{+2} per mole of media.

$$H_2Media + (Na,K,Li)^{+1} \overset{Q_{S1}}{\leftrightarrow} (Na,K,Li)HMedia + H^+$$

$$H_2Media + 2(Na,K,Li)^{+1} \overset{Q_{S2}}{\leftrightarrow} (Na,K,Li)_2Media + 2H^+$$

$$H_2Media + 0.5(Mg,Ca)^{+2} \overset{Q_{S3}}{\leftrightarrow} (Mg,Ca)_{0.5}HMedia + H^+$$

$$H_2Media + (Mg,Ca)^{+2} \overset{Q_{S4}}{\leftrightarrow} (Mg,Ca)Media + 2H^+$$

The strength of the rigorous approach is that it uses standard equilibrium reactions, a selectivity coefficient, and non-ideal interactions for each adsorbing ion. Thus, it incorporates temperature, concentration, and pH effects automatically.

Both approaches include adsorption with all ions if they are developed: H^+, Li^+, Na^+, K^+, Mg^{+2}, Ca^{+2}, Sr^{+2}, Ba^{+2}, Fe^{+2}, and Al^{+2}. The media molecular weight is defined by its molar exchange capacity (grams of media per mole of Li^+ adsorbed). The media enthalpy (for heats of reaction) is referenced to Na2TiO3. These values are not precise but are satisfactory for first-pass development. The enthalpy of reactions for H_2TiO_3 and Li_2TiO_3 species was adjusted to match adsorption vs. temperature data.

RESULTS – FITTING ADSORPTION AND DESORPTION DATA USING EMPIRICAL APPROACH

We used adsorption vs. time data from a private communication to define the reaction rate expression[i]. We set the media's formula weight to a value that would produce a lithium exchange capacity of 5 meq Li/g media (35 mg/g) and used the measured data to parameterize the kinetic coefficients. This data included concentration vs. time as temperature and pH varied. Then, using the brine composition, the experimental pH (5 and 8), temperature (20, 40, and 60C), and the concentration vs time plots to define the kinetic coefficients. Figure 1 is a curve fitting plot of adsorption rates on a proprietary DLE media.

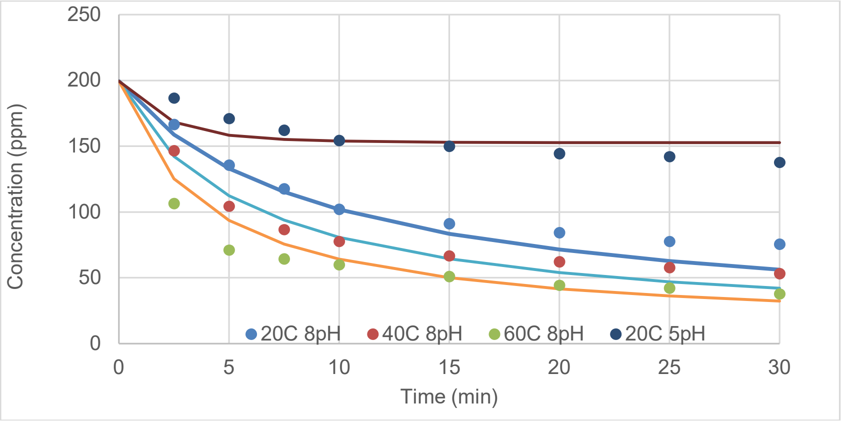

Figure 1 - Curve fitting of adsorption data vs time and temperature

We obtained good agreement with the measurements at pH 8, and limited alignment with data at pH 5. The best fit plots produced the following values. The reactants and products are measured in activities and the volume is in m³.

$$Rate = \left(\left[3.4x10^{13} * e^{2112/T(K)} * (HIX^{1} * Li^{0.6} * H2O^{0})\right] - \left[2.8x10^{13} * e^{-97/T(K)} * (H3O^{1.19} * LiIX^{1.17})\right]\right) * V_{liq}$$

There were no uptake rates for Na^+, K^+, Mg^{+2}, and Ca^{+2}, so we used the lithium uptake rates for the other cations, and limited the extent to which these other ions adsorb to 1.5 mg/g (for Na and K) and 3 mg/g (for Mg and Ca).

