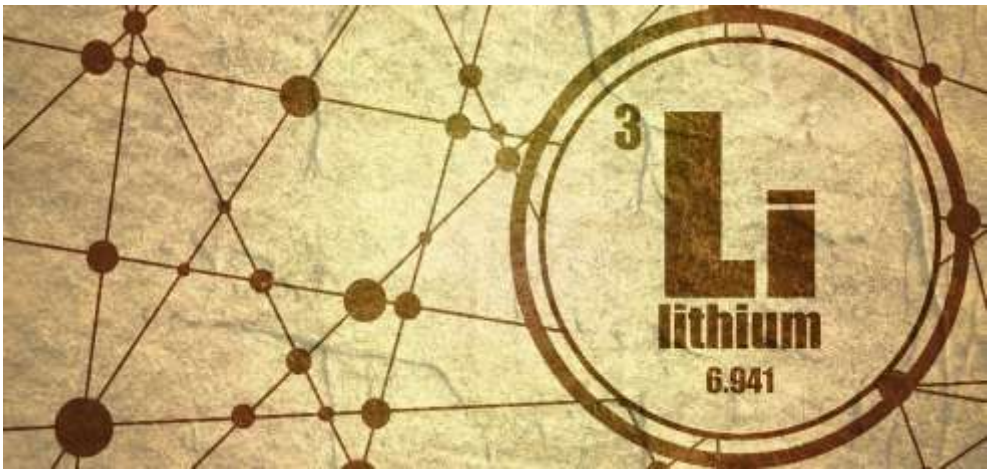
OLI systems, inc.

think simulation | getting the chemistry right



Breakthrough chemistry simulations for lithium processing

Using simulation to maximize your investment return in lithium extraction and processing

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Updated to V10 chemistry, February 2020

Introduction

Photo taken at the edge of the largest salt plain in the world, the Salar the Uyuni, in the Bolivian Andes.

The worldwide demand for lithium is expected to increase over tenfold in the next decade. This creates significant opportunities for the lithium industry, as companies race to get production to market. Traditional lithium extraction from ores, or evaporation from Andean salars have been the basis for most production schemes. Profitability comes from improving on methods to increase yield, purity, or to drive down costs. As with other industries, improved process design using mathematics and chemistry principles is one way to gain this profitability edge.

Process simulation deficiencies

Process simulation of lithium production has historically addressed some, but not all aspects of optimization. What has been lacking is the rigorous chemistry that is critical to compute true mass, chemistry, and energy balance within the process. This includes accurate solubility characterization, effects of high salinity, temperature, and acidity, and lastly the prediction of complex double/triple-salts. These missing features have made true simulation out of reach of all major flowsheet tools. Consequently, the industry has relied on "bucket chemistry," or empirical approaches that roughly and imprecisely characterize the behavior of lithium processes.

OLI Systems electrolyte thermodynamics

OLI Systems, Inc., a global electrolyte chemical technology leader for nearly five decades, is uniquely positioned to move beyond bucket chemistry for lithium processing. OLI can supply the missing mission-critical aspect of rigorous chemistry simulation.

OLI Systems has a proven framework for predicting the properties and solubilities of ore and salar processing, from the kiln outlet and high saline brines to carbonate purification. OLI also has the most complete modeling tool that integrates solid-phase properties to the electrolyte solution from which the form.

Bottom line: OLI Systems' framework is sufficiently robust and extendible to deliver an accurate simulation of your lithium production process.

OLI Systems' lithium initiative

OLI Systems began its lithium (and potash) initiative in 2012. We understood quickly that a comprehensive research effort was required to model accurately, such a complex system - Li-Mg-Na-K-Ca-SO_4-CO_3-Cl-OH. This research work took several years to pursue and required a team of thermodynamicists to develop the required parameters. The outcome is a series of phased-in model predictions.

