AQSim
OLI electrolyte solutions

The demand for a new user interface for ESP
Introducing OLI Flowsheet ESP

If your company licenses a commercial process flowsheet simulator: stay with it! OLI as an embedded property method is a viable option when electrolyte simulation is a minor part of your project. However, when electrolytes are the primary reason for simulation, AQSim recommends software designed specifically for this reason. To that end, OLI has updated their electrolyte-based, steady-state process flowsheet simulator, ESP with a new User Interface (UI). The product, OLI Flowsheet ESP is planned for release in 2015.

Why ESP is important to industry

ESP is differentiated from other commercial flowsheet simulators by its focus on rigorous electrolyte thermodynamics. Such a software tool requires three key characteristics: unit operations relevant to electrolytes; rigorous thermodynamic models that capture the unique properties of electrolytes; and a database sufficiently large to enable modeling of commercial operations.

Electrolyte-based flowsheet simulators differ considerably from hydro-carbon, mining, or heat/material balance simulation tools

An electrolyte-based, flowsheet simulator UI differs from hydrocarbon, mining, or heat/material balance simulation tools because the user's needs are different. For example, an effective electrolyte flowsheet simulator contains the following features:

- An input method to enter ion analyses and to reconcile for measured properties such as pH, charge balance, total dissolved solids, and alkalinity;
- Methods to enable redox reactions, and to suppress the formation of specific, kinetically slow oxidation states;
- Methods to convert ions to molecular flows;
- Reports and plotting packages tailored and optimized for reviewing a stream's speciation, thermophysical properties, and elemental/oxidation-state material balance.

These interface features are examples of how electrolyte flowsheet simulation is unique, and an interface focused on these needs is critical for those involved in such processes.

Business justification

OLI electrolyte thermodynamics remains industry's principal electrolyte engine

Three market forces led OLI to develop ESP Original in 1991 and to redevelop OLI Flowsheet ESP in 2013. The first is the ongoing market need for a commercial electrolyte-based, process simulator. OLI recognized this need in 1991 during the original ESP development.

The second is that no existing commercial flowsheet tool using a contemporary interface is designed around water-based operations as the primary user-base.

The third is that OLI electrolyte thermodynamics remains the industry's principal electrolyte engine, and the core units of ESP: solids separator, evaporator, multi-stage electrolyte distillation, membranes, etc. remain critical to contemporary process design. Thus, there was strong business justification to redevelop this software.

Finally, the redevelopment of ESP in 2013 was motivated by repeated requests from the present ESP Original client base to update this interface.

Where ESP can make a difference

The ESP software simulates electrolyte-based processes in multiple industries: oil and gas production, refinery water processing, mineral purification, chemical production, water treatment, and numerous other systems. The number and type of applications are broad. Appendix A lists some general applications. .

ESP simulates a variety of "electrolyte-based" processes

"Electrolyte-based" means that electrolytes are the focus of the process simulation. However, these processes can also contain hydrocarbons and various other nonelectrolyte components. OLI uses an enhanced SRK in the Aqueous framework and SRK/UNIQUAC in the Mixed Solvent Electrolyte framework to model hydrocarbons and other nonelectrolytes present in the process.

The original ESP software

The original ESP software (ESP Original) was developed under the sponsorship of an eight-company consortium that ran between 1991 and 1994. The internal code and the user interface were written in FORTRAN. This software, despite its 20-year-old interface is still used by hundreds of clients, and its longevity is evidence of its excellent electrolyte simulation capabilities, despite lacking a modern interface.

ESP's longevity is evidence of its excellent electrolyte simulation capabilities

ESP Original contained five programs: ESP Process, CSP Corrosion, OLI Databook, OLI Toolkit, and OLI Estimate. ESP Process was the electrolyte flowsheet simulator, and it is a new UI for ESP Process, which is the focus of this document.

The letters ESP stood for Environmental Simulation Program. Environmental clean-up was the original focus, modeling steady-state, water-based operations such as scrubbers, strippers, water treatment, etc. OLI has since broadened and generalized the name into Electrolyte Simulation Program because the software's applications expanded beyond environmental operations.

Short-cut approach

Given the technical robustness of ESP Original, OLI's ongoing improvements in ESP's convergence techniques, and additions and improvements to ESP blocks, the OLI development team recognized that a new UI overlaid on the original ESP solver would be sufficient to re-launch this product.

