Chapter 1 **Welcome to OLI**

Who is OLI Systems?

OLI Systems was founded in 1971 by Dr. Marshall Rafal. During the past four decades OLI has developed, at a cost of almost $30,000,000, commercial computer software which has established the company as the world leader in simulating aqueous-based chemical systems

OLI's unique capability is providing the world with the only **predictive thermodynamic framework** for calculating the physical and chemical properties of multi-phase, aqueous-based systems. This framework is applicable to most multi-component mixtures of chemicals in water, and is predictive over almost any conceivable temperature, pressure and concentration of interest.

Employing this unique and powerful framework, the OLI Engine, supported by a very large, in-place databank, allows users to predict the chemical and phase behavior (including aqueous, vapor, non-aqueous liquid and multiple solids), of most mixtures of inorganic or organic chemicals in water. The resulting phase separation into aqueous, vapor, organic liquid and multiple solids is performed automatically. In the laboratory, in steady-state or dynamic process conditions or in the natural environment, the OLI Engine is broad-based and accurate.

OLI's world leadership is reflected in many ways, including authorship of AIChE's Handbook of Aqueous Electrolyte Thermodynamics. OLI software is used by nearly all of the largest companies in the Chemicals and Oil & Gas sectors of the Chemical Process Industries (CPI) as well as companies in other sectors such as Metals and Mining, Forest Products and Pharmaceuticals. In addition, OLI software is used extensively in Environmental, E & C and Basic Research.
OLI has created several widely-used products:

OLI Engine

OLI's aqueous thermodynamics are at the heart of the OLI software. OLI Engine refers to the thermodynamic database, thermodynamic framework, and supporting numerical computation to simulate the chemical and phase behavior of aqueous-based systems.

OLI Studio

Never has aqueous chemistry problem solving been easier. The OLI Studio combines ease of learning, ease of use with the power of the OLI Engine. It supports single and multiple point calculations, utilizing OLI's extensive PUBLIC databanks. **Ionic input is possible.** The OLI Studio allows customers to input, store, manipulate, adjust and reconcile laboratory data, with facilities to adjust laboratory errors in pH and charge balance.

OLI Express

Prior to the Analyzers, access to the OLI Engine was through OLI Express. It supports single *ScratchPad* and parametric *Survey* calculations for investigating chemical behavior, pH, solubility, multiple phases, speciation, and other phenomena.

Environmental Simulation Program (ESP)

ESP is OLI's **steady-state flowsheet simulation** package capable of simulating rigorous environmental unit operations including stripping/scrubbing, pH control, ion exchange, biotreatment, clarification, UF/RO, electrodialysis, and many others. Feedback control and recycle convergence are included.

Corrosion Analyzer (now part of the OLI Studio)

CSP provides a framework to **analyze metal and alloy redox solution chemistry** for any mixture of chemicals at almost any condition of interest. The package provides for real-solution stability diagrams (e.g., Pourbaix and Yield) and accurate prediction of electrical conductivity and ORP. CSP supports calculation of predictive rates of corrosion for a limited set of chemistry.

DynaChem

Dynamic is a **flowsheet simulation** package for time-dependent and transient processes. DynaChem includes support for scheduled entry feeds, PID control, open and closed loop, feedback and feed-forward, multi-cascade, adaptive gain, pH, compositional control and many others. Operator intervention to introduce upsets, manually adjust valves and control settings is also possible.

OLI Studio ScaleChem

OLI Studio ScaleChem is OLI's solution for **oil-field applications** including surface and subsurface mineral scale prediction, saturation profiles, and produced/formation water mixing. OLI Studio ScaleChem is based upon accurate fitting of binary, ternary and quaternary data up for several common scales, and many more "not-so-common" scales!

OLI is comprised of an extraordinary staff of advanced degree scientists and engineers who enable OLI to maintain a high-level of Research & Development while offering a full range of Support Services and Professional Services.

What does OLI Systems do?

