OLI Information Series

think simulation | getting the chemistry right

OLI databanks
Options for adding or modifying simulation parameters

Contents

OLI databank extension options

MSE: OLI electrolyte thermodynamic framework

OLI has developed a comprehensive thermodynamic framework called MSE. This framework makes it possible to predict the properties of a stream with virtually any composition. The combination of thermochemical properties, interaction parameters, and a numeric solver enables the software to provide an accurate representation of the chemistry and phase behavior of multicomponent systems.

These thermochemical properties and interaction parameters undergo constant revision by OLI's thermophysical modeling team; a team passionate about delivering the most accurate representation of fluid chemistry available. The result is a Databank containing over 6,000 species and covering 80+ elements.

Options available for extending the OLI databank

There are occasions where this databank is missing species or interactions parameters. In such cases when species are missing (e.g., a particular solid phase), it may be critical that the species be added, if it is important to the equilibrium state of the system being studied.   In cases where interaction parameters are missing, the model may still provide 'reasonable' results, because of the robust long-term electrostatic model built into the theory. However, it is usually best to eliminate uncertainty and lower the risk by developing interaction parameters for the missing species.

In situations where a client would like to extend the OLI databank, three options are available:

- *OLI Thermophysical Modeling Service*
  OLI experts develop new species and/or new interaction parameters for the species of interest and deliver them in a private databank. This is co-funded work that will ultimately be added to the OLI databank and available to all clients. OLI provides a cost share for this option.

- *OLI Regression Service*
  OLI provides a bundle package consisting of 3-days training, OLI REGRESS and OLI Databook software, and consulting time. This package is designed to get the client started in their work and to help them be successful in developing a private databank

- *OLI Training*
  3 days of training and courtesy access to the OLI REGRESS and OLI Databook software for a one-time 6 month period. Consulting by thermophysical modelers may be purchased a la carte

OLI Thermophysical Modeling Service

With this option, clients provide a list of target component(s) that are expected in the system. OLI gives the modeling work priority treatment, and delivers early results to the client via a private databank. Clients also receive the OLI proprietary validation spreadsheet for the commissioned chemistry.

If the data used in this work is sourced from the public domain, then the new simulation parameters will be added to the OLI databank during the next major release. If the data used is private to the client (i.e., client's experimental data), this data is combined with published data, and the combined set is used to create the private database. The OLI databank will be updated using regressions from the published data only.

Types of data needed for regression

OLI conducts a literature search to locate experimental data for both pure component properties and for mixtures. The types of properties that OLI collects include:

- Vapor-liquid equilibrium (*VLE)* data
- Osmotic coefficients (or activity of water) in aqueous solutions;
- Activity coefficients in completely dissociated aqueous systems
- Solubility of salts in water, organic solvents and mixed solvents;

OLI databank extension options

- Acid dissociation constants as a function of solvent composition;
- Titration curves and pH values (as a frequently desirable alternative to the reported equilibrium constants)
- Complexation constants for systems that form complexes; in general, raw titration data are preferred to complexation constants that were obtained by processing titration curves;
- Spectroscopic speciation data, typically obtained from Raman or NMR spectroscopy
- Gibbs energy of transfer of electrolytes;
- Densities;
- Heats of mixing and dilution;
- Heat capacities

Finding sufficient experimental data for modeling

Contrary to what some clients assume, OLI has no laboratory facilities. Instead, OLI's literature search relies on extensive data mining techniques to gather all relevant published experimental data on the chemistry of interest. Sometimes there is an abundance of data (that unfortunately can on occasion be contradictory) and in other cases data is scarce.

When there is insufficient data to complete the thermophysical modeling project, the following options are available: OLI can assist the client in locating a third-party laboratory to generate the data, or OLI can use estimation methods to develop properties and parameters for some classes of components.

