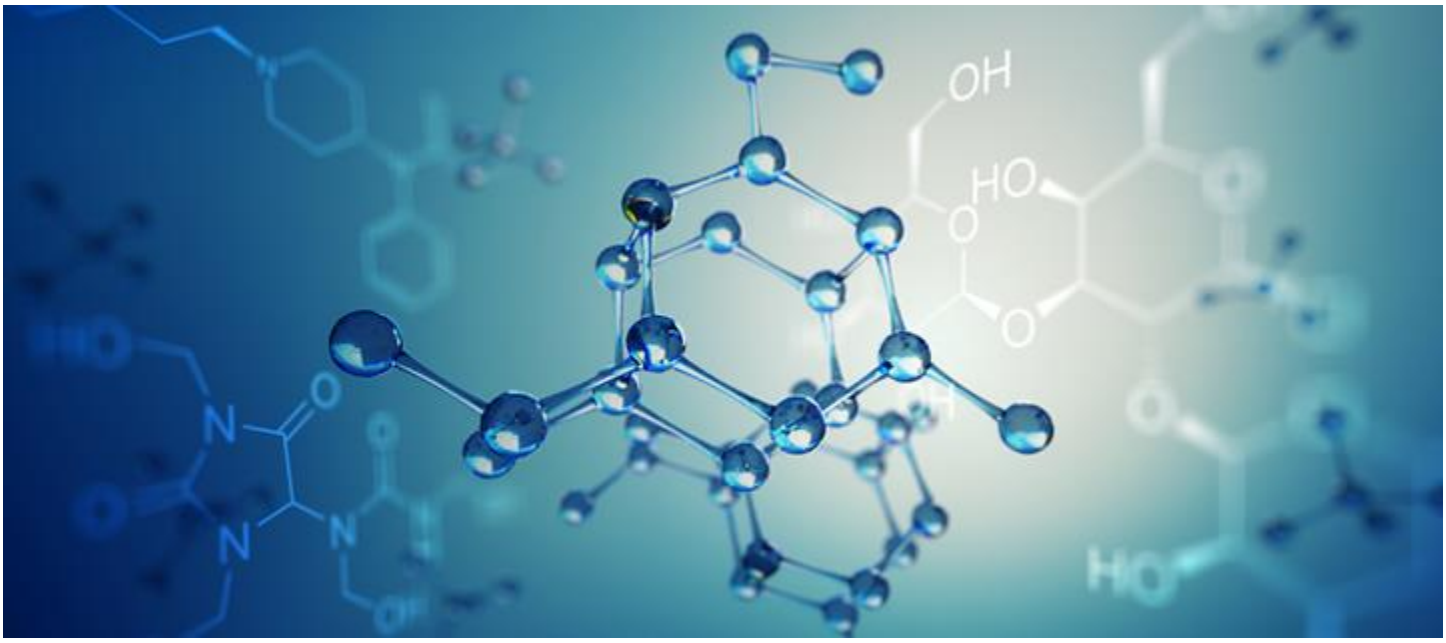
think simulation | getting the chemistry right



Transforming electrolyte chemistry modeling applications

Pioneer the future of water chemistry with rigorous chemistry analysis

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TECHNICAL BRIEF

Introduction

The chemical engineering landscape is undergoing major shifts that are challenging companies to evolve their approach to technology, chemistry, and mathematics. With the development of new advances—such as the Internet of Things (IoT), process modeling and simulation software, advanced analytics, and more—the industry is realizing greater performance, yields, cost-efficiencies, and more widespread applications including faster time to market. Today's companies must capitalize on these advancements to promote strategic growth, respond rapidly to market needs and to streamline operations.

Pursuing digital transformation empowers companies to hone their business strategies, from design optimization to production. This not only prepares them to satisfy evolving trends, but it also allows them to find new ways to significantly reduce CAPEX and OPEX by adopting the right tools and capabilities. Digital transformation is key to harnessing the full power of chemistry data, enabling more comprehensive insights for descriptive and prescriptive outcomes to fuel growth and success. As a result, savvy companies are investing in new, effective innovations in order to enhance process automation as well as their capacity to collect and analyze data and operationalize insights gleaned from the data.

