Enhancing process water management with rigorous chemistry insights

Electrolyte chemistry modeling applications for waste water treatment

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TECHNICAL BRIEF

Introduction

The water treatment landscape is undergoing major shifts that are challenging companies to evolve their approach to technology, chemistry, and mathematics. With the development of superior tools and capabilities, the industry is performing more efficiently, cost-effectively, and environmentally friendly than ever. Today's companies must capitalize on these advancements to streamline operations, respond rapidly to market needs, and ensure compliance.

Complying with environmental regulations is vital to operating in an effective and ecofriendly. Environmental regulations provide strict guidelines for gas, water, and solid waste—some of which require scrubbing noxious components like SOx, NOx, Hg, and other pollutants from gases, reducing or eliminating waste water discharge to the environment, and anticipating and preventing dangerous chemical reactions. When harmful components affect water-based processes, they can trigger results like changes in pH or temperature, which can have a severe impact on the environment.

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 challenging for engineers to analyze. The market's current simulation software for water treatment lacks the rigor and accuracy required to safely and successfully manage water in industrial processes. With untapped technological capabilities and chemistry expertise and complex outcomes to predict, adhering to evolving federal and state regulations can pose a major challenge for water treatment facilities. As a result, companies are seeking more effective and economical ways to remove contaminants and toxins from waste water, making operational processes safer for workers and more environmentally friendly.

This game-changing effort requires rigorous water chemistry expertise to model behavior and analyze the risks associated with different components in water. While water chemists have the ability to calculate many of these scenarios, it is virtually impossible to determine every potential outcome or achieve conclusively accurate results with manual calculation. Companies need a new breed of technology to deliver precision insights, optimize water management and treatment, and dramatically reduce risk. Transformative capabilities like water chemistry simulation and in-depth chemistry analysis are foundational to success, enabling companies to streamline processes, increase cost-efficiencies, and operate without incident.

Waste water treatment companies must pursue digital transformation to operate at peak efficiency and effectiveness. The ultimate goal for water treatment is to eliminate waste water discharge altogether. However, current technologies are merely scraping the surface of water treatment applications. Digital transformation is key to harnessing the full power of chemistry data, capturing descriptive and predictive insights, and accelerating and improving critical processes. Companies who invest in leading innovations are investing in a successful future.

The drive to market leadership

OLI Systems, Inc. is uniquely positioned to help companies effectively treat waste water, with a powerful combination of simulation software and extensive water chemistry expertise. OLI Systems solutions utilize electrolyte thermodynamic elements that are essential to designing and optimizing water treatment operations, empowering faster and highly accurate electrolyte simulations to transform industrial processes. The application of electrolytes equips companies to accurately model and predict the most challenging water chemistry behavior, unlike anything else on the market. This exclusive approach helps companies improve decision-making and effectiveness to realize the best course of action for any given situation. As chemical properties change and become more complex, OLI Systems' unique software will continue to deliver comprehensive water treatment simulations for high-quality predictions.

OLI Systems is preparing process industries to tackle their most complex water chemistry challenges with a combination of market-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, ensure that waste water is scrubbed of all noxious components prior to disposal. Based on the set of equations, OLI

Systems supports three distinct <u>thermodynamic models</u> including the Mixed Solvent Electrolyte (MSE) model, <u>MSE-SRK model</u>, 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 Systems 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 Systems 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, particularly as companies strive to comply with increasing environmental regulations.

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 most demanding water management issues. OLI Systems customers 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 Systems 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 Systems 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 Systems has the ability to think and compute beyond the empirical data, a key differentiator that is helping OLI Systems and their companies achieve market leadership. Whether companies require updates every 10 seconds, 15 minutes, or hour, OLI Systems provides rigorous chemistry analysis with near-time results to uncover progressions of change. By automating these processes, companies can benefit from faster, more accurate outcomes to help them operate safely, proactively, 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 Systems 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 Systems software can be used to evaluate the components of a water sample; the customer could then manage an app that notifies them when the water has been scrubbed for disposal. In the future, OLI Systems will utilize machine learning tools to analyze vast quantities of IoT data to deliver predictive and even preventive insights in real-time. The <u>possibilities for electrolyte modeling applications</u> are endless, and OLI Systems is pioneering the journey.

Virtual research & development

Research and development (R&D) is a lengthy and resource-consuming process for water treatment facilities 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 Systems 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 Systems 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 Systems will help to increase the cleanliness of industrial waste water as well as

properly configure experiments to explore thermodynamic activity, cut preparation time and operating costs, operate in an ecofriendly way, and accelerate time to insight.

Process simulation

Optimizing water treatment and reuse is a crucial mission for today's companies. Fresh water is an essential resource that is quickly reaching scarcity. Higher-income countries treat 70 percent of their waste water 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 waste water.

Water chemistry insights empower chemists with increased confidence in their recommendations, and allow companies to streamline purification and disposal processes, boost water reclamation, and achieve ideal operating conditions. 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 advanced simulation capabilities to perform chemistry analysis and dramatically improve industrial water management.