As the recognized experts in modeling aqueous electrolyte thermodynamics, backed by a large in-place databank, we provide computer software tools to solve your problems quickly and accurately for:

Aqueous Simulation

It is essential for scientists and engineers to understand the effects of aqueous chemistry of their processes. This includes the effects of trace components, pH, temperature, and other factors on their process systems. Over the past 30 years, OLI has refined software which accurately models multiphase, multi-component aqueous solutions for virtually any mixture of chemicals. The basis for OLI's Software is the "OLI Engine." The OLI Engine is made up of the Solvers and the Databanks.

The OLI Databank contains proprietary coefficients for the prediction of thermodynamic, transport, and physical properties for **80 inorganic elements** of the periodic table, and their associated aqueous species, as well as **over 8000 organic species.** Thus, most mixtures of chemicals in water can be modeled, provided the solvent of the solution is water.

Upon the user's request, the aqueous model can incorporate redox chemistry, co-precipitation and reaction kinetics. Also available are surface phenomena such as ion exchange, surface complexation and molecular adsorption. Transport properties such as electrical conductivity, viscosity and diffusivity are also available.

Oil-Field Chemistry

ScaleChem is software which assesses potential scaling problems for oil-field applications. The ability to calculate the high temperature and pressure effects typically found in oil-field production is solved using the OLI Engine. OLI Systems is a recognized leader in the world of aqueous chemistry, and has a generalized modeling capability, the OLI Aqueous Thermodynamic Model which is being applied here specifically to the problems of the oil-field industry.

Corrosion Chemistry

Most corrosion problems are addressed by treating the symptoms. A treatment plan would constitute:

- ***measuring corrosion rates,***
- ***determining life expectancy,***
- ***Regularly replacement of corroded material and equipment.***

Corrosion Analyzer and CSP are unique software used to investigate **the Rate of Corrosion** and determine the **causes of corrosion before they happen**, allowing preventive actions to be evaluated and implemented. This includes choosing correct operating conditions and corrosion resistant materials.

Elemental and alloy metal oxidation and reduction reactions for 79 inorganic elements and thousands of species are available in the OLI Databank. The software automatically generates the redox reactions and the resulting species and solves for the equilibrium conditions using its predictive thermodynamic model.

Because of OLI's unique, predictive aqueous model featuring accurate activity coefficients, the corrosion software offers a few types of real-solution diagrams for your analysis. Our competitors only offer idealized solution diagrams and none of a general prediction of rates of uniform corrosion.

Real Solution Pourbaix Diagrams

Graphical depiction of EH vs. pH for any mixture of chemicals in water is available to evaluate stable and meta-stable corrosion and redox products. This allows assessment of the effect of passivating species in real solutions without any simplifying assumptions.

Real Solution Stability Diagrams

Flexible selection of independent variables and graphical depiction of local and global equilibria in various projections is available in CSP. Depictions include EH vs. composition and composition vs. pH for any chemical mixture, including trace components, to assess stable and meta-stable species in real solutions.

Uniform corrosion rates and predicted polarization curves are featured in OLI's unique Rates of Corrosion calculations. Single-Point and Multiple-Point calculation points are available.

Process Modeling

The Environmental Simulation Program (ESP) is a steady-state process simulator with a proven record in enhancing the productivity of engineers and scientists. With applications industry-wide, the software is not only applied to environmental applications but to any aqueous chemical processes.

A wide range of conventional and environmental unit operations are available:

Mix	**Precipitator**	**Feedforward**
Split	**Extractor**	**Crystallizer**
Separate	**Component Split**	**Clarifier**
Neutralizer	**Incinerator**	**Sensitivity**
Absorber	**Compressor**	**Membrane (UF, RO)**
Stripper	**Bioreactor**	**Electrodialysis**
Reactor	**Manipulate**	**Saturator**
Exchanger	**Controller**	**Dehydrator**

ESP provides the engineer or scientist accurate answers to questions involving complex aqueous systems. Design, debottlenecking, retrofitting, troubleshooting and optimizing of existing or new processes is easy with ESP. Upstream waste minimization, as well as the waste treatment itself, is possible with ESP. The dynamic response of a process can be studied using the dynamic simulation program, DynaChem, to examine control strategy, potential upsets, scheduled waste streams, controller tuning, and startup/shutdown studies.

Process Flow-sheeting and Control

Process flow-sheeting with multiple recycles and control loops are allowed. Feed-forward and feedback Controllers and Manipulate blocks help to achieve process specifications.