Chemical engineers work to understand chemical properties under a range of conditions in order to produce and transform materials, and design, simulate, and optimize their processes. Water is one of the most versatile chemicals on the planet impacting almost all process industries—from Metals & Mining and Oil & Gas to Nuclear Energy. Water used in industrial processes and waste water produced must be treated and carefully disposed of to avoid harmful effects like scaling, corrosion, and pollution. The challenge is, water is a highly reactive electrolyte, and its unique chemical properties make it incredibly complex for engineers to analyze and predict. The market's current simulation software for water treatment lacks the rigor and accuracy required to safely and successfully manage water in industrial processes. Digital transformation is critical for engineers to capitalize on the full power of simulation software, enabling them to study the volatile behavior of electrolytes and achieve accurate water chemistry insights to fuel ongoing innovation and ensure competitive advantage.

The drive to market leadership

A strong technology base in conjunction with a unique framework is putting OLI Systems, Inc. at the forefront of water chemistry expertise. OLI is working to increase the speed and consistency of electrolyte simulation and to change the way the industry approaches chemical applications. Its rigorous, first-principles approach lets clients screen vast quantities of data to pinpoint critical and potential issues and achieve desired results, equipping them with the right chemistry to transform their operations. This exclusive approach helps clients improve decision-making and effectiveness to realize the best course of action for any given situation.

OLI is preparing clients to tackle their most complex water chemistry challenges with a combination of industry-leading thermodynamic frameworks, data parameters, and software innovations. These three vital components make up the OLI Engine:

- OLI's revolutionary electrolyte thermodynamic framework. The framework contains thermodynamic equations that explore water chemistry properties, enhance phase prediction, and accurately model any chemistry in water. The framework supports a range of diverse chemistries, using binary (one compound and water) and ternary (two compounds and water) systems. Based on the set of equations, OLI supports three distinct thermodynamic models including the Mixed Solvent Electrolyte (MSE) model, MSE-SRK model, and Aqueous model.
- The OLI Data Bank. This is an ever-evolving library of species, phases, and chemical reactions managed by a team of OLI thermodynamicists. Data is expertly compiled from troves of literature citations and experimental data, to develop the parameters that expand the range—temperature, pressure, and composition—of the software prediction. Parameters include coefficients for an equation of state, used to describe the behavior of a system at a reference, or an ideal state, and then activity coefficients that describe the ion-ion interactions in a system.
- Mathematical convergence techniques. OLI has developed numerical algorithms and convergence techniques that can solve highly complex and non-linear equations. As the chemistry changes, the math itself changes, making the mathematical behavior of electrolyte chemistry unique and challenging. This aspect of the OLI Engine is in fact essential when attempting to simulate the multi-phase behavior of electrolyte systems.

Together, these components are transforming how engineers approach water chemistry processes. With advanced software, data, and algorithms, the OLI Engine provides the most precise and comprehensive answers to the industry's most demanding issues. OLI

clients have the game-changing opportunity to predict thermodynamic variables and to model the behavior of virtually any combination of chemicals in water. And now, OLI's unique approach to electrolyte science is spearheading the science into areas of simulation that, as recently as ten years ago, would have been considered impossible to do.

OLI solutions are unlike anything on the market, with the capacity to predict the properties of so many electrolyte-based processes. While most of the market operates on interpolative models with a limited number of data points, OLI employs a predictive model to calculate outside the range of known values. Moving forward, OLI's vision is to apply advanced analytics across the entire periodic table—leveraging chemical data, modeling software tools, and intelligent analytics to enact the power of prescriptive insight. Although this is a massive undertaking, OLI is already well-positioned to cross a range of applications in a variety of industries and locations—from nuclear power plants in France to the salt flats in Bolivia. The ability to think and compute beyond the empirical data is a key differentiator that is helping OLI and their clients achieve market leadership. Whether clients require updates every 10 seconds, 15 minutes, or hour, OLI provides rigorous chemistry analysis with near-time results to uncover progressions of change. By automating these processes, clients can benefit from faster, more accurate outcomes to help them operate efficiently and cost-effectively.