RESULTS – FITTING MEASURED ADSORPTION AND DESORPTION DATA USING RIGOROUS APPROACH

Wang et al[ii] studied adsorption of metals from a heavy brine on their H_2TiO_3 media. Ion concentration for Ca^{+2}, Mg^{+2}, Na^+, K^+, and Li^+ in the brine, was reported as 55, 58, 1.6, 0.5, and 1.56 g/l, respectively. They reported maximum adsorption capacities for these metals on their material at pH 8.8 and 25 C, this data is presented in Table 1.

Table 1 - Estimation of the equivalent weight of the media based on the different cation adsorption capacity.

Cation	Reported adsorption capacity in mg/g	Reported adsorption capacity meq /g	% of sites accessible to cation	TiO3 eq wt g/eq
H^+ (stoichiometric)	20.43	20.43	100	**48.94**
Li^+ (all sites)	36.3	5.24	25.6	
Li^+ (site 1)		5.14	25.1	**194.6**
Li^+ (site 2)		0.10	0.50	
Na^+ (site 2)	1.93	0.08	0.40	
K^+ (site 2)	1.99	0.05	0.25	
Mg^{+2} (site 2)	2.58	0.21	1.0	
Ca^{+2} (site 2)	3.53	0.18	0.86	

Li^+, Na^+, K^+, Mg^{+2}, Ca^{+2} (site 2)		**0.62**	**2.51**	**1604**

We created two sets of adsorption reactions to accommodate the two reported adsorption sites (site 1 and site 2) for Li^+, H^+, Na^+, K^+, Mg^{+2}, and Ca^{+2}. The first reaction (site 1) adsorbs Li^+ and H^+. It has a capacity of 5.14 meq/g and a formula weight of 194.6 g/mol. The second reaction (site 2) adsorbs all cations and has a capacity of 0.62 meq/g and formula weight of 1604 g/mol. The chemical reactions created were:

$$HMedia(1) + \ Li^{+1} \overset{Q_s}{\leftrightarrow} LiMedia(1) + H^+$$

$$HMedia(2) + (\ Li^{+1}, K^{+1}, Na^{+1}) \overset{Q_s}{\leftrightarrow} (Li, K, Na)Media(2) + H^+$$

$$HMedia(2) + 0.5(Ca^{+2}, Mg^{+2}) \overset{Q_s}{\leftrightarrow} (Ca, Mg)_{0.5}Media(2) + H^+$$

We then fit the experimental data (symbols) using selectivity coefficients. The results are shown in Figure 2. There is good fit for lithium (left plot) and reasonable fit above pH 7 for the other metals (right plot). The right plot fits can be improved by modifying the surface interaction parameters.

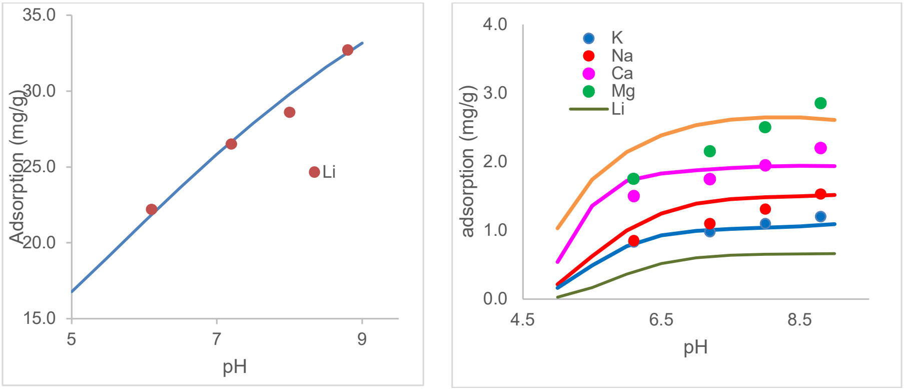

Figure 2 - Curve fitting Li, K, Na, Mg, and Ca adsorption on an HTiO3 media from a high concentration chloride brine

The computed selectivity coefficients (Q_s) for each metal were (log scale) -6.6, -4.4, -5.2, -6.8, and -6.8 for Li^+, Na^+, K^+, Mg^{+2}, and Ca^{+2}, respectively (before adjustment by activity coefficients). These values are based on the adsorption maximum values and the brine compositions reported by the authors. These selectivity coefficients are specific to the brine and the media. More intrinsic selectivity coefficients can be produced if the media is tested in simpler salt-water solutions like, NaCl-H_2O, KCl-H2O, $MgCl_2$-H_2O, and $CaCl_2$-H_2O.

