

IDEAS

OLI thermodynamic engine



The challenge: To accurately predict the type, quantity, and physical state of components in a process



The solution: Simulate. Predict. And profit.

IDEAS OLI is an advanced thermodynamic engine that helps to predict the type, quantity, and physical state of the components in a process.

The IDEAS OLI engine combines the user-friendly capabilities of the IDEAS simulator with OLI, the world's leading solver for aqueous speciation.

The IDEAS OLI engine works together with IDEAS to conduct a variety of steady-state mass and energy balances complete with chemistry predictions.

It can also provide more dynamic predictions, such as reactions in tanks. For example, the mass fractions in tanks are calculated auto-

matically, so the final chemistry (for example, pH) can be plotted at each time step. The IDEAS OLI engine even lets the user predict reactions in pipes, such as precipitation and heat exchanger reactions. A full list of features is provided below.

Extensive phases

Large multicomponent systems can be modeled using the OLI software. The solution engine covers not only complex aqueous systems, but also nonaqueous, organic, and inorganic components including solids, liquids, and gases.

Chemistry prediction

With the specialized databases available, the OLI engine can predict the chemistry of multiphase systems (for example, aqueous liquid, vapor, organic, and solid) at al-

most any condition, with an effective range from -50 °C to 300 °C, 0-1500 bar and 0-30 molal.

Redox chemistry

OLI provides for the option of automatically including redox chemistry thermodynamics. A databank supports calculations involving redox of pure metals as well as alloys.

Combined with our in-place databank, redox chemistry can be studied for real solutions, including trace components.

Solid surface/aqueous sorption phenomena

OLI provides for the possibility of partitioning to a solid phase via coprecipitation, surface complexation, ion exchange or molecular adsorption (including carbon adsorption).



Benefits

- Complete steady-state mass and energy balances with chemistry predictions
- Predict tank reactions with mass fractions to plot final chemistry
- Predict precipitation and heat exchanger reactions in pipes



Predictive models for principal transport properties

OLI provides rigorous predictive models and supports databanking for electrical conductivity, viscosity, and self-diffusivity over the full range of conditions.

Thermodynamic and derived thermodynamic properties

OLI has a large thermodynamic database that covers most periodic elements. This includes the aqueous phase speciation, along with associated phases speciation chemistry and thermodynamics, for 79 inorganic elements and more than 3,000 organic molecules, including many organic electrolytes.

OLI provides for the rigorous computation of the principal thermodynamic properties including Gibbs free energy, enthalpy, entropy,

heat capacity, and volume. It also supports derived thermodynamic properties such as density, osmotic pressure, and ORP. The following items are included in the IDEAS OLI product:

- OLI Databanks: PUBLIC, GEOCHEM, LOTEMP, and COMPLEX
- OLI Interface DLLs: AUTOGEN and HYPCALC
- IDEAS OLI libraries: Material Properties OLI and Transmitters OLI
- OLI Data Locator Program: This stand-alone program assists users in translating the OLI species names to conventional as well as IUPAC names

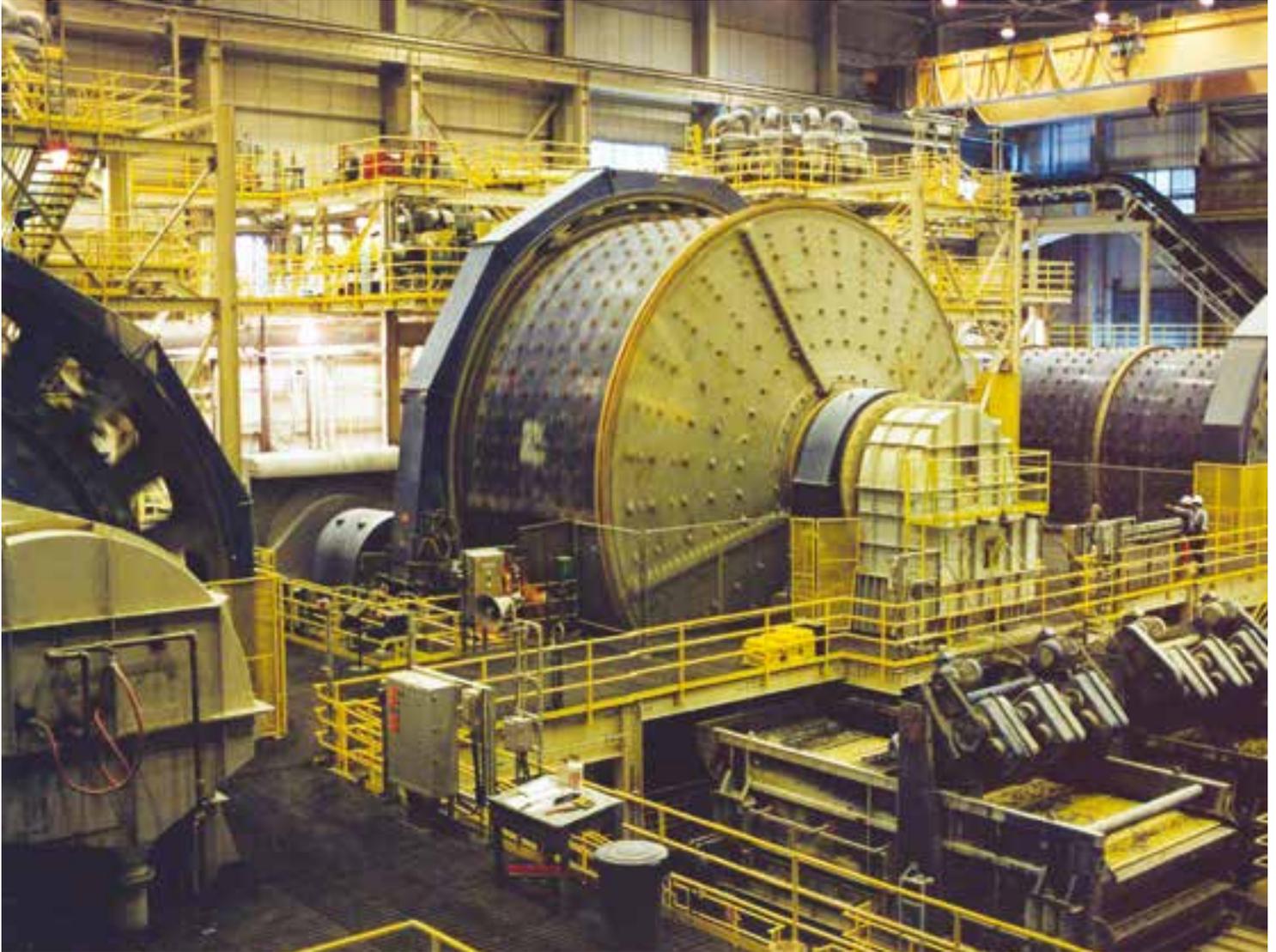
Other OLI products available

In addition to OLI integration within IDEAS, we are also able to offer these other OLI programs:

- Corrosion Simulation Program: This stand-alone tool provides the calculation of metal and alloy redox stability at almost any aqueous chemical condition of interest. Real-solution stability diagrams (for example, Pourbaix and Yield) can be plotted along with accurate prediction of electrical conductivity and ORP.
- OLI Column: This steady-state object can be used as a distillation column, steam stripper, absorption column, liquid-liquid extraction column, as well as a reactive distillation column. This object must be used to model a primarily aqueous system.

Automation solutions

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