A new UI overlaid on the original ESP solver code is sufficient

This UI-update approach allowed OLI developers to implement this tool without seeking new industry input via a current consortium. OLI typically relies on organizing industry consortia to specify and steer requirements for software under development. Instead, OLI is working on a straight translation of the original ESP blocks and features. Because no specifications are changing, a very strict conversion protocol is also possible so that ESP Original cases may be easily read by OLI Flowsheet ESP.

OLI Flowsheet ESP

OLI Flowsheet ESP retains ESP's Original user-work process, one that is standard among many current flowsheet simulators:

- *Model Build*, a facility to define the chemistry model;
- *Process Build*, a facility to specifies the input for the unit operations;
- *Process Analysis*, a calculation engine and output for solving the flowsheet and monitoring the solver process; and,
- *Summary*, a reporting tool to review the results.

All ESP Original capabilities will be retained

All of ESP Original capabilities will be retained, including full chemistry model capabilities with the OLI Aqueous (AQ) and Mixed Solvent Electrolyte (MSE) thermodynamic frameworks.

OLI Flowsheet ESP Unit Operations

ESP Original contains thirty-five process blocks classified into six general categories (**Error! Reference source not found.**). OLI Flowsheet ESP rollout beginning in 2015 will contain most of the blocks in the conventional, multi-stage and controller categories. As development continues into 2016, the remaining blocks will be added to new releases, until conversion is complete.

From the initial release, existing ESP Original clients will be able to migrate cases to OLI Flowsheet ESP. There will be an alternate 'block reader' for blocks not yet converted to the new UI, so all cases should work in OLI Flowsheet ESP.

Some OLI Studio code is used as a basis in some of OLI Flowsheet ESP

One note about translating blocks: Several ESP Original blocks contain multiple configurations. For example the existing Separator block can be configured as a two-, three- or four-phase separator (four process blocks in a single object). Therefore, the final OLI Flowsheet ESP interface will likely contain many more units than the thirty-five blocks listed in **Error! Reference source not found.**. In addition, engineering development to create new units will expand this list over time.

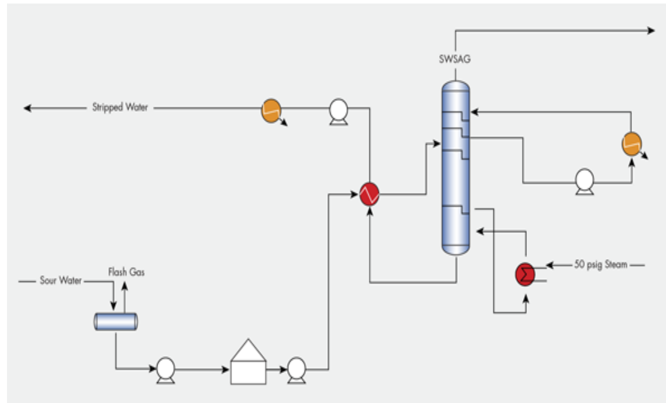
Communication with OLI Studio

OLI Flowsheet ESP will import and export streams to and from the OLI Studio for more detailed stream studies or for corrosion simulation calculations.

Furthermore, OLI Studio code is used as a basis in some of OLI Flowsheet ESP. In addition, existing OLI Studio features are being upgraded to share common features with OLI Flowsheet ESP. Thus, a secondary benefit of this work is an upgrade to the OLI Studio code.

ESP Example: Sour Water Stripping

Sour water stripping is a common gas processing and refining operation. The diagram below displays the various units involved. The main unit is the multi-stage stripper. Ancillary units include heat exchangers, pumps, flash tank and storage tank.

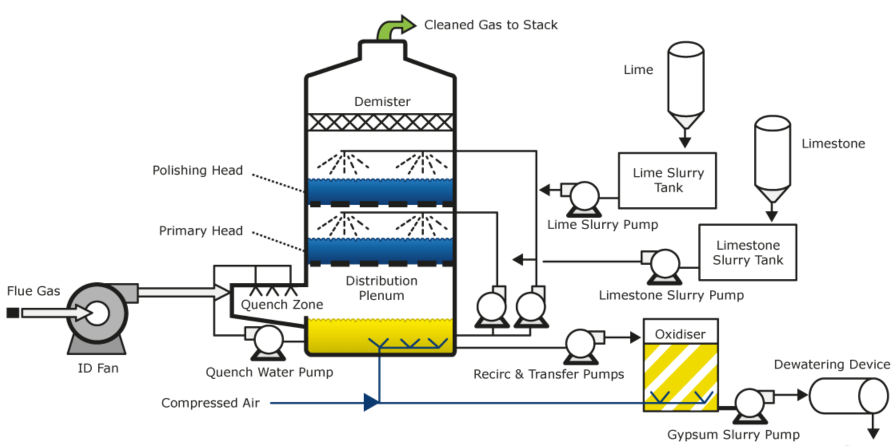


There are two non-equilibrium limits to sour water stripping. The first is the mass transfer of volatile solutes (NH_3, H_2S, CO_2) to the vapor phase. The second is the heat transfer between the tower bottoms and the injected sour water.

