

Electrolyte Modeling Basics (EMB) Syllabus

This 2-day course explains both electrolyte thermodynamic principles as well as hands-on training in electrolyte simulation techniques. Participants will begin by formulating problems in Stream Analyzer V3.2, the simplest and most direct way to study the OLI electrolyte thermodynamic framework. Beginning with the ionization of components in water to form charged species (e.g., $\text{NaCl} \rightarrow \text{Na}^+ + \text{Cl}^-$ in the presence of H_2O), participants study electrolyte speciation, ion pairs, complexation, and overall solution behavior. Course material works with scale tendencies, activity coefficients, and equilibrium constants. Oxidation/reduction and its impact on the physical properties of materials will be addressed. The second day of the class is tailored to the interests of those participating. Topics may include applications in electrolyte flowsheet simulation and corrosion simulation.

Day 1 Introduction to OLI Electrolytes through the Analyzer software

The first day of the course is an introduction to OLI technology through software mechanics. Participants work on standard calculations such as calculating the isothermal properties of a salt in water, boiling, dew, and precipitation points, and pH adjustments. Participants then apply these calculation types to multiple-point/survey calculations and mixtures of two or more streams. Participants then learn how water analyses are converted to process streams.

As part of this work, participants are introduced to the concept of electrolyte speciation; ionization of components in water to form charged species (e.g., $\text{NaCl} \Rightarrow \text{Na}^+ + \text{Cl}^-$ in the presence of H_2O). From this basic reaction, participants learn about ion pairs, complexation, and overall solution behavior.

General functions

- Single Point calculations
- Multiple Point calculations
- Mixer Calculations
- Water Analyses

Theories and Application

- Mixed-Solvent vs. Water-Solvent electrolytes
- Selecting Phases
- Azeotropes and other observable phenomena

Day 2 Intermediate Calculations

The first part of the second day is used to complete any first-day work and to answer software and scientific questions about OLI software. Following this users learn how to enter organic pseudocomponents using PVT data or pre-generated data.

The remaining time is reserved for working on advanced software features, such as oxidation-reduction, flowsheet simulation, electrochemical stability diagrams, Corrosion diagrams, and practical applications specific to the attendee interests.

As part of the second day, process simulation software (ESP or OLIPro) may be used.

Functions and features

- Entering Pseudo-components and Assays
- Oxidation-Reduction and Stability diagrams
- Customization options – plots, reports

(Based on participants' interests, we will select from the applications in the following two sections)

Single-point, survey, and single-unit Applications

- Distillation – vapor-liquid-solid calculations (e.g., azeotropes, column scaling)
- Cl₂ and acid gas absorption
- Sour gas and other corrosive environments
- Sublimation-salting (gas-solid equilibrium)
- Product yield – solids precipitation
- Mineral scale prediction

Multi-unit Process Simulation Application

Distillation towers

Gas scrubbing/treating

Process/Waste-water treatment

Other user applications