OUTOTEC HSC CHEMISTRY

Outotec HSC Chemistry is the world's most popular thermochemical calculation software. Its modeling and simulation platform is a valuable tool for process research, development, design, and digitalization, as well as for estimating variables such as process efficiencies, yields, and environmental footprints. The software makes it possible to carry out quick and easy thermodynamic and mineral processing calculations on a standard computer.

BENEFITS

- Develop new processes and improve existing ones through modeling and simulation
- Develop process flowsheet models and test ideas prior to lab or pilot stages
- Apply complex calculations in minutes
- Estimate the environmental footprint of processes for Life Cycle Assessment
- Apply complex process theory in an easy-to-use format
- All the tools and databases you need in a single package

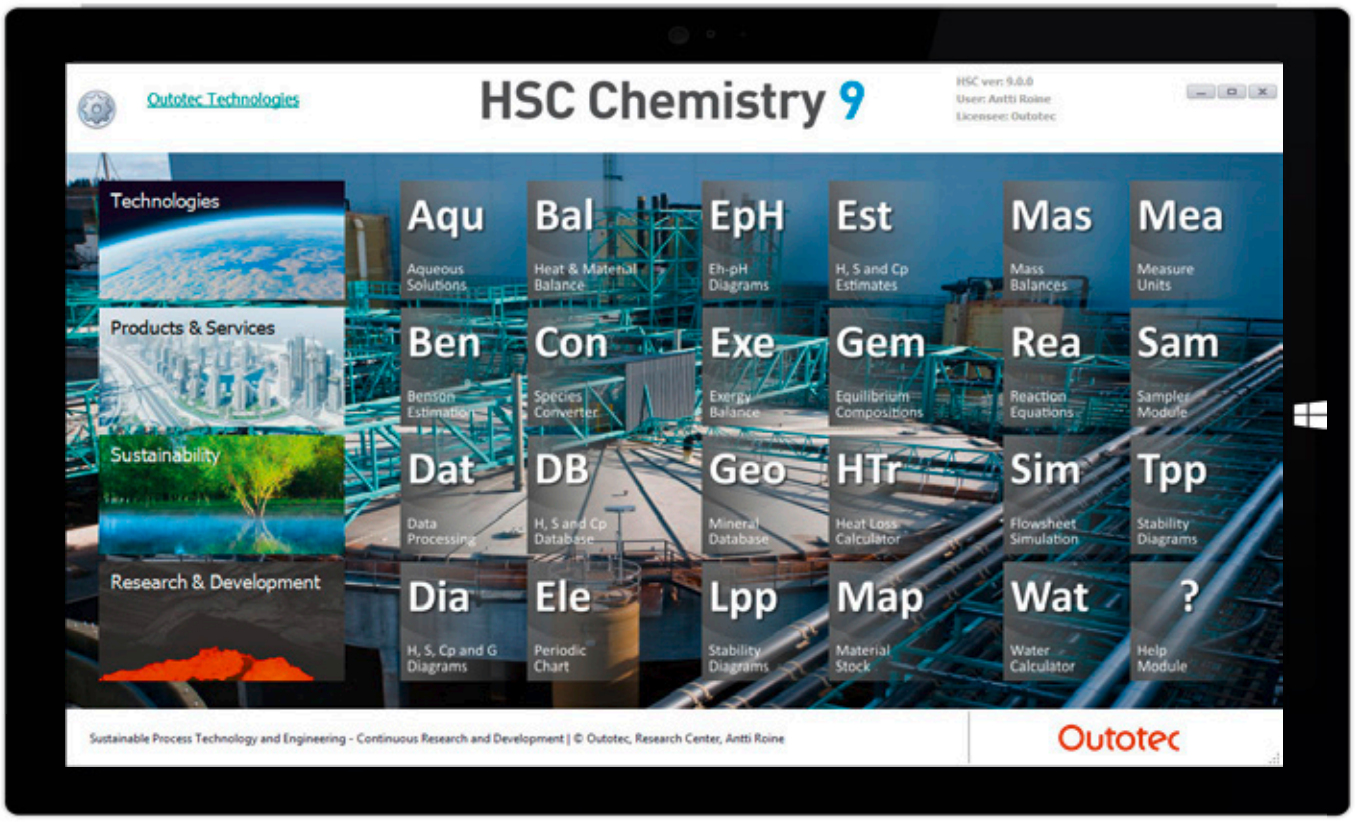
MAKE ELEMENTS WORK FOR YOU

Every element has its own unique features and properties that determine how it behaves in chemical molecules, species, and processes. Outotec HSC Chemistry helps you to understand, control, and master this behavior in chemical processes.

HSC is one of the first software packages to combine versatile chemical, thermodynamic, and mineral-processing features. Thermochemical calculations are useful, for example, when developing new chemical processes and improving existing ones. Because the software enables you to make quick and easy calculations using a standard computer, it has a wide range of educational, industrial, and research applications.