We used the same parameters to simulate the adsorption data from Zhang et al[iii]. They produced a pure H_2TiO_3 and polyvinyl benzene treated H_2TiO_3, and studied lithium adsorption on that media. Figure 3 is a plot of the adsorption isotherm for the two materials. There is good agreement between the measurements and predictions for the pure H_2TiO_3 material but initially, poor agreement for the PVB-treated media. To compensate for this, we created a separate media, PVB-TiO_3. We calculated an equivalent weight for pure H_2TiO_3 media at 208 g/eq and for the PVB-TiO_3 media at 230 g/eq. The computed selectivity coefficients for the PVB-TiO_3 were (log scale) -6.8, -7.7, -6.9, -9.3, and -9.3 for Li^+, Na^+, K^+, Mg^{+2}, and Ca^{+2}, respectively (before adjustment by activity coefficients). Each of the metals are 1.1 log-unit lower than values shown above.

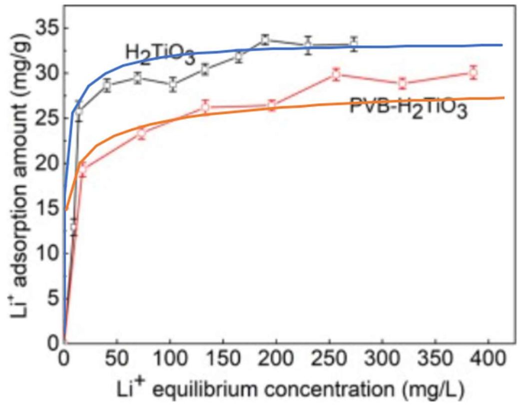

Figure 3 - Matching equilibrium sorption curve and capacity for a H_2TiO_3 and PVB-H_2TiO_3

Figure 4 is a plot of the calculated and measured adsorption vs. pH for the same materials. The model predicts lithium uptake quite well for the H_2TiO_3 media but not for the PVB-H_2TiO_3 media. It will be necessary to use different selectivity coefficients and equivalent weights for the commercial material as compared to the pure material.

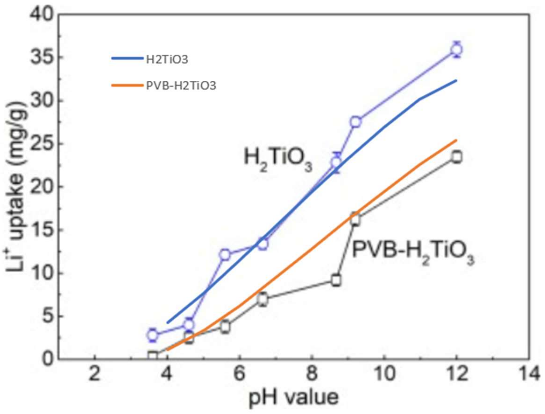

Figure 4 - Comparing simulated and reported uptake vs pH curves using parameters regressed for the equilibrium sorption curve

APPROACH TO SIMULATING THE DIRECT LITHIUM EXTRACTION PROCESS

Figure 5 is an image of the flow diagram used to simulate direct lithium extraction process with DLE media. The units represent a single contactor vessel undergoing four extraction process steps: lithium adsorption, brine rinsing, media regeneration with HCl, and a final rinse.