Today, automated processes are rapidly exceeding the performance capabilities of human beings; thus, as chemical data collection and analysis become increasingly streamlined, OLI plans to leverage transformative methods like IoT analytics, cloud computing, and machine learning to revolutionize chemistry modeling with greater simplicity and accuracy. For example, OLI software can be used to evaluate the scale tendency of a water sample; the client could then manage an app that notifies them when the scaling tendency begins to reach saturation. In the future, OLI will utilize machine learning tools to analyze vast quantities of IoT data to deliver predictive and even preventive insights in real-time. The possibilities for chemistry modeling applications are endless, and OLI is pioneering the journey.

Virtual research & development

Research and development (R&D) is a lengthy and resource-consuming process for companies across all industries. Even in lab environments, having a generous budget does not necessarily ensure quick or accurate outcomes. The problem is that many companies lack a simple way to target lab experiments.

OLI is equipping today's scientists and engineers with virtual R&D capabilities, helping them to simulate experiments to lower the costs and time required for physical testing. In addition to streamlining experiments, virtual R&D software also enables companies to determine the exact experiment that must be run and guides lab technicians in choosing the correct configurations, which dramatically reduces lab work. This technology allows even technicians with limited training to perform the right experiment, and to derive virtual insights to understand what's happening in the real world.

OLI will consult with companies to virtualize a number of tests, including autoclave experiments, to achieve desired products. By virtualizing R&D efforts in lab environments, OLI will help to increase the purity and yields of industrial processes as well as properly configure experiments to explore thermodynamic activity, prevent overdesign, cut preparation time and operating costs, and accelerate time to insight.

Process simulation

Optimizing resource consumption and reuse is a crucial mission for today's companies. As valuable materials grow progressively scarce, the ability to reduce consumption and improve a resource's usability becomes crucial to success.

Fresh water is one essential resource that is quickly reaching scarcity. Higher-income countries treat 70 percent of their wastewater while middle-income countries treat only 38 percent, and lower-income countries focus even less on water reclamation, treating 28 percent. By 2030, half of the global population will face water scarcity. In an effort to conserve this precious commodity, companies must strive to reuse water multiple times before disposing it as wastewater. Water engineers recognize this trend and are investigating the options of reusing this resource through some simulation work as well as through laboratory and pilot-plant testing.

While this foray into simulation is an important step in water conservation, the use of simple chemistry models, that is, empirical (or fixed) formulas and simplified equations, can significantly handicap water chemistry simulation success and reliability. As a result, companies are seeking a new breed of simulation capabilities to perform chemistry analysis and limit the use of fresh water.

OLI is driving the performance of water engineering with the OLI Flowsheet: ESP, a revolutionary software that delivers electrolyte flowsheet simulation. Process simulation enables engineers to uncover new options for maximizing the use of water and other resources. With OLI Flowsheet: ESP, companies can model a variety of systems to determine what happens to water at various pH levels, temperatures, pressures, ion concentrations, and many other variables.

OLI Flowsheet: ESP features a membrane unit. The unit uses first-principles-based permeabilities—in place of empirical permeabilities—that delivers highly accurate results. OLI is developing five types of membrane simulations. The most popular is Reverse Osmosis (RO), which allows process engineers to simulate real process waters and that enables process optimization. This disruptive technology is transforming the way companies approach industrial wastewater treatment as well as redefining the way we think about water as a resource.

Corrosion modeling & prediction

Understanding corrosive environments is another important application in electrolyte chemistry modeling. In this space, companies must quantify the active, corrosive component in their operating environment that places the integrity of their equipment at risk. Corrosion modeling provides an insight on which companies can capitalize to select the most effective and least expensive solution that minimizes risk and maximizes production operations.

The ability to predict corrosion is key to optimizing a company's capital investments. For example, a company may select a pipe with a higher degree of alloy—such as titanium—to prevent catastrophic failure. This action is called "alloying up." However, utilizing a more expensive material might not be necessary for that particular environment. Leveraging simulation software could direct engineers to a carbon steel pipe, which is much more economic and equally effective for their environment.