HSC also contains modules for mineral processing and particle calculations, which are integrated with an extensive mineral database.

Modules and databases are accessed via a dynamic and fully customizable menu.



Available at www.outotec.com/HSC

HSC CALCULATION MODULES

The modules included in HSC Chemistry have been designed to help solve real problems in industrial processes or to decrease the amount of expensive trial-and-error chemistry at the R&D stage. The software contains 24 modules connec-ted to 12 integrated databases. The modules operate like independent programs, each with its own interface.

Rea – Reaction Equations module

The Reaction module is used to analyze chemical reaction equilibrium and energy requirements, and for calculating dissolution heats and vapor pressures. It features an illus-trative and intuitive user interface, as well as comprehen-sive graphing tools. Calculation results can be collected on several sheets, allowing comparison and visualization of the results on the graphs.

Bal – Heat & Material Balances module

The Heat & Material Balances module is used to esti-mate the heat and material balances of one or more balance areas. It includes an intuitive user interface and graphing tools, as well as predictive text entry for chem-ical formulas. Users can modify the interface according to their own requirements. The module also calculates exergy balances.

HTr – Heat Transfer module

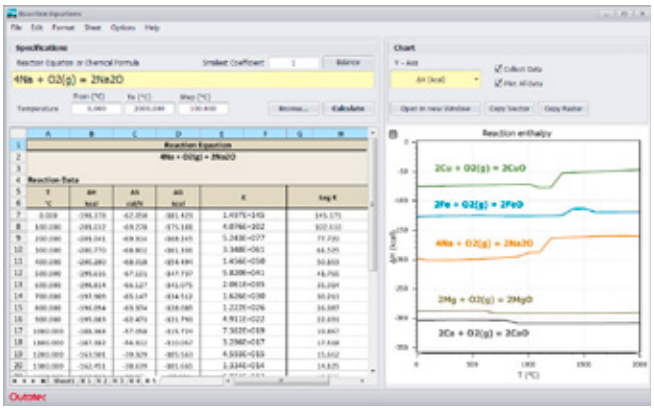
The Heat Transfer module estimates the heat losses and heat transfer of reactors of varying capacities and with given walls and linings, making it an extremely useful tool during the thermal design stage. It features a clear and easy-to-use interface, simple measurement unit changes, extensive and up-to-date databases, as well as data refer-ences. The "Specify Layer Type" dialog makes it easy to specify layer properties.

Gem – Equilibrium Compositions module

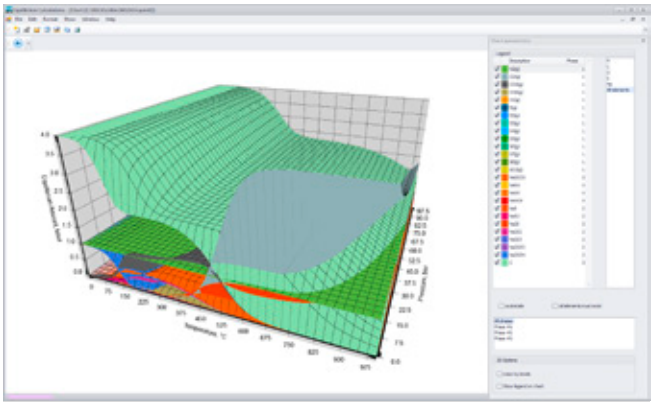
Gibbs equilibrium calculations are a practical way to investigate and study the effect of raw materials and process variables on the products of chemical reactors. This helps when estimating recovery levels, identifying opportunities to reduce the environmental footprint of the reactor, and setting the limits of sustainability before proceeding to the lab stage. The Gibbs Energy Minimiza-tion (GEM) method is used in the calculations.

Gem – Cell Equilibrium module

Cell calculations have been integrated into the Equi-librium module. These calculations use the same GEM routine as the main equilibrium module, making it possible to calculate the phase compositions and cell volt-ages of electrochemical cells and plot 2D and 3D charts in electrochemical systems with the discharge level on the x-axis.



Screen capture from the Rea - Reaction Equations module



Screen capture from the Gem - Equilibrium Compositions module

The software contains 24 modules connected to 12 integrated databases.

HSC CALCULATION MODULES

Aqu – Aqueous Solutions module

The Aqueous Solutions module contains non-ideal aqueous electrolyte models and databases. It estimates a number of water-solution properties – such as activity coefficients, enthalpies, boiling point elevations, and freezing point depressions – as a function of composition and temperature. The module works as a standalone tool for calculating water solution properties, but can also be used to estimate the behavior of water solutions in the equilibrium module.

Tpp – Stability Diagrams module

The Tpp Stability Diagrams module calculates phase-stability diagrams using partial pressures on both axes, or with temperature on the x-axis and partial pressure on the y-axis. This module calculates the diagram on the basis of minimum Gibbs energy.

