

## Electrolyte Modeling Basics (EMB) Course

January 2020

**Instructor:** Diana Miller, PhD

**Time:** 2 days (One 3-hour web session each day)

**Course Description:** Training in electrolyte simulation techniques using OLI Studio: Stream Analyzer

**Summary:** The Electrolyte Modeling Basics course is designed to train attendees on how to use OLI software and its underlying chemistry principles. At the end of the course, participants will be able to formulate and build their own applications and interpret the data presented in reports and plots. Participants will leave with a qualitative image of how ions and molecules behave in water and a better understanding of properties like alkalinity and pH.

### Class Content

This workshop will teach electrolyte chemistry concepts and electrolyte simulation techniques.

#### Day 1

- Introduction to **OLI Studio: Stream Analyzer** simulation
- The User Interface – Workspace and Tool bars
- Stream Definition – Enter components, composition, and conditions such as T, P, etc.
- Types of calculations (**Chapters 2 and 3**)
  - Single point calculation using variety of equilibrium methods: Isothermal flash, bubble / dew points, solubilities, set pH, etc.
  - Single and dual surveys to study trends using independent variables of T, P, composition, and pH
  - Contour plot
- Review stream results
  - Identifying the main report tables
  - Output interpretation, including customization of plots and reports
  - Contour plots
  - Exporting data

#### Day 2

- Water Analysis (**Chapter 4**)
  - Entering ionic inflows
  - Scaling Tendencies and Scaling Index
  - Converting an ionic inflow into a molecular inflow

- Mixers (**Chapter 5**)
  - Water Incompatibility
  - Titration curve
- A brief introduction to **OLI Studio: Corrosion Analyzer (Chapters 6 and 7)**
  - RedOx reactions (Chapters 1)
  - Pourbaix Diagrams
  - Corrosion rates
  - General Corrosion Rates
  - Localized Corrosion Propensity
  - Polarization Curves

You will also become familiar with the following electrolyte chemistry theory

- Electrolyte speciation, acid-base chemistry, and other common chemical reactions
- Basic electrolyte thermodynamics for equilibrium constants and activity coefficients
- Precipitation/Dissolution and vapor/liquid reactions
- Oxidation-Reduction redox potential