OLI simulation technology

General introduction

think simulation

getting the chemistry right

May 2019

Discussion outline

- Introductions
- Simulation to address chemistry / corrosion / process applications
- A closer look at the software
- OLI access

Individual introductions

Individual introductions
Your group
Your simulation interest

What are <u>your</u> biggest water chemistry challenges?
- ✓ Know whether scaling will occur?
- ✓ Simulate your process to find corrosion problems?
- ✓ Maximize water re-use?
- ✓ Optimize your water-based process?
- ?

& introducing OLI Systems …

OLI Systems: Proven water chemistry leadership

A unique combination of capabilities

- Physical property modeling
- Electrolyte Property database
- Simulation software

A unique group of professionals

Most comprehensive electrolyte chemistry based solutions

Sustained innovation research & development

Think simulation!
Getting the chemistry right

Expertise and resources

Global recognition

Simulation power: the OLI Engine

Frameworks

- Three electrolyte thermodynamic frameworks available
- MSE — No concentration limits, pressure 1500 bar, temperature up to 90% of the critical T of mixture
- **MSE-SRK — For upstream oil & gas: a variation of MSE using SRK for 2nd liquid to remove discontinuities**
- AQ — Legacy framework, excellent for many systems, good ability to extrapolate on new systems

Structure

- Equation of state (EOS) for the reference state properties — **Helgeson-**Kirkham-Flowers-Tanger EOS
- Activity models for the excess properties — **Minimization of Gibbs Free Energy**
- Equations for all models are published, many peer-reviewed papers

Databases

- OLI databases = OLI's competitive edge
- Close to 6000 species, 81+ elements of the periodic table
- Validation spreadsheets available for all MSE, MSE-SRK parameters

OLI simulation modeling benefits

Reduce and focus lab testing ruling out what is infeasible

Anticipate changes before they occur: “what-if T, P, pH trends towards…”

Model system complexity with thermodynamic accuracy

Compare alternatives when looking for optimal performance

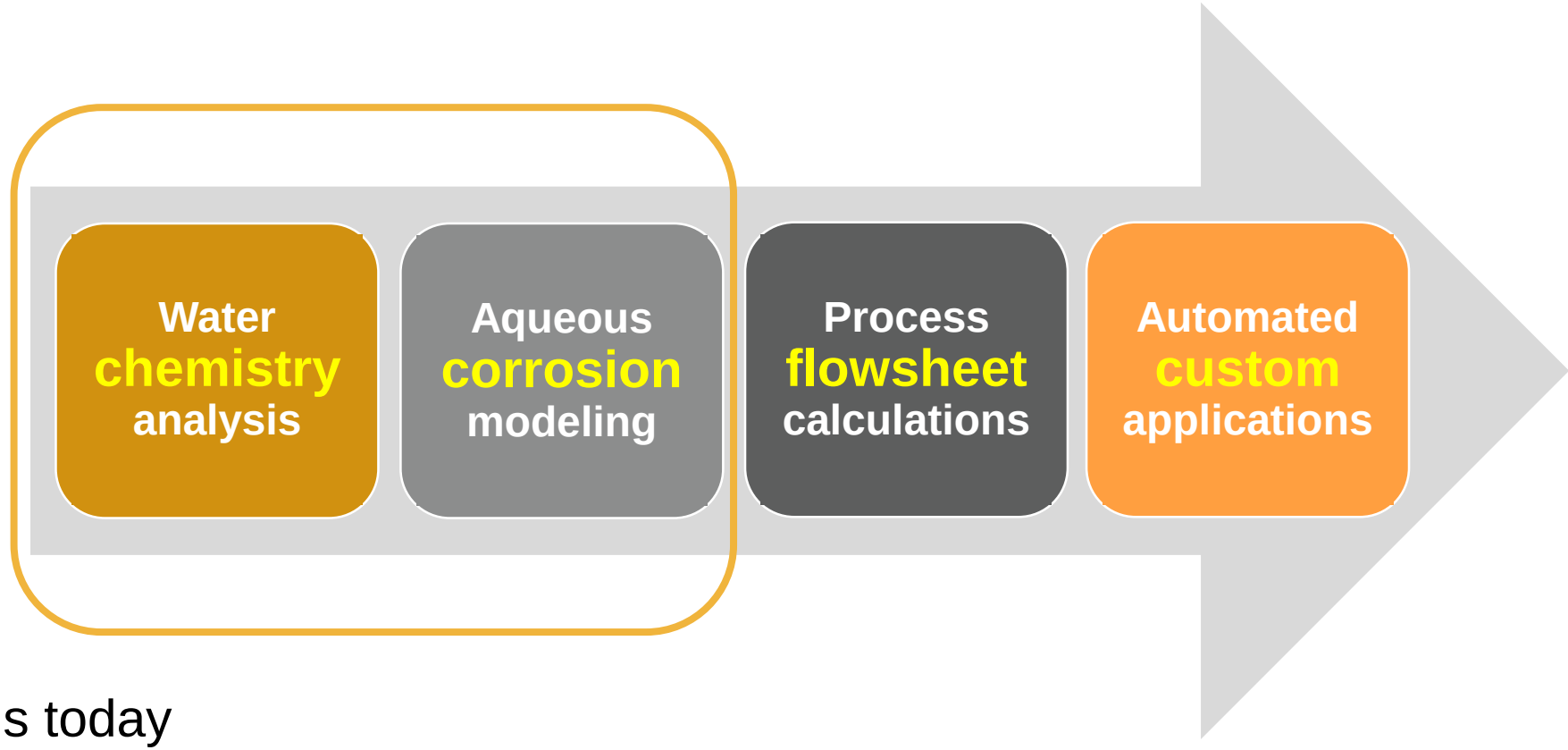
Identify bottlenecks that could limit yield, cost savings