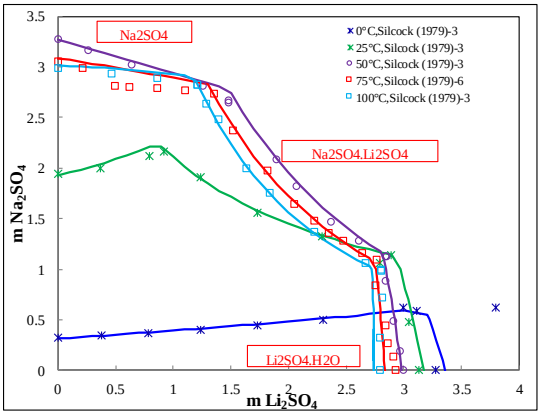
Lithium phase 1 and potash chemistry is complete

As of 2019 with the release of OLI V10, a major subset of OLI Systems' lithium chemistry initiative is complete. OLI's simulation capabilities include:

Fundamental sulfate – chloride systems

Binary systems:

- Lithium sulfate: $Li_2SO_4 – H_2O$
- Lithium chloride: $LiCl – H_2O$



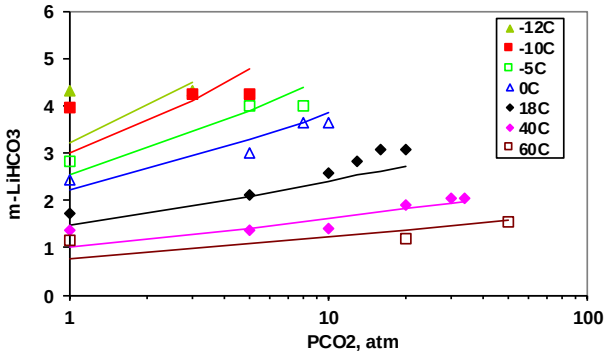
Ternary and quaternary systems:

- Lithium & potassium sulfates: $Li_2SO_4 – K_2SO_4 – H_2O$
- Lithium & potassium chlorides: $LiCl – KCl – H_2O$
- Lithium, sodium & potassium sulfates: $Li_2SO_4 – Na_2SO_4 – K_2SO_4 – H_2O$
- Lithium & sodium chlorides: $LiCl – NaCl – H_2O$
- Lithium & magnesium sulfates: $LiCl – MgSO_4 – H_2O$
- Lithium & magnesium chlorides: $LiCl – MgCl_2 – H_2O$
- Lithium & calcium sulfates: $Li_2SO_4 – CaSO_4 – H_2O$
- Lithium & calcium chlorides: $LiCl – CaCl_2 – H_2O$
- Lithium sulfate & chloride: $Li_2SO_4 – LiCl – H_2O$
- Mixed $Li – Mg – SO_4 – Cl – H_2O$ system
- Mixed $Li – Ca – SO_4 – Cl – H_2O$ system

Fundamental hydroxide and carbonate systems

Binary systems:

- Lithium hydroxide: $LiOH – H_2O$
- Lithium carbonate: $Li_2CO_3 – H_2O$



Ternary systems:

- Lithium carbonate & hydroxide: $Li_2CO_3 – LiOH – H_2O$
- Lithium & sodium carbonate: $Li_2CO_3 – Na_2CO_3 - H_2O$
- Lithium carbonate & chloride: $Li_2CO_3 – LiCl - H_2O$
- Lithium carbonate & carbon dioxide: $Li_2CO_3 – CO_2 – H_2O$
- Lithium chloride & carbon dioxide: $LiCl – CO_2 – H_2O$
- Mixed $Li – Na – CO_3 – Cl$ system

Lithium in acid environments for processing and recycling

Ternary systems:

- Lithium chloride & hydrochloric acid: $LiCl – HCl – H_2O$
- Lithium sulfate & sulfuric acid: $Li_2SO_4 – H_2SO_4 – H_2O$

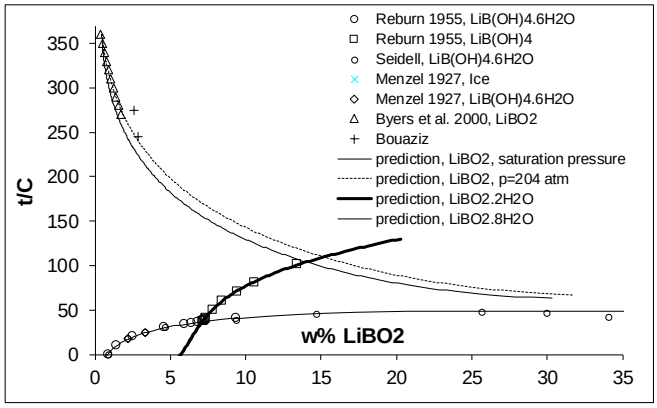
Lithium borate systems for Li production:

Binary systems:

- Lithium metaborate: $LiBO_2 – H_2O$
- Lithium borate: $Li_2B_4O_7 – H_2O$
- $LiB_5O_8{\cdot}5H_2O$: $LiB_5O_8{\cdot}5H_2O – H_2O$

Ternary systems:

- Lithium hydroxide & various lithium borate species
- Li borates, lithium chloride, sodium chloride
- Lithium chloride & H_3BO_3



Systems related to Li hydrometallurgical processing, purification and recycling

Binary systems:

- Lithium fluoride: $LiF – H_2O$

Ternary systems:

- Lithium & nickel sulfates: $Li_2SO_4 – NiSO_4 – H_2O$
- Lithium & cobalt sulfates: $Li_2SO_4 – CoSO_4 – H_2O$
- Lithium & cobalt chlorides: $LiCl – CoCl_2 – H_2O$
- Lithium & zinc chlorides: $LiCl – ZnCl_2 – H_2O$
- Lithium & ammonium sulfates: $Li_2SO_4 – (NH_4)_2SO_4 – H_2O$
- Silica & lithium chloride: $SiO_{2(am)} – LiCl – H_2O$
- Lithium chloride and methanol, ethanol, formic acid

Li nitrate systems for caliche sources and thermal energy storage systems

Binary systems:

- Lithium nitrate: $LiNO_3 – H_2O$

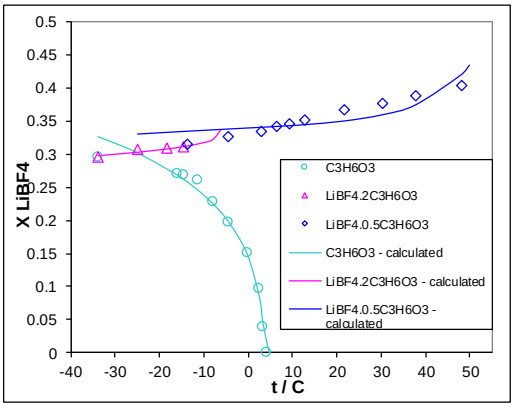
Ternary systems:

- Lithium & sodium nitrates: $LiNO_3 – NaNO_3 – H_2O$
- Lithium & magnesium nitrates: $LiNO_3 – Mg(NO_3)_2 – H_2O$
- Lithium & calcium nitrates: $LiNO_3 – Ca(NO_3)_2 – H_2O$

Systems related to battery electrolytes

Solutes include:

- Lithium hexafluorophosphate $LiPF_6$
- Lithium tetrafluoroborate $LiBF_4$
- Lithium perchlorate $LiClO_4$

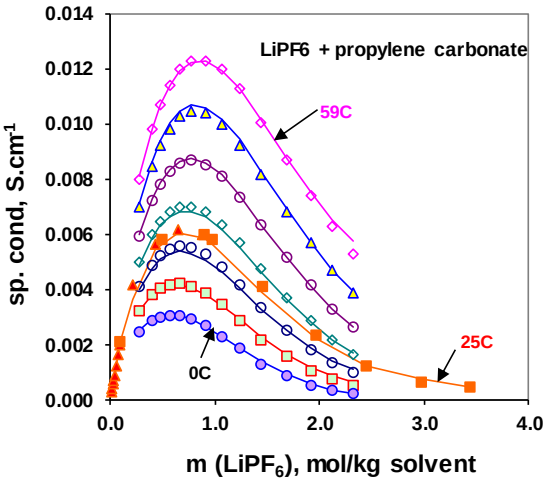


Solvents include selected pure and mixed carbonates

- Dimethylcarbonate
- Diethylcarbonate
- Ethylenecarbonate
- Propylenecarbonate

Electrical conductivity

The OLI Systems framework also has the ability to model transport properties. Here is an example of the electrical conductivity of lithium hexafluorophosphate and propylene carbonate. The model is predictive and built in this case on underlying experimental data.



