

## Mixed-Solvent Electrolyte Model Regression Course 2020 Syllabus

1. **Focus:** The Regression Course will focus on teaching the attendees to develop parameters for the Mixed-Solvent Electrolyte (MSE) model, which is incorporated in the OLI software. This course is for the people who want to master the OLI thermodynamic model in order to add their own chemistries.
2. **Objective:** The objective of the course is to show the attendees the full process of obtaining the MSE model parameters, which starts from collecting the relevant experimental data, learning the structure of OLI databanks using OLI Databook, creating private databanks using Chemistry Wizard, generating models and running regressions.
3. **Topics:** The course will take 3 full days and cover the following topics:
  - General information about the course and thermodynamic background
  - Speciation in chemical systems and types of data necessary for regressions
  - OLI Databook: A tool for creating and managing databanks
  - OLI Databanks: Their structure and adding new databanks
  - Chemistry Wizard: A tool for creating new models and dbs files
  - Creating and customizing chemistry models for new systems
  - Learning the structure of input files for regression and our regression program
  - Running regressions using OLI Regression Console
  - Reviewing and understanding regression output files and troubleshooting
4. **Documents:** Prior to the course, the attendees will receive the following documents:
  - Additional information (e.g., concentration conversions, apparent properties)
  - Documents (e.g., Regression Course.pptx, examples of Excel files containing experimental data)
  - A private databank PRIVDB.ddb for learning and practicing
  - Regression cases containing input and output regression files
  - OLI publications about the MSE model and its applications (pdfs files)
5. **Custom cases:** Attendees are encouraged to bring a chemistry system of their interest and relevant experimental data, which would include one or more of the following types:
  - water activity or osmotic coefficients
  - mean activity coefficients for fully dissociated salts
  - solid-liquid equilibrium data (solubility)
  - vapor-liquid equilibrium data
  - liquid-liquid equilibrium data
  - speciation (e.g. ionization or hydrolysis constants, pH)

- enthalpies of mixing or dilution
- solution heat capacity data

We would appreciate it if attendees would inform us about specific chemistries of their interest at least one week before the course. We will prepare examples that cover similar chemistries or use our standard examples during the 3<sup>rd</sup> day of the course.