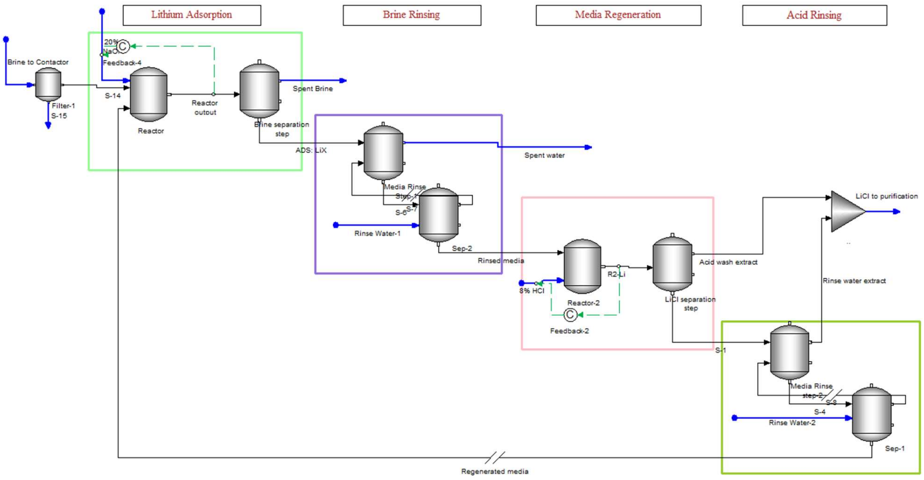

Figure 5 - Simulation flow diagram for testing the two DLE reaction approaches.

We simulated the lithium extraction process at 25 C and 1 atm using the above flow diagram with both the empirical and rigorous reaction methods. The following parameters were used for the modelling:

- Media mass / capacity reported in Table 1
- A generic Salton Sea brine composition (see below)
- Brine feed rate of 10 kg/min
- Lithium adsorption at pH 8 and controlled using 20% NaOH
- Lithium removal at pH 0.5 or 1 and controlled using 8% HCl
- Pure water at 5.5 g water/g media was used for rinsing brine off media
- Pure water at 2.5 g water/g media was used for rinsing acid off media to recover Li^+
- 10 wt% entrained liquid on the media at the start of each process step
- Filtered inorganic solids from the brine upstream of the extraction process

We then varied the following parameters:

- Brine to media mass ratio between 6 mg Li/g media (excess media) and 40 mg Li/g media (insufficient media). We expected to see a higher concentration of unwanted salts, Na, K, Mg, and Ca in the final extractant when using media in excess of lithium.

- Contact time for the adsorption and regeneration between 15 and 60 minutes (same value for each step). This is done for the empirical (kinetic) reactions only to study the impact on lithium uptake and on the final composition of the Li in the purification stream.

Figure 6 provides a visualization of the Na and Cl concentrations in the entrained liquid after each step. The jump in concentration following the regeneration is the Na release from the media and from the HCl added to release the lithium.

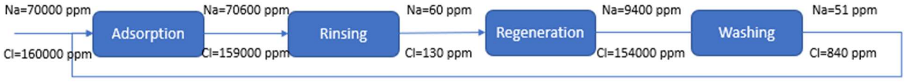

Figure 6 - impact of 10% entrainment on the sodium and chloride concentration in contact with the media through the four extraction steps

We used a generic Salton Sea brine in our simulation work. This brine has roughly half the ionic strength of the Wang et al brine, Table 2. The far-right column is the activity coefficient ratio between the generic Salton

Sea water and the Wang et al brine. It is based on the following equation, where Q' is the activity coefficient ratio. The equation is written reactants over products and the media phase is assumed to have unit activity:

$$Q' = \frac{\gamma_{M^{+z}}^{1/z} * \gamma_{H_2O}}{\gamma_{H_3O^+}}; \qquad ratio = \frac{Q'_{Salton\ Sea}}{Q'_{Wang\ et\ al\ brine}}$$

A ratio >1 indicates that metal adsorption from generic Salton Sea water is enhanced relative to the Wang et al brine. Lithium adsorption affinity is computed to be suppressed by 12% while Na^+, K^+, Mg^{+2}, and Ca^{+2} adsorption is computed to be enhanced, with K^+ adsorption enhanced by 7.2x. Uptake differences are further affected by the absolute metal concentrations in solution. Potassium concentrations for example are 17.6x greater in the generic Salton Sea brine. The effect of these differences is that the metal adsorption efficiency between the two brines will differ.

Table 2 - Comparison of the brines used to create the selectivity coefficients and to simulate lithium extraction.