Gain confidence in decisions when backed by thermodynamics

Study regulatory limits and what is needed to meet them

Evaluate operational, environmental impact ahead of making changes

OLI technology brings competitive edge



Focus today

OLI Studio: ScaleChem

OLI Studio: Corrosion Analyzer

Water chemistry analysis

OLI Studio ScaleChem

or

Stream Analyzer

Equilibrium based

Solid-liquid-vapor-organic phase distribution

Multi-component systems

Physical & chemical property calculations

Advanced mechanisms

- **Kinetics framework**
- **Reduction / oxidation**
- **Mass transfer**
- **Surface reactions**

Advanced properties

- **ORP**
- **Water activity**
- **Transport properties**
- **Osmotic pressure, etc.**

Aqueous corrosion simulation

OLI Studio: Corrosion Analyzer

Thermodynamics of corrosion

Real-solution Pourbaix diagrams, taking all ion-ion interactions into account

Uniform (general) corrosion rate

Computer-generated polarization curves &

underlying, diffusion limited anodic & cathodic reactions

Localized corrosion

Corrosion potential vs repassivation potential, calculating the worst-case pitting rate

Remaining asset life

Given time, pit depth, area, a statistical model that calculates time to failure

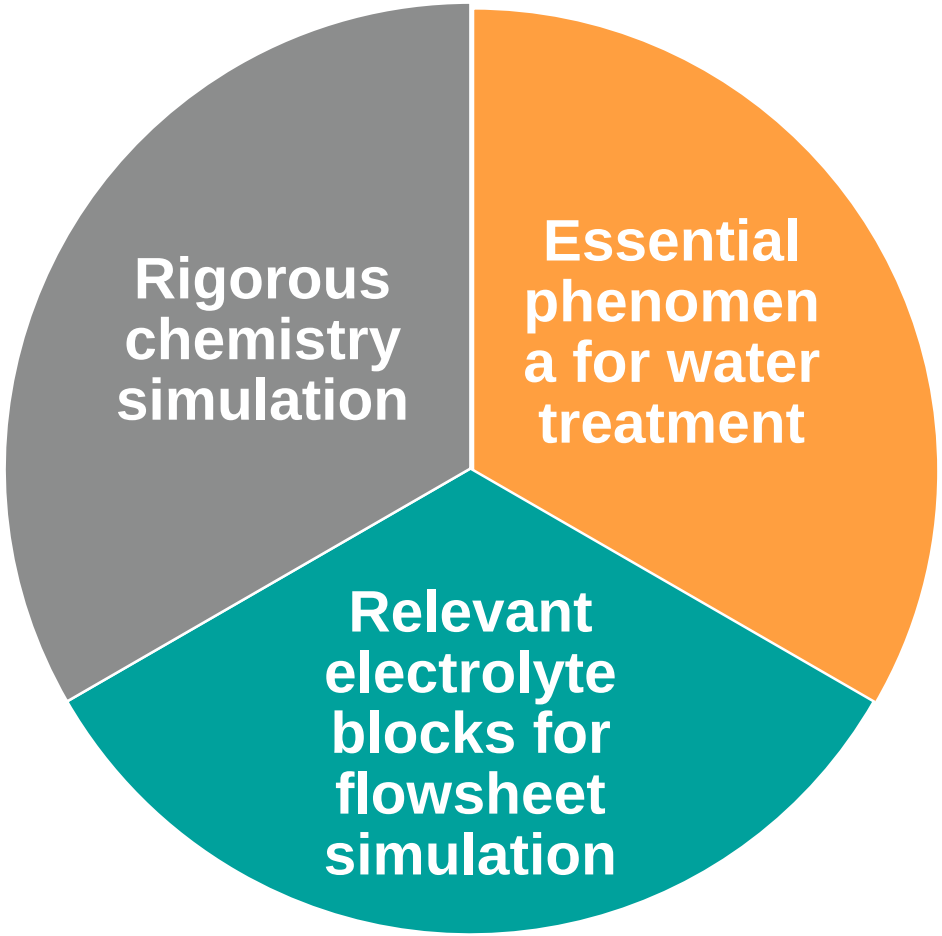
Process flowsheet simulation

OLI Flowsheet: ESP

When electrolytes are primary

OLI Flowsheet: ESP

- **Multiple units, recycle**
- **Fullest implementation of OLI technology (kinetics, ion exchange)**
- **Reverse osmosis unit**
- **Target: industrial water treatment**



