OLI Technical Differentiators

TARGET APPLICATION: LITHIUM MINING SIMULATIONS

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Key lithium mining techniques

Extracting lithium from each source - saline lakes (salars), lithium-bearing minerals, lithium-bearing clays, recycled batteries, oilfield produced water, hydrothermal deposits, and seawater - employs a different chemical process. Understanding the chemical mechanisms of each process enables efficient and sustainable production and enables engineers to maximize yields while lowering operations costs and maintaining environmental compliance.

Lithium is extracted from salt brines in a two-step process. First the brine is evaporated to raise the lithium concentration and to precipitate unwanted salts like NaCl, $CaSO_4$, and KCl. Lithium is then extracted from the bittern by one of several chemically-intensive processes.

Lithium from silicate ore follows a multi-step extraction procedure. The Li-bearing minerals, spodumene, petalite, or lepidolite are removed from the rock by sorting or other separation process. This ore is then roasted to change the crystal structure, making it more susceptible to acid leaching. Then an acid solution extracts the lithium, and this pregnant leach is sent through a series of chemical washing and separation steps to concentrate the lithium and removing impurities.

Lithium from waste materials like batteries follows yet another set of extraction procedures. Metals are leached from the waste using a strong acid. Following this step, transition metals (Cd, Ni, Mn, and whatever else it contains) are separated. The lithium is then purified with chemical precipitation.

Importance of electrolyte science to optimize the design and operation of lithium mining processes

Lithium extraction from salt basins is a wholly electrolyte-based process. In fact, because of the high concentrations and because there are many different elements in the water (multicomponent), it is next to impossible to perform an accurate mass balance of the process without a rigorous model. Evaporation does not form simple salts like NaCl or KCl. In fact, double and even triple salts precipitate as concentrations increase. Thus, the pond overflow composition will differ from any composition estimated using a basic water chemistry program.

The principle science behind lithium extraction in any of the above forms is understanding the properties of these very concentrated electrolyte solutions. Salar brines have salinities in the hundreds of thousands of mg/l and extracting lithium from batteries creates a black mass that does not resemble any normal liquid phase. Perhaps the only fluid that is recognizable as a normal water is the pregnant leach extracted from the silicate rock. That fluid still needs to flow through a series of reaction and separation processes before it is purified. Thus, without critical understanding of this science, designing and operating processes must rely on heuristics and past experience to produce optimal results.

Producing lithium from saline brines is time consuming, complicated, and highly dependent on the climate and the weather in the region of the brine deposit. Factors like evaporation rate, lithium grade, by-products produced, and purity levels impact the speed, cost, and product yield. This makes accurate simulation and modeling critical to maximizing production yields and lowering costs. By-products like potassium can be sold to increase profits while separating impurities from lithium is the most expensive part of the brine refinement process.

Unique elements of OLI Systems technology

The mathematical behavior of electrolytes is challenging. Composition changes, hydrate formation, and phase transformation can lead to solution properties that are not easily predicted and often counterintuitive.

Accurate modeling of lithium processing therefore requires an accurate knowledge of phase equilibria and speciation in multicomponent aqueous and organic systems. OLI's unique MSE thermodynamic model contains an accurate treatment of mixtures containing lithium with important anions (sulfates, chlorides, borates, nitrates, hydroxides, carbonates, etc.) and cations (sodium, potassium, calcium, magnesium, ammonium, nickel, cobalt etc.). In many cases the phase behavior is complex or even counterintuitive. Such behavior can be accurately predicted by MSE. In addition to the chemistries mentioned above, lithium and cobalt phosphate chemistry is under development and will be included in the next version of the software.

Deep expertise in solution chemistry

A key technology element is modeling *solution chemistry*, i.e., the ability to predict the properties of the water and the salts it contains. When we developed the salar database, we include the solubilities of twenty-seven important salts that can play a part in salar evaporation. We also harness our capabilities in ion exchange, adsorption, and solvent extraction to help clients develop more environmental-friendly and more cost-effective processes.

A unified framework

We suggest a unified OLI solution for all your electrolyte design and production work - to be the primary/only property package used in every software tool for any type of aqueous chemistry situation. This will result in greater consistency across the various technology teams, and represent the single source of thermodynamics that, when necessary, can be modified as needed. This is what will be possible when working with an expandable framework that could address any chemistry, and even include your own nonelectrolyte (hydrocarbon) equation of state if desirable.

The cornerstone of lithium extraction modeling and simulation

The Mixed-Solvent-Electrolyte (MSE) thermodynamic framework is the foundation model. The Li chemistry enables accurate model predictions under a broad range of conditions. New properties can be added to this database as a development project as required.

Furthermore, the framework can be extended to incorporate other mechanisms including solvent extraction, ion exchange and related phenomena. It can also be used to simulate the use, reuse and discharge of mining water as well as to manage the reliability of operating units like cooling towers and heat exchangers.

Thus, a single, unified mathematical model can be used for all processes including the core extraction and purification as well as ancillary operations such as water treatment and equipment reliability.