OLI Systems is driving the performance of waste water treatment with the OLI Studio and OLI Flowsheet: ESP. OLI Studio software helps customers quickly assess the properties of their water supply, according to a specific set of conditions or a range of chemical properties. OLI DynaChem, one component of the OLI Studio, can be used to examine control strategy, potential upsets, scheduled waste streams, controller tuning, and more. Companies who leverage this software will have the ability to study pH and compositional control, batch treatment interactions, and multistage startup and shutdown with multicascade and adaptive control. Meanwhile, OLI Flowsheet: ESP augments every stage of the water treatment process—this includes providing customers with an intuitive understanding of how chemical conditions will affect operations as well as the optimum set of changes required to enhance the process end-to-end. This revolutionary software delivers electrolyte process simulation which enables engineers to uncover new options for maximizing the use of water and other resources.

A new, central feature of OLI Flowsheet: ESP is the reverse osmosis (RO) membrane simulation tool, which allows companies to simulate real process waters outside of manufacturer's specifications. The RO membrane is the first of a series of specialized water treatment blocks and a critical advancement for the water management industry. This block combines rigorous electrolyte chemistry to RO calculations, using customer-defined chemistry environments to determine how a membrane will perform. Now, companies can simulate unique membranes into a real process flowsheet. Membrane technology is transforming the way companies approach industrial waste water treatment as well as redefining the way we think about water as a resource.

OLI Systems is working to create the ideal waste water treatment solution. In addition to the RO membrane, plans include developing membranes simulations for forward osmosis, nanofiltration, ultrafiltration, and electrodialysis. Together, these five types of membranes will empower unparalleled modeling for water treatment. Furthermore, recent chemistry innovations (i.e. arsenic, struvite, boron, iodine, selenium, and mercury) are significantly enhancing the accuracy of existing models. As a result, waste water treatment chemical processing has never been more accessible or precise. OLI Systems' arsenic and struvite chemistry is another crucial update that dramatically optimizes water treatment. This novel capability works to predict phase equilibria and speciation of arsenic in water, in the presence of Ca, Fe, and CO_2 and in acidic environments as well as predicting the formation of struvite in waste waters. With this groundbreaking development, water treatment organizations can predict what will happen to arsenic—one of the most toxic components in natural and industrial waters—and calculate the possibility of scaling in pipes due to struvite in water treatment.

OLI Systems is setting the standard for water management by advancing water chemistry simulation, membrane technology, and chemistry expertise to redefine traditional processes. As new regulations and industry challenges emerge, savvy companies will look to the latest tools and capabilities to expand their operations, optimize water use and reuse, and ensure environmental compliance.

Modeling & prediction

Water chemistry is not intuitive. With countless variables affecting chemistry behavior, many companies struggle to predict and prevent corrosion, scaling, and other issues associated with waste water.

Understanding corrosive and scaling environments is a critical application in electrolyte chemistry modeling. Corrosion and scaling modeling provides insights into the most effective solution to eliminate risk and enhance water treatment. OLI Systems software is the key to unraveling these complex problems, with the capabilities to calculate process water solubility and optimize water reclamation. OLI Systems performs these valuable simulations without disrupting operational processing, by analyzing data from sensors in water streams—at recycling centers, process plants, and numerous other locations—in order to read corrosion or scaling potentials, optimize water usage, predict the concentration limits of ions before they precipitate in water, and create the safest and most efficient process water environment.

OLI Systems offers unique and dynamic solutions for simulating water treatment and water reclamation processes, including thermodynamic models which allow companies to analyze the most challenging water types and salinities—from lake water or seawater, to brackish well water, salt-saturated oilfield waters, and a variety of industrial effluents. In short, OLI Systems software model complex salt solutions with a range and level of accuracy that simply cannot be achieved elsewhere. This breakthrough capability promises to enhance the safety and efficiency of industrial operations, and allow water treatment facilities to reach optimal levels of performance and compliance.

Alliance partners

Advanced software and an expansive knowledge of water chemistry are growing increasingly important in the water treatment landscape. To further these trailblazing advancements, OLI Systems is working with alliance partners like Schneider/AVEVA, Honeywell, Aspen, and others to expound on process design applications. OLI Systems' one-of-a-kind technology is a critical component in today's simulation and modeling software. By adding electrolytes to flowsheet simulators, OLI Systems can deliver the most comprehensive and accurate insights right to your fingertips.

The ability to model RO membranes inside a process flowsheet is one of many steps OLI Systems is taking to help customers drive productivity and success. These disruptive technologies with rigorous chemistry applications go beyond companies' basic needs, to rapidly transform their unique processes. OLI Systems is avidly partnering with companies who want to bridge the gap between traditional processes and reaching their optimal performance, paving the way to groundbreaking innovations like zero-liquid discharge, and much more.

Innovation is integral to achieving the desired physical and chemistry outcomes. OLI Systems and alliance partners are working tirelessly to accelerate process design innovation, empowering process engineers to simulate a water treatment schemes into a process flowsheet as well as enabling companies 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 Systems the go-to partner for any water chemistry challenge. With the most accurate, rigorous capabilities and a client-friendly approach, OLI Systems is prepared to address a wide range of industry needs, equip companies for future growth and success, and work vigorously to develop new electrolyte chemistry modeling applications.

OLI Systems continues to provide water treatment companies with the right software to fulfill their evolving chemistry and data requirements. As electrolyte modeling and analysis become increasingly vital, OLI Systems' 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.

For more information on how digital transformation is improving waste water treatment, and to learn about personalized assessments and trainings to empower your business contact OLI Systems.

For more Information

www.olisystems.com

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