	Brine composition (ppm)		Equivalent conc (eq/kg H_2O)		Activity coefficients (kg/mol)		Activity coefficient ratio
Ion	Wang et al	Generic Salton Sea	Wang et al	Generic Salton Sea	Wang et al	Generic Salton Sea	
H_2O	1000000	1000000	55.5	55.5	0.52	0.76	
H_3O^+	$3.0e^{-8}$	$1.9e^{-7}$	$1.6e^{-9}$	$1e^{-8}$	13.7	4.2	
Li^{+1}	1769	200	0.25	0.039	12.4	2.3	0.88
Na^{+1}	1814	70000	0.08	4.1	3	1.1	1.8
K^{+1}	567	10000	0.014	0.35	0.4	0.6	7.2
Mg^{+2}	67641	2000	5.6	0.22	28.6	1.5	1.3
Ca^{+2}	62583	20000	3.1	1.34	12	0.9	1.2
Sr^{+2}		650					
Ba^{+2}		100					
Fe^{+2}		20					
Cl^{-1}	319720	160000					
HCO_3^{-1}		15					
SO_4^{-2}		50					
BOH_3		1500					
SiO_2		10					
CO_2		50					
IS (m)	13.6	6.9					

RESULTS – SIMULATING EXTRACTION PROCESS USING EMPIRICAL REACTIONS

Table 3 contains the results for the empirical exchange simulation. The contact time is set to 30 minutes, the lithium to media mass ratio in the contactor is set to 20 mg/g. The adsorption step is set to pH 8, and the regeneration step is set to pH 0.5. The spent brine column contains the calculated lithium concentration of 71 mg/l. This represents 65% lithium capture. The simulated lithium concentration exiting to the purification process is 4872 mg/l and pH 1.9. Both values are after mixing the HCl extraction step with the pure water media washing step. The regenerated media is calculated to *still* contain lithium after the acid extraction. The final column shows that the regenerated media still contains 18.5 mg/g of lithium (50% of the available sites). This indicates that the HCl did not extract all the lithium. We suspect our kinetics may not be valid at very low pH's because there was no data to regress in this region.

Table 3 - Base case simulation using pH 8 in spent brine and pH 0.5 in LiCl to purification.

Species conc. (mg/l)	Feed Brine	Spent Brine	LiCl to purification	Regenerated media (mg/g)
Li^{+1}	200	73	4872	18.5
Na^{+1}	70000	70545	1250	<0.01
K^{+1}	10000	9943	230	<0.01
Mg^{+2}	2000	1981	124	<0.01
Ca^{+2}	20000	19836	484	<0.01
Ba^{+2}	100	35.5	<0.1	…
Cl^{-1}	159240	158971	26704	…
pH	5.1	8.0	2.0 (after rinsing)	…

Figure 7 is a plot of the lithium extraction efficiency as contact time and Li:Media loading vary. A minimum of 20 mg/g loading is required to achieve 75% removal efficiency. At this loading ratio, the contact time would be greater than 30 minutes. At 10 mg Li/g media loading, nearly 100% of the lithium is removed from the brine. This is not surprising, since at this loading only one in three of the available adsorption sites can be filled. This creates problems because the other ions are in excess and continue to adsorb on the sites that are available to them. The net effect is an enrichment of the impurities adsorbed relative to the lithium.

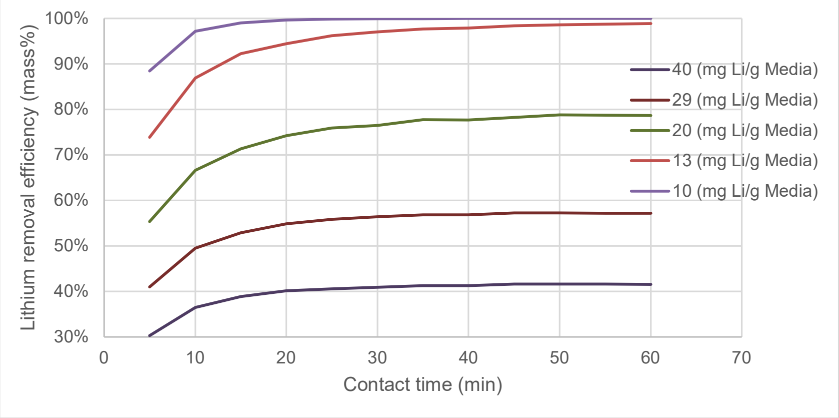

Figure 7 - Lithium extraction efficiency as a function of contact time and Li:Mg loading.