Battery simulation studies

Why is electrical conductivity important in battery studies?

A battery electrolyte should have sufficiently high electrical conductivity and should remain thermodynamically stable in the liquid phase over a wide temperature range. This can be achieved by creating appropriate formulations containing a lithium salt such as $LiPF_6$ and highly polar organic solvents such as various alkyl carbonates.

OLI System's MSE model makes it possible to predict the electrical conductivity and phase equilibria in such mixtures, thus helping to optimize the composition of the battery electrolyte. The model is calibrated by reproducing selected experimental data in binary systems within their experimental uncertainty (as shown in the diagrams on the right-hand side) and then it can predict the behavior of more complex battery systems. Consider for a moment the sophistication required for a software to predict such systems!

Capability in the OLI software platform

With the release of OLI V10.0, a major subset of OLI Systems' lithium chemistry initiative is complete. It includes over sixty Li-containing phases and species as shown in the following matrix. Among the Li-only containing species are double salts with K, Mg, Ca and others. This allows phases like LiKSO4 (in salars) and LiAl(SiO3)2 (spodumene) to be modeled properly in the overall plant operations.

Table 1 - Matrix of Li-containing species (solid and aqueous) in the V10 database.
The values in each box represent the number of species present with that set of elements.

	Li-only	Li-K & Li-Na-K	Li-Mg & Li-Ca	Li-Na-Al	Li-F	Li-Co & Li-Al
SiO2	4					3
B, B(OH)3	9				3	
NO3 / NO2	3					
AsO4	1					
Alcohol / Org Acid	10					
CrO4 / MoO4	2					
CO3/SO4	6	4	2	1		
OH/Cl/Br/F/I	12		5			1

Other studies OLI Systems' simulation enables

The implementation of the complete lithium chemistry system provides engineers with the ability to design more efficient processes, and to predict better than ever before, the yield and purity of their products. Measurable quantities like pH, conductivity, concentrations, and TDS, now are firmly rooted in a fundamental physico-chemical basis.

To assist clients in deploying this data, OLI Systems' simulation packages include:

- OLI Studio where clients can use the survey capability to calculate the effect of evaporation or leaching on lithium processes.
- OLI Flowsheet: ESP where clients can design entire processes, such as an evaporation pond process
- OLI Engine in <Alliance Partner Products> where clients can use OLI in an existing Alliance Partner flowsheet to obtain rigorous chemistry analysis of process streams

Looking ahead: partnering with OLI Systems to extend the lithium chemistry initiative

More remains to be done. As we move into the lithium-based transportation economy, all sources of lithium ore (clays, recyclables, etc.) are potentially cost-competitive alternatives. To make such alternatives feasible, OLI will be available as a resource to provide a deeper understanding of these chemistries.

We have plans to pursue this chemistry further, and we are seeking industry partners to help steer and specify this work. A one-time investment can reap years of benefit, and using the OLI framework as a proven delivery vehicle is a low-risk investment. You have the assurance that OLI will work with you to "get the chemistry right." And, there is no other simulation company who is positioned to extend this work.

Partnering with OLI can increase your competitive edge and bring your process ideas early to market. You can selectively help us co-fund chemistry that is mission-critical to your operation. As an additional feature, the selected graphs in this technical brief are part of OLI's validation spreadsheet system which will be open for the lithium chemistry only to OLI's lithium chemistry initiative partners.

Some of the possible chemistries that we will be tackling include:

- Remaining borate chemistry
  to completely model the behavior of borates in brines associated with Li production; this will be based on recent experimental data obtained at the University of Guelph; this work is currently under way
- Chemistry required for modeling lithium recycling processes
  to augment the database with parameters for hydrometallurgical systems that include various transition metals (e.g., the components of lithium batteries) as well as lithium
- Chemistry required for modeling lithium-based working fluids
  lithium with bromides, molybdates, etc.

Take action now!

To find out more about how your business can gain the intelligence you need in understanding your lithium processes through accessing the OLI software, or to find out how to partner with OLI on the lithium chemistry initiative, please contact us at sales@olisystems.com and mention this technical brief to arrange a free Application Assessment for your lithium chemistry challenges.

For more Information

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