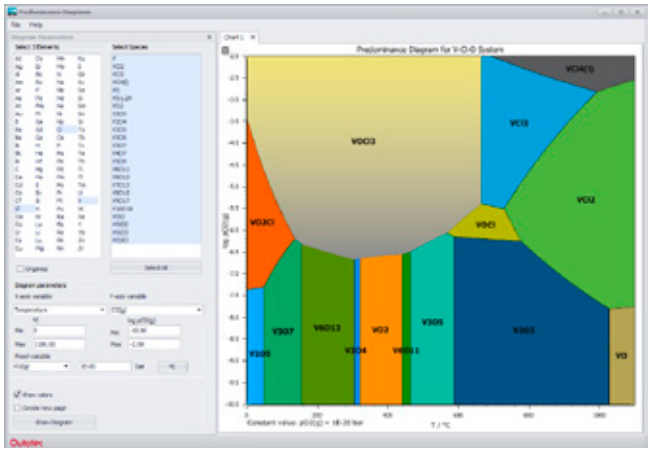
Lpp – Stability Diagrams module

Lpp stability diagrams show the stability areas of condensed phases in a ternary system in isothermal conditions, with the remaining constraints on the other axis. This module generates isothermal phase-stability diagrams of three-element systems. These are also known as predominance area diagrams or Kellogg diagrams.

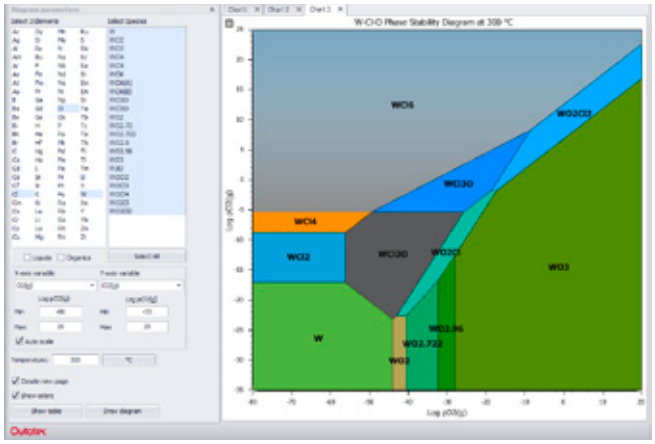
EpH – Eh-pH Diagrams module

E-pH diagrams, also known as Pourbaix diagrams, show the thermodynamic stability areas of different species in water solutions. These areas are presented as a function of pH and electrochemical potential scales. Usually, the upper and lower stability limits of water are also shown as dotted lines. This module makes it possible to create diagrams with any combination of temperature, concentration, and element, unlike traditional Pourbaix handbooks, which give only a limited number of combinations.

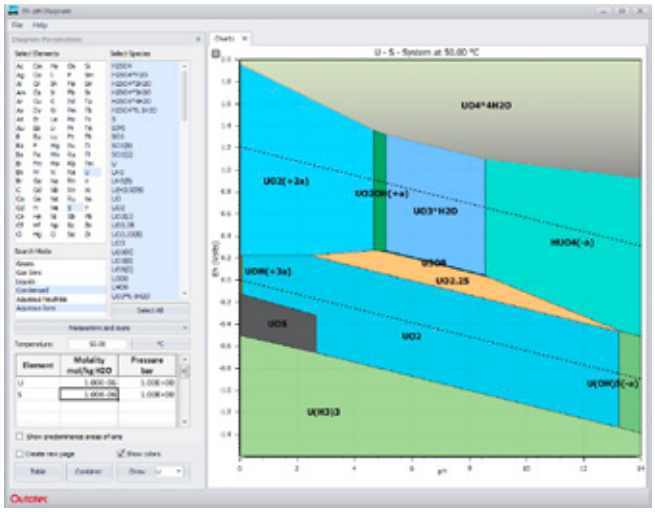
With the high-quality charting routine you can create visually impressive diagrams for reports and publications.



Screen capture from the Tpp – Stability Diagrams module



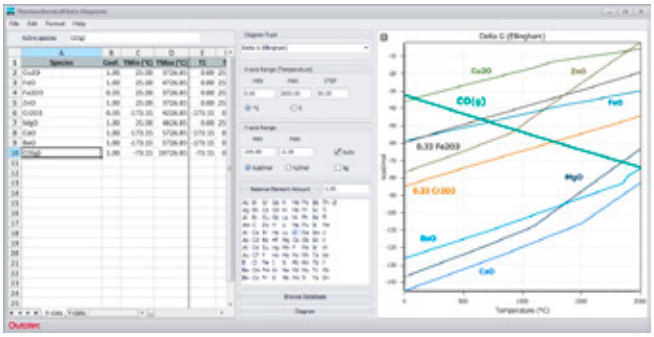
Screen capture from the Lpp – Stability Diagrams module



Screen capture from the EpH – Eh-pH Diagrams module

Dia – H, S, Cp, G Diagrams module