Figure 8 is a plot of the Li$^+$ concentration in the purification stream vs. contact time and Li:Media loading ratios. The lithium concentration increases with contact time for each of the Li:Media loading ratios except one. At the lowest ratio (10 mg Li/g Media), there is insufficient lithium remaining in the brine to occupy the available sites (above discussion). This has two effects, the first is that more HCl is needed to achieve the 0.5 pH, diluting the metals concentration in the purification stream. The second is that the impurities concentration in the purification stream increases relative to lithium. This is shown in Figure 9 where at low Li:Media loading ratio, there is a higher impurity:Li equivalent ratio in the purification stream. The increase is significant below the 20 mg Li$^+$/g media loading.

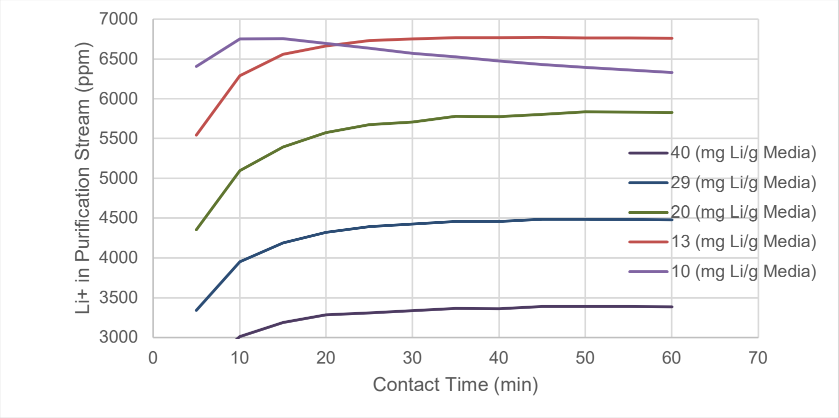

Figure 8 - Lithium concentration in the purification stream as a function of contact time in the extraction step and the Li:Media loading ratio.

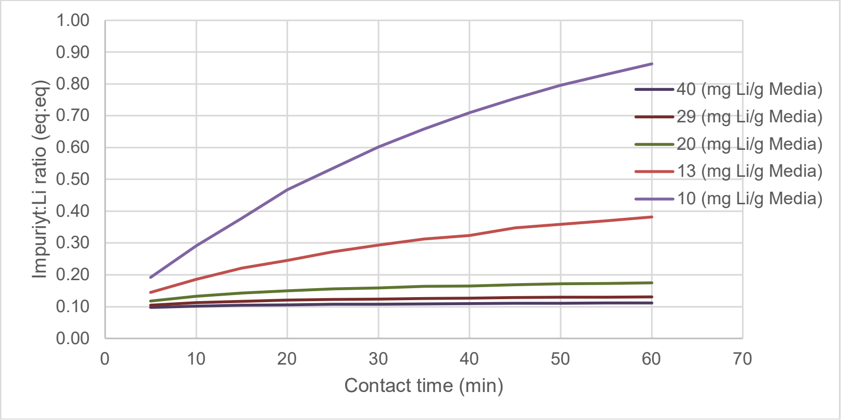

Figure 9 – The Impurity:Li ratio in the Purification stream as a function of contact time and Li:Media loading ratio

RESULTS – SIMULATING EXTRACTION-PROCESS USING RIGOROUS ION EXCHANGE

Table 4 contains the simulation results using the rigorous adsorption approach. The lithium loading is set to 20 mg Li/g media, the contactor pH for lithium extraction is set to pH 8, and the HCl recovery step set to pH 0.5. The software computes 15 ppm Li^+ remaining in the spent brine, which is approximately 93% recovery. The slightly higher Na^+ in the spent brine is from NaOH addition, and the lower cation concentration is from adsorption onto 10% of sites available to these ions. This simulation approach differs from the empirical approach in that reactions come to equilibrium.

Table 4 – Base case simulation using a Li/media load of 20 mg/g, a pH 8 for extracting lithium, and a pH 0.5 for removing the lithium.