The multi-stage stripper is designed to incorporate mass-transfer effects on tower performance.

ESP Example: Gas Scrubbing Applications

The basis of gas-scrubbing is that the gas-phase to be treated contains components that absorb into an electrolyte phase. A combustion gas containing SO_2 can be scrubbed using an alkaline scrubbing solution. This alkaline scrubbing solution can be regenerated using compressed air to oxidize SO_2 to SO_3, which then precipitates as a sulfate salt. The inflows are then limited to inexpensive lime ($Ca(OH)_2$), limestone ($CaCO_3$), and air.



The application is modeled in ESP using a multi-stage absorber, a sparging tank, mixers, pumps, filters, controllers, and recycle-stream calculators.

There are two mass transfer limited reactions; SO_2 absorption into the alkaline solution within the tower, and O_2 absorption to the spent alkaline solution in the sump and oxidizer tank. There is also a rate limitation reaction in SO_2 to SO_3 oxidation.

Tools necessary to manage these non-equilibrium limits are part of the ESP code.

Converting ESP cases

There is an existing body of ESP cases, which already can be brought into the Flowsheet ESP environment. Where unit operations have not yet been converted, integrity of the blocks will be maintained, calculations will be permitted, and full stream reporting will be enabled.

Remaining programs in Original ESP

What are OLI's plans for the other parts of the original ESP development? OLI has already transitioned OLI Toolkit, CSP Corrosion, Water Analyzer, and ElectroChem to OLI Studio in 2003. ESP Process is being released as OLI Flowsheet: ESP in 2015. No plans have yet been announced for OLI Databook, OLI Estimate, DynaChem, FraChem and ReaChem.

For information on how to become a beta-tester for OLI Flowsheet: ESP, please contact Pat McKenzie, Business Development Director for OLI at

pat.mckenzie@aqsim.com
1-973-998-0240 x112

Also please note that OLI Flowsheet: ESP will be demonstrated and discussed at OLI's upcoming Simulation Conference on 21-22 October 2014
http://marketing.olisystems.com/conference

Appendix A: Example ESP Applications

Flue gas scrubbing
Sour water stripping
SAGD water reuse
Oil-gas-water scaling in field production
Salar lake lithium recovery
$(NH_4)_2SO_4$ evaporator recovery
CaF_2 recovery
Amine sweetening
CO_2, NH_3 recovery
Claus plant sulfur recovery
Beryllium recovery
$NaHCO_3$ purification
Sulfate stripper
HF/SO_3 distillation
$Ca(OH)_2/Mg(OH)_2$ purification
Coke oven gas purification
Perovskite - TiO_2 reaction design
Refinery amine unit
Evaporator-crystallizer
Optimization
Kraft process: chemical recovery
Jetwater: Water purification design
Microchip fabrication: Water recovery system
Flakt Modo process: Flue gas oxidation
Process water evaporation /crystallization
Zero liquid discharge
SynGas shift/recovery
Mechanical vapor recompression
NH_3 stripping and purification
SAGD evaporator feed boil-up
MEG/MeOH recovery/produced water
Tailings pond water chemical fate
Armanda Lake remediation
Landfill leachate fate and transport

Appendix B: List of Existing ESP Process Blocks

Conventional block

Mixer
Split
Separator
Heat Exchanger
Compressor
Calculator

Multi-Stage blocks

Absorber
Stripper
Liquid-Liquid Extractor

Environmental blocks

Reactor
Neutralizer
Precipitator
Incinerator
Crystallizer
Saturator
Dehydrator
Membrane
Electrodialysis
Electrolyzer

Bioreactor blocks

Bioreactor
Clarifier

Controller blocks

Controller
Feed Forward
Manipulate
Sensitivity
Energy Transfer

Crystallizer blocks

X-crystallizer
Filter
Settler
MSMPR Crystallizer

Specialized blocks

E-Cell Model
Autoclave
Downhole Calculator
Brine-Oil-Gas Saturator
Brine-Solids Saturator