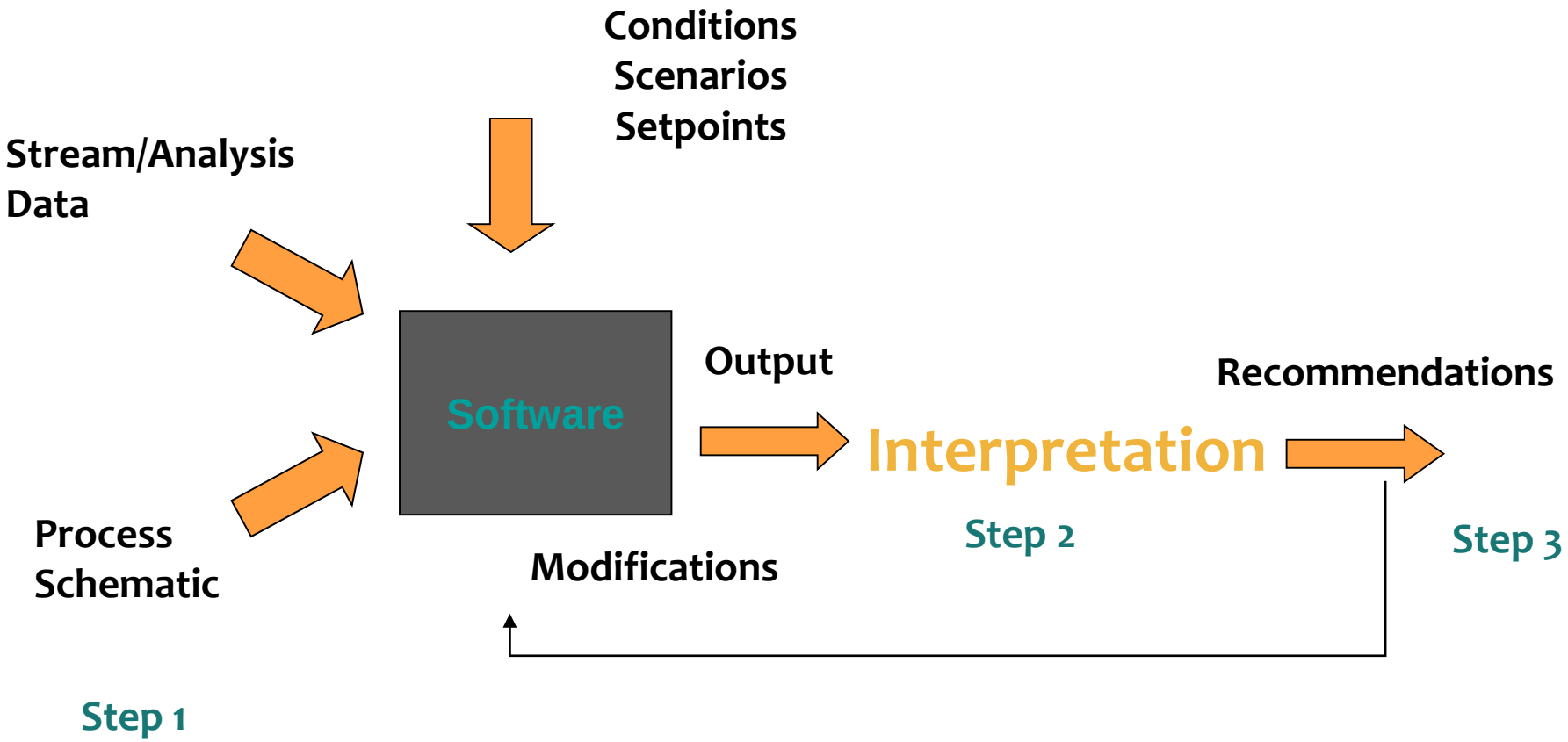
Selected applications that are possible

Autoclaves	Evaporative crystallization	Flue gas desulfurization	Steam generation
Strippers and scrubbers	Gas sweetening and regeneration	Cooling towers and cycle up	Pond evaporation
Lime softening	Syngas purification	Clay-resin fixation	Desalination