Species conc. (mg/l)	Feed Brine	Spent Brine	LiCl to purification	Regenerated media (mg/g)
Li^{+1}	200	15	5094	1.3
Na^{+1}	70000	70270	2640	
K^{+1}	10000	9914	274	
Mg^{+2}	2000	19001	2409	
Ca^{+2}	20000	19790	13	
Ba^{+2}	100	0	0	
Cl^{-1}	159240	154977	38772	
pH	5.1	7.9	1.4 (after rinsing)	

Figure 10 is a plot of lithium concentration in the extracted purification and spent brine streams as a function of pH when the Li:Media loading is 20 mg/g. The pH where lithium is computed to be at its maximum concentration is 7.5. Above this pH, lithium concentration in the purification stream decreases. This is for three reasons; 1) the lower lithium concentration reduces the extent of the adsorption reaction; 2) the impurities continue to adsorb because they are not in limited concentrations; and 3) more HCl is used to bring the pH to 0.5, which dilutes the lithium in the purification stream.

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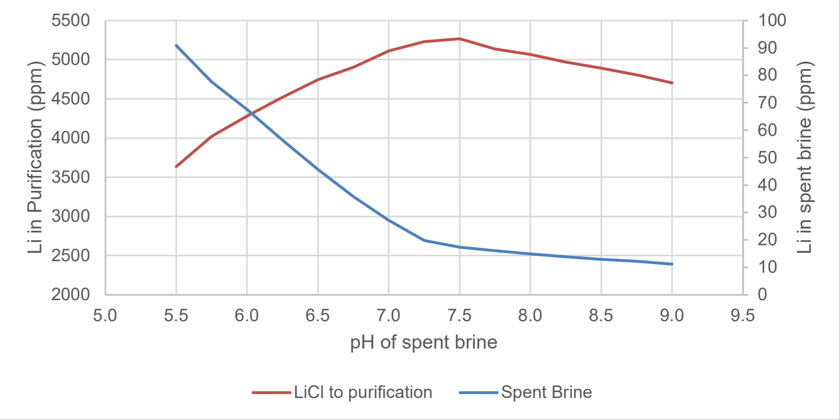

Figure 10 - Lithium concentration in *LiCl to purification* stream and spent brine as a function of target pH in the spent brine when the Li:Media loading is set to 20 mg/g.

Figure 11 is the computed lithium concentration in the *LiCl to purification* stream as the pH of the extraction step varies and as the Li:Media loading varies from 10 mg/g (excess media) to 40 mg/g (insufficient media). The highest Li^+ concentrations are computed to be at high Li:Media loadings and between pH 6.5 and 7. There is a marked decrease between the 27 and 20 mg/g loading at lower pH. At extraction above pH 7.5, there is no difference in loading effects above 20 mg/g.

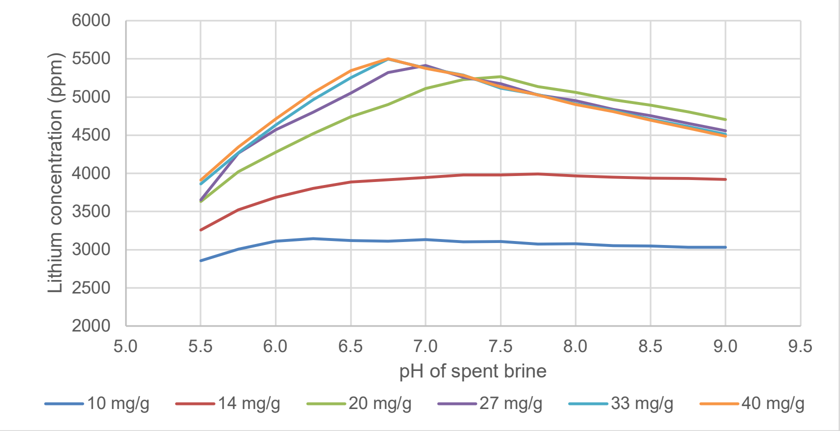

Figure 11 - Lithium concentration in purification stream as a function of spent brine pH and Li:Media loading

Figure 12 is a plot of the percentage of the feed brine Li^+ that is extracted. The 40 mg/g and 33 mg/g Li^+ loadings plateau above 6.7 pH, because the salinity effects on the Li^+ activity coefficient impacts overall adsorption. We will investigate this in future studies to determine the significance of ionic strength on lithium extraction. At loadings of 20 mg/g and lower, more than 90% of the Li^+ is computed to be extracted at pH 7.5 and higher.

