think simulation | getting the chemistry right

Expanding electrolyte chemistry modeling applications for the Oil & Gas Industry

Transform end-to-end operations with rigorous water chemistry analysis

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TECHNICAL BRIEF

Introduction

The Oil and Gas (O&G) 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 widespread applications that enable faster time to market. Today's O&G companies must capitalize on these innovations to promote strategic growth, respond rapidly to market needs, and drive production.

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 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 energy production and growth. As a result, savvy O&G companies are investing in new, effective innovations to enhance process automation as well as their capacity to collect and analyze data and operationalize insights.

Understanding chemical behavior under a range of conditions is vital for O&G companies to produce and transform materials, particularly when it comes to designing, simulating, and optimizing their unique processes. Water is one of the most complex and versatile chemical substances on the planet—and water used in industrial processes 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 O&G companies 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 increase yields and ensure competitive advantage.

The drive to market leadership

Today's companies are seeking advanced water chemistry technologies and capabilities to enhance Upstream O&G production. 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 O&G 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 energy companies 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 environment.

OLI is preparing O&G 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 MSE-SRK bolsters O&G production with the ability to assess supercritical components at extreme pressures as well as mixtures containing supercritical components at transitional points between vapor and liquid states. The increased functionality of the MSE-SRK model supports any chemistry a client may need for production. This comprehensive tool is driving greater levels of performance and insight to companies across the O&G sector—from energy production companies to corrosion testing laboratories.
- OLI Data Bank 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. These comprehensive datasets allow O&G

companies to carefully analyze their environments in order to protect operating equipment and materials, streamline operations, optimize waste water management, and much more.

- 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, particularly as O&G companies produce massive amounts of water during production.

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 O&G 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, allowing energy companies to operate successfully across remote and extreme environments. 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, O&G companies can benefit from faster, more accurate outcomes to improve energy production with increased efficiencies and profits.

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 O&G engineers could then manage an app that notifies them when the scaling tendency of a pipe 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 in the O&G sector are endless, and OLI is pioneering the journey.

Virtual research & development

Research and development (R&D) is a lengthy and resource-consuming process for energy companies. 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 O&G companies to determine the exact experiment that must be run and guides 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 O&G 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 energy producers as well as properly configure experiments to explore thermodynamic activity, prevent overdesign, cut preparation time and operating costs, and accelerate time to value.

Process simulation

In the Upstream O&G sector, a major dilemma is finding ways to streamline production and increase yield while reducing the cost of operations. Exorbitant amounts of money and manpower are required to design and build facilities, manage materials and equipment, extract resources, and cost-effectively dispose of water. 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. While O&G uses significantly less water than sectors like agriculture or power generation, energy companies have a critical role to play in protecting the quality and safety of water sources and expanding water reuse.

O&G wells bring large amounts of water to the surface. In fact, wells can produce 20X more water than oil or gas, and this water is often saline and unsuitable for surface disposal. Producing this water can also lead to costly and sometimes catastrophic corrosion, solids buildup (fouling or scaling), emulsion, and reservoir souring problems. Because this water isn't environmentally friendly, companies must find ways to evaporate it to salts, reinject it, or treat it—all of which require time, money, and resources. OLI Systems' process simulation assists companies in handling industrial water. This critical technology determines the most cost-effective and efficient way to process water: Should it be treated to remove solids? Is it too saline to be disposed of in surface waterways? Can it be injected back into the well? Will it damage operating equipment? Solving these complex questions is the difference between a successful Upstream operation and one that loses time and revenue. 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, O&G companies are seeking a new breed of simulation capabilities to perform chemistry analysis and limit the use of fresh water.

OLI is driving water chemistry analysis 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. Utilizing the MSE-SRK thermodynamic model, this powerful flowsheet simulator delivers a superior way to plan and execute O&G operations. Now, OLI Systems supports a broader range of applications, enabling better phase predictions for even extreme conditions and honing oilfield process modeling with greater accuracy and the usability of electrolytes. As a result, OLI Systems can assist clients in designing the ideal facility to suit their unique environments.

Scaling & corrosion modeling

Another major challenge for O&G companies is mitigating scaling and corrosion. When hydrocarbons are produced (the chief components of petroleum and natural gas), salt-rich water in the same process can cause a number of issues. One of the most common issues is fouling in which, over time, mineral scale buildup chokes off tubing. As water clogs or corrodes pipelines—which can be over a mile long—companies are forced to pause operations, pull up pipeline, install new pipes, and then resume operations. This cuts off all revenue for an expensive and time-consuming fix with costly materials that increases operational costs and reduces profitability.

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. 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.

Similar to determining scaling tendencies, 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 energy production.

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.

Water chemistry is not intuitive. With countless variables affecting chemistry behavior, many O&G companies struggle to predict and prevent scaling and corrosion issues. The prescriptive approach is to utilize modeling and simulation to avoid these occurrences altogether. OLI software is the key to unraveling these complex problems, with the capabilities to pinpointing how and why a problem will occur and how and where to treat it. By uncovering these insights, OLI Systems creates a personalized treatment option to help companies prevent issues and achieve optimal production.