Multi-stage evaporation	Chemical recovery and purification	Claus plants	Wastewater treatment

Templates & expert setup help available

Process simulation: Interpretation is key!

Training and expert opinions help establish experts in your company



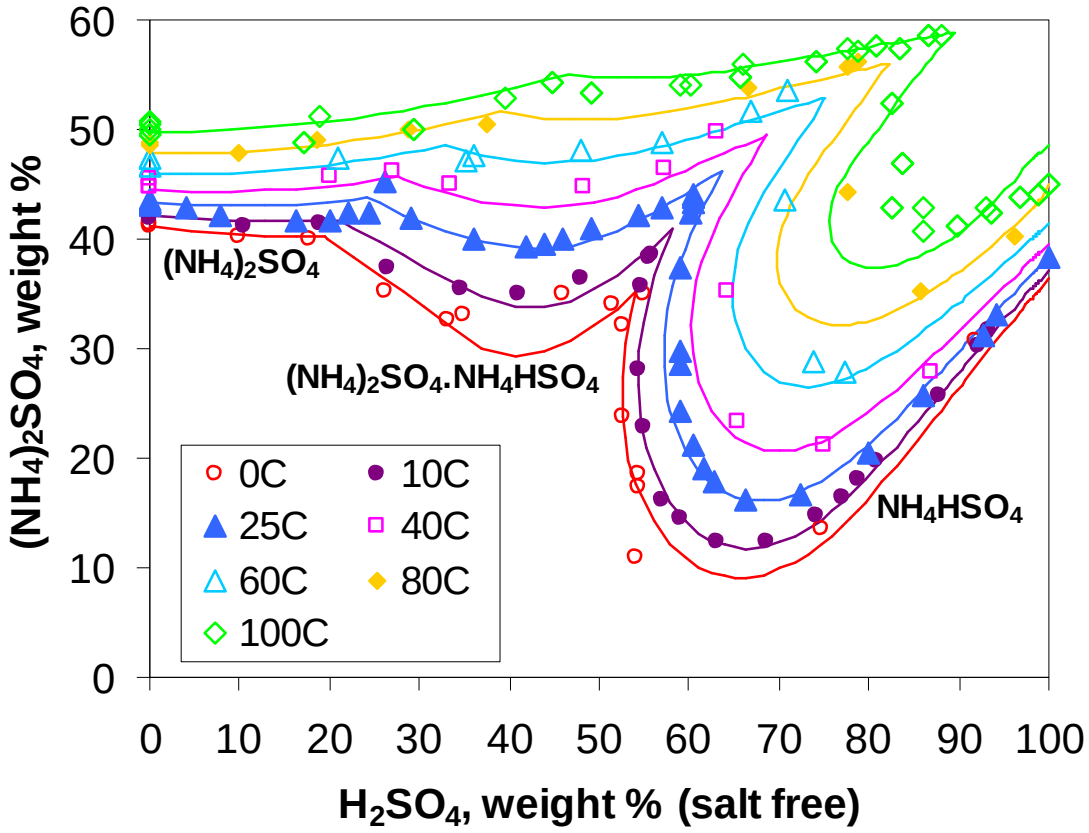
OLI Validation Plots increase confidence