Time and cost of the OLI thermophysical modeling process

Once a client specifies a target chemistry including any related key components, OLI prepares a fixed cost estimate to complete this work. The estimate is based on the number of days needed to complete each species and their binary / ternary interactions. The cost is estimated based on the expected complexity of the system.

Sometimes the estimate can be staged or broken into phases. In these cases, the client can co-fund the first phase and use the simulation parameter results to show early success and motivate additional phase funding within the client company.

Work is scheduled as soon as OLI receives a purchase order for the modeling, and work can begin as soon as a contract is signed. Typically, OLI can start work on client components within a month of scheduling. The time estimate given in days is for actual time, not elapsed time. Further, if modelers encounter any difficulty, more time at OLI's expense may be accrued. Please double the amount of actual days as the first indication of when a private databank might be made available.

Why choose Thermophysical Modeling service?

This is the best choice when:
- You have mission-critical simulation work that requires the most accurate parameters possible
- You lack the interest, time or expertise to extend the databank yourself
- You would like validation spreadsheets containing the comprehensive literature search results, the experimental data from the literature, and plots showing experimental data versus OLI model results

OLI Regression Service?

The OLI Regression Service is a good choice when a client wants to establish OLI regression expertise in their organization. For this approach, OLI recommends a bundle of 3 days of training (given by OLI thermophysical modelers), access to OLI REGRESS and OLI Databook software, and a thermophysical modeling support retainer for 3 days for question and answers, and setup and interpretation guidance by OLI's modeling team. Training can be at OLI or at a client's location

Software used

OLI databank extension options

- OLI REGRESS – the actual regression software that has file-driven input
- OLI Databook – a viewer onto the OLI databank (in beta test now for general client distribution in V11

Challenges when performing OLI data regressions

OLI designed this service to ensure a client's success in developing private data. There are a few factors that led OLI to this approach:

- An extensive knowledge of OLI framework internals is needed to be successful in OLI regressions.
- Electrolytes are mathematically challenging, and this is reflected in skill level needed
- The REGRESS software is low-level with an MS-DOS-like interface that can be difficult to master in today's computing environment.
- The present OLI regression training (the three-day class in this bundle) leaves a gap between the classwork time and the skill necessary to complete a client regression.

Bundling the software, the training, and a support retainer together is OLI's best recipe for your success in performing OLI regressions.

Why choose the OLI Regression service?

This is the best choice for extending the OLI simulation parameters for your chemistry, when:

- You have an ongoing need to add components and insufficient funds to have OLI do it for you
- You have someone skilled in physical chemistry who understands regressions and can commit the necessary time to completing the work successfully
- You have company data and would like to develop a limited, local model for just your conditions

OLI Regression Training

OLI periodically offers a 3-day regression training course at OLI's office. This is a public class which needs a minimum registration of four participants. This class may also be given onsite at a client location for a client's own physical chemists.

The OLI REGRESS software is given upon request to clients; there is no charge.

The OLI Databook software, the viewer onto your private databanks, will be available for leasing in V11, or can be received as part of the bundle in the Regression Service. A courtesy evaluation copy of up to 6 months can be extended with the training

Why choose the OLI Regression Training?

This is the best choice for extending the OLI simulation parameters for your chemistry, when:

- You have limited funds available for this activity
- You have someone skilled in physical chemistry who understands regressions and can commit the necessary time to being successful at regressions
- You are able to commit the time it will take to master the subtleties of OLI internals in order to be successful in formulating your own cases

For more information

Additional resources

If you would like to understand more about OLI's electrolyte thermodynamic framework, OLI has several peer-reviewed papers. Selected papers may be accessed at http://downloads.aqsim.com/OLI-Introduction

If you would like to discuss any of the options for extending the OLI databank with simulation parameters for your chemistry, please contact OLI at oli.info@olisystems.com

Author: Pat McKenzie, OLI Systems
Contributions by: Andre Anderko, Anthony J (AJ) Gerbino, OLI Systems

www.olisystems.com