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.

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 O&G companies to simulate a water treatment schemes into a process flowsheet as well as enabling process engineers to accurately predict the behavior of virtually any combination of chemicals in electrolyte solutions.

Summary

The O&G sector relies on transformative technologies to harness deep water chemistry insights, assess risk, and optimize operations end-to-end. These capabilities are essential to explore potential complications, drive efficiencies, and determine the most effective way to produce energy resources for maximum profit and minimum risk. Moving forward, OLI Systems will provide predictions as well

as solution outcomes for O&G production. This will expand scale inhibition, corrosion inhibition, water analysis interpretation, and other critical tasks to help clients operate not only efficiently and cost-effectively, but also prescriptively. Table 1 in the Appendix shows OLI's current capabilities for the Oil & Gas industry.

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 O&G companies 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.

Appendix: Table 1: Key OLI Systems, Inc Capabilities for the Oil & Gas Industry

Segment	Process/ Application	Use Cases for Electrolyte Chemistry	OLI Systems, Inc. Modeling and Simulation Capabilities
Upstream Oil & Gas	Sag-D	Higher steam quality (e.g. >80%) and silicate scaling	• Scaling Prediction and Inhibition • Scale Treatment • Remediation • Corrosion Prediction and Inhibition / Green Technology • Mercury Removal • Autoclave simulation • H2S removal from gas and liquid • MEG Recovery • Gas Hydrate Prevention • Gas Well simulation for enhanced oil recovery • Scaling and Corrosion in HPHT conditions for Extreme Reservoir Production
		calculate chemical dosing rates / chemical treatment	
		Optimizing silica removal, Surface complexation	
		Optimizing Ion Exchange purification	
		Boiler feed water clean up	
		Steam injection and mineral dissolution	
		water separation from bitumen (skimming)	
		Whole plant simulation for water mass balance	
		Reservoir mixing	
	Production: flow assurance	Enable designing experiments for Corrosion testing using autoclaves	
		Creating recipe for the lab tech	
		Enhance Engineering Design for Corrosion Scientist	
		Injection water compatibility, scaling predictions	
	Production	Scaling and Corrosion of production assembly	
	Exploration and drilling	Drilling fluid chemistry	
	Completion	Drilling fluid chemistry	
	Abandonment	Drilling fluid chemistry	
	Industrial Water Treatment -	Treat water before discharge to the environment	
	Regulatory Compliance - (RCRA)	Flue gas removal from water in treatment process	
Midstream	Transmission	Pipeline corrossion: from the field into the refinery or gas plant	• Top of line corrosion • Corrosion prediction • Corrosion in CO2 transmission • Gas hydrate prevention • Natural gas odorants
Refining / Downstream Oil & Gas	Desalter	Demulsifier, wash water, organic acid additon	Scaling of desalter with calcium bearing salts
	Furnace	High temperature evaporation, phase separation	Sulfidic corrosion
	Atmospheric column	Water/Organic acid/high salt condensation and corrosion	Organic acid and salt condensate corrosion
	Vacuum column	Heavy organic acids, naphthenates, NH3 and H2S formation	Amine salt corrosion
	Overheads	Amine-HCl Salting point, ionic dew point, Chemical and wash water dosing rates	Dew point corrosion
	Hydrotreating	NH3 and H2S formation and evaporation to overhead line	Condensed NH4SH and NH4Cl corrosion
	Reforming	Corrosion in fired heaters, reactors, transfer pipework, NH4Cl, HCl corrosion	
	FCC	Salting point, ionic dew point, corrosion	
	Hydrocracker	NH3 and H2S formation and evaporation to overhead line	NH4Cl corrosion
	MEROX	Converting mercaptans to disulfides, to remove sulfur	Optimize disulfide formation
	Coking unit	CO2, H2S, NH3 gas production	Acid gas condensation and corrosion
	Alkylation unit	HF regeneration, catalyst regeneration	HF corrosion
	Amine Gas treater	Acid base removal of H2S from the gas, Amine regeneration	heat stable salt formation, corrosion, absorber and regenerator optimization
	Claus, Scot	H2S to SO2 and S. Recovery in scot tail gas unit (TGU)	elemental sulfur corrosion, unit optimization
	Sour Water Treatment	Stripping water of NH3, CO2, H2S	condensed water corrosion in reflux, Unit optimization
	Cooling Towers	Cooling water cycle-up	Scale prediction, water optimization, chloride (O2) corrosion
	Wastewater treatment	Re-using the water in their process plant	Optimize water reuse, simulate effluent quality
	Gas Sweetening	Removal of H_2S from Produced Gas Streams	Chemical Analysis
	Debutinzer, Depropanizer	Dehydration unit efficiency, water entering unit	Condensed water Corrosion
	Regulatory Compliance -RCRA	Flue gas removal from water in treatment process	Water quality

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