One OLI client, a fullstream provider of integrated oilfield products, is harnessing OLI technology to optimize simple and effective corrosion testing. With one of the largest hydrogen sulfide labs, this client must maintain a safe and efficient way of running corrosion tests. OLI simulation software allows the company to evaluate corrosive gases under elevated temperature and pressure conditions and reduces the need for physical and potentially dangerous lab experiments. By measuring precise phase properties and pressures, the software provides key information to select the right operating materials, which can save exorbitant amounts of time and money.

Other material scientists see the OLI Studio: Corrosion Analyzer as a vital component for studying polarization curves, replacing the costly lab work that would generate them. Through the polarization curves, clients can analyze the behavior of different chemistries and their relative contribution as corrosive components. Corrosive environment simulation greatly reduces the number of required experiments while fueling corrosion mitigation, and OLI is at the forefront of these cutting-edge capabilities.

Scaling modeling & prediction

Like corrosion, scaling is a massive detriment to industrial processes which can lead to severe inefficiencies, decreased production, and even catastrophic failure. This makes process scaling is a major concern for today's companies. For example, in the upstream oil and gas industry, as deposits build up in production lines, companies face greater risk of lost production—from reduced pipe flow to rising internal pressure causing pipes to explode. Furthermore, approximately 20 percent of well production globally disrupted by scaling.

To combat this staggering statistic, OLI is employing classic scale modeling techniques to examine reservoir conditions (i.e. temperature, pressure, and ion concentration). These models allow companies to predict scaling in different sections of pipes with varying pressures and temperatures, and alert them to escalating saturation levels.

Water chemistry is not intuitive. With countless variables affecting chemistry behavior, many companies struggle to predict and prevent scaling issues. OLI software is the key to unraveling these complex problems, with the capabilities to calculate process water scalability and optimize water reclamation. Right now, OLI does this valuable simulation work offline of the plant. OLI's current target will be for OLI software to analyze data from sensors in water streams—at recycling centers, process plants, and numerous other locations—to read scaling potentials, optimize water usage, or predict the concentration limits of ions before they precipitate in water.

OLI's approach analyzes solubility, indicating when ions will precipitate and crystallize. Many clients utilize OLI software to understand how much of a component can be present in water before the solubility point is reached. This becomes increasingly difficult as water sources can hold dozens of impurities or trace materials. This breakthrough capability promises to enhance the safety and efficiency of industrial operations, and allow clients to reach optimal levels of productions.

Alliance partners

To further these trailblazing advancements, OLI is working with alliance partners like Schneider/AVEVA, Honeywell, Aspen, and others to expound on process design applications. OLI's one-of-a-kind technology is a critical component in today's simulation and modeling software. By adding electrolytes to flowsheet simulators, OLI can deliver the most comprehensive and accurate insights right to your fingertips. OLI technology, after all, is the same in Alliance products as it is in OLI's standalone software.

This process is integral to achieving the desired physical and chemical transformation of highly valuable materials. Whether working as an OLI Engine inside an alliance partner product, or in OLI's standalone software, there is no comparable process simulator on the market. This positions OLI to accelerate process design innovation, empowering process engineers to simulate a water treatment schemes into a process flowsheet as well as enabling clients to accurately predict the behavior of virtually any combination of chemicals in electrolyte solutions.

Conclusion

OLI Systems, Inc. is committed to furthering electrolyte science, everywhere. The company is expanding and enhancing the ability to simulate electrolytes wherever they exist, making OLI the go-to partner for any water chemistry challenge. With the most accurate, rigorous capabilities and a client-friendly approach, OLI is prepared to address a wide range of industry needs, equip clients for future growth and success, and work vigorously to develop new electrolyte chemistry modeling applications.

OLI continues to provide clients with the right software to fulfill their evolving chemistry and data requirements. As electrolyte modeling and analysis become increasingly vital, OLI's objective is to transition from simple user-centric calculations to augmenting human thinking with machine learning. This ambitious pursuit will not only improve accuracy, but it will ultimately empower the best course of action in any environment.

Contact OLI today to learn more about the industry-leading advancements that can drive your operating potential.

For more Information

www.olisystems.com

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