A benefit of Silver, Gold, Platinum service levels

NH_3, H_2SO_4, H_2O

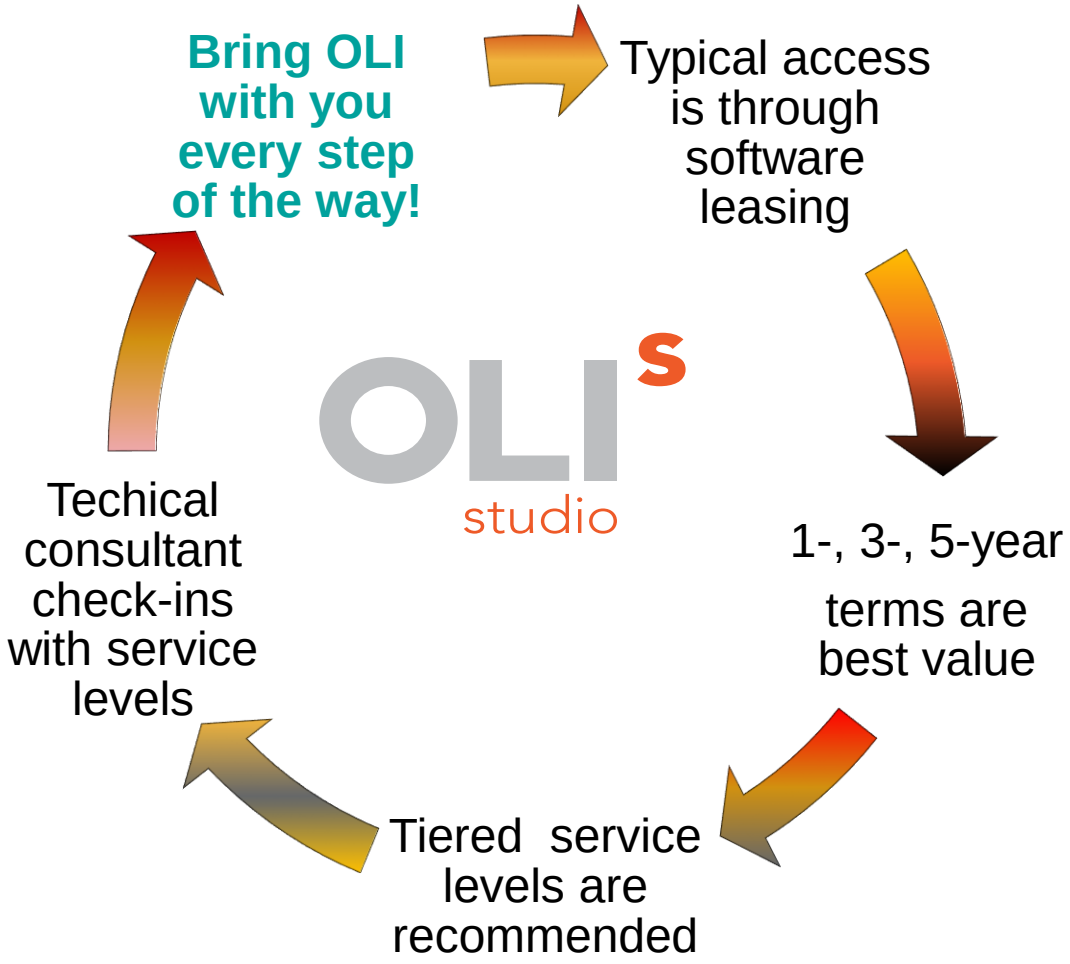
100% water to 100% sulfuric

Symbols are experimental points
Curves are OLI predictions



Your system available to you upon request

Working with OLI



Service levels to ensure your success!

Combining training, support, consulting, data validation bundles

LIMITED
Installation, configuration, break-fix and bugs

Included

STANDARD
For building confidence in your electrolyte simulation work

PREMIUM
When you want and need mission-critical success in your work

SUPERIOR
OLI onsite training and consulting to ensure your success

Pre-paid Service Levels

www.olisystems.com

Thanks for your attention!