Selected processes that benefit from this unified framework unique to OLI

Lithium evaporation from brines

OLI technology enables

- Accurately predict lithium speciation during evaporation to increase yields √
- Extract **'high purity'** lithium, boron, and potassium salts – leading to higher grade products that command a price premium. √

Lithium extraction / separation from brines

OLI technology enables

- Simulate lithium **adsorption** over a broad range of compositions, extractant materials and operating conditions (flow rate, temperature, adsorbent type, extraction process) √
- Simulate **solvent extraction** over a broad range of compositions, solvents, and extractants (when the material is selected for addition into the database) √
    - Currently all predictions are based on experimental data. The simulation capability unique to OLI dramatically lowers costs, increases productivity and speed to market.

Lithium extraction from pegmatite ores

OLI technology enables

- Calculate the lithium extracted from the ore **and separation from impurities** (Mg, Ca, etc.).
- Optimize water treatment plant to maximize chemical and water recovery and to minimize treatment chemical addition.

Battery recycling

OLI technology enables

- Enhance lithium and high value metals yield from battery waste √
- Develop a unified and standardized metals recovery (and recycling, if appropriate) process that spans lithium ion and lead acid batteries

Regeneration of Extracting Materials

OLI technology enables

- Increase utilization of resins/ ion sieves and adsorbents to reducing processing costs √
- Enhance recovery of extractant materials to improve operational efficiency √

Materials Selection

OLI technology enables

- Optimize performance, cost and risk with materials selection using accurate simulations.

Plant equipment/ Asset Integrity

OLI technology enables

- Accurately predict acid corrosion and localized corrosion (H_2SO_4, HCl, HNO_3, H_3PO_4, sulfide corrosivity) to mitigate risk of unplanned downtime √
- Predict mineral scaling to improve operational efficiency of cooling towers and heat exchangers √

Water and wastewater treatment

OLI technology enables

- Enhance use, reuse, and discharge of mining water
- Remove contaminants that limit the usability/reuse of water √

√ OLI unique features not available in most other simulators and chemistry packages!

Implications of not having access to the OLI Capabilities

Without the OLI technology these calculations cannot be performed satisfactorily:

- Heats of reactions between ore and leaching/digesting chemicals (acids and bases)
  - Complex reactions that cannot be simulated with a simple simulator; lower yields, and higher costs

- Acid gas generation from kiln operations - these acids (SO_2, SO_3, HCl) require downstream scrubbing, including the proper scrubbing solution flow rate and materials of construction.
  - Elevated corrosion risk and reduced asset reliability.

- The leaching/digesting process releases metals from ore minerals other than spodumene. Feldspars, micas, quartz, amphiboles, etc. release metals during the strong acid or base processing. These metals in turn, impact chemical treatment downstream and impact final product purity
  - Less efficient purification process; increased costs

- Chemical hardness (Ca, Mg), transition metals, and silica removal are heavily dependent on chemical addition. Optimizing this operation can be done only with the use of a rigorous chemistry simulation
  - Higher chemical treatment costs; more expensive purification process.

- Element like boron, tantalum, rare earths, etc., that are present in the ore can provide a secondary revenue stream. These elements can be harvested once the plant chemistry is designed to isolate and purify these materials
  - Reduced revenue from sale of secondary products like tantalum

- Plant optimization including reducing chemical consumption, sludge production, and increased Li_2CO_3 (or LiOH) purity can be accomplished more predictively when a rigorous chemistry calculation tool is included
  - Reduced operational efficiency and higher operations costs.

Selected key chemical mechanisms √

Now available through OLI research or through past sponsored research projects

- Solution chemistry and solubilities √
- Acid leaching
- Evaporation and crystallization
- Solvent extraction √
- Surface complexation and ion exchange √
- Thermophysical properties prediction
- Thermodynamic database of toxic contaminants; removal of arsenic, selenium, mercury, etc. and their reactivity √
- Reverse osmosis (RO) √
- Transport properties and surface tension prediction √
- Mineral scaling prediction √

- General and localized corrosion prediction for *carbon steel, nickel-base alloys, stainless steels, duplex alloys, Cu-Ni alloys, and pure Cu, Ni, and Al* √

√ OLI value-added and differentiated capabilities

Professional services

- Access to experienced OLI mining industry consultants *(with Silver, Gold, Platinum service)*
- Access to corrosion engineers and scientists to extend the corrosion model
- Access to thermophysical modelers to extend the chemistry into other scavengers, polymers, etc.
- All levels of standardized and customized training onsite or via web
- Expert setup and interpretation services
- Best practices advice based on process simulation and design experience with commercial clients

… Where would you be without OLI technology?

- Lower yields and higher production costs
- Inefficient, higher cost purification process
- Reduced revenue streams from sale of secondary by-products
- Higher risk of catastrophic equipment failure due to scaling, corrosion
- Higher experimental costs
- Lower staff productivity
- Increased regulatory risk from inability to treat, manage and reuse water, wastewater
- Increased risk of making poor engineering decisions
- Lower engineering productivity due to inconsistent models
- Lack of insight to chemical processes
- Increased gap in knowledge in how to address water chemistry challenge