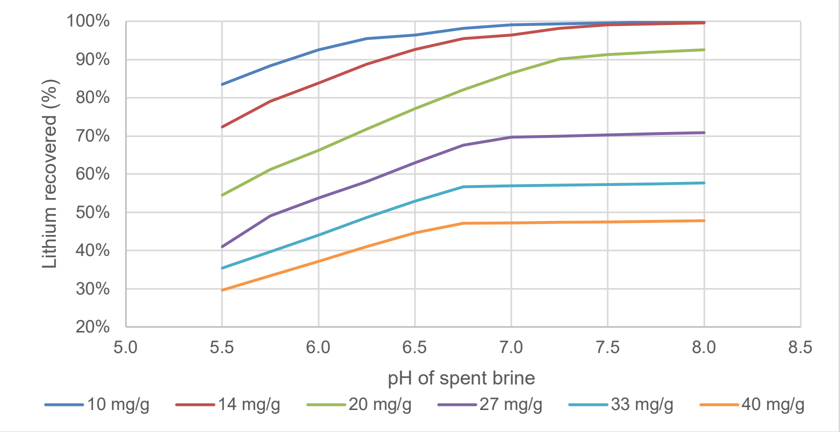

Figure 12 - Percent of lithium recovered from brine vs spent brine pH and Li:Media loading.

Figure 13 is the calculated impurity:Li ratio as a function of pH and Li:Media loading ratio. At low contactor pH, the impurity/Li ratio in the purification stream is low. The optimum ratio is calculated to be approximately 20 mg Li/g media loading. Below this ratio, there is insufficient lithium to extract to all available sites, but there are also additional sites for the impurities to adsorb. The worst-case scenario is the 10 mg/g loading. Compared to the 20 mg/g loading, there are twice as many sites for Na^+, K^+, Mg^{+2}, and Ca^{+2} to adsorb, and so their extraction is doubled. However, if we consider pH 7, there is only 15% additional lithium adsorbed when the loading is 10 mg/g vs 20 mg/g (Figure 12). Consequently, the impurity:Li ratio increases in the extraction.

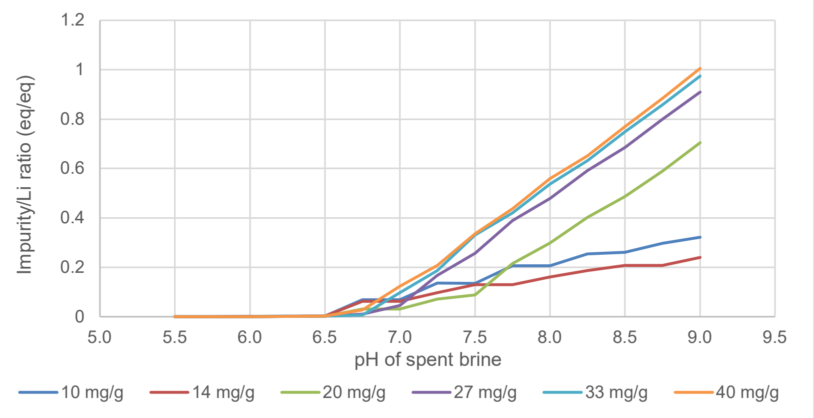

Figure 13 - Impurity:Li ratio in purification stream vs pH of spent brine and Li:Media loading

SUMMARY

We incorporated direct lithium extraction into a thermodynamic model to test whether it is feasible to simulate with precision the lithium extraction process. We used two modelling methods: empirical uptake and release calculations using proprietary media and kinetic reactions, and rigorous uptake and release using surface ion exchange reactions.

We can achieve reasonable curve fitting of laboratory uptake data using both approaches. We identified non-ideal adsorption vs. pH effects. This appeared in the kinetic and rigorous approach. These non-ideal adsorption behaviors should be resolved by using a more complex kinetic equation for the empirical approach and surface activity parameters for the rigorous approach. Both will be part of future work.

Finally, we used a process simulator to model the mass balance using the two uptake models (empirical and rigorous). We were able to predict in a semiquantitative way the impact of contact time, pH, and media reuse (recycle) on overall process performance. Future work will focus on using more complex kinetic equations in the process simulation.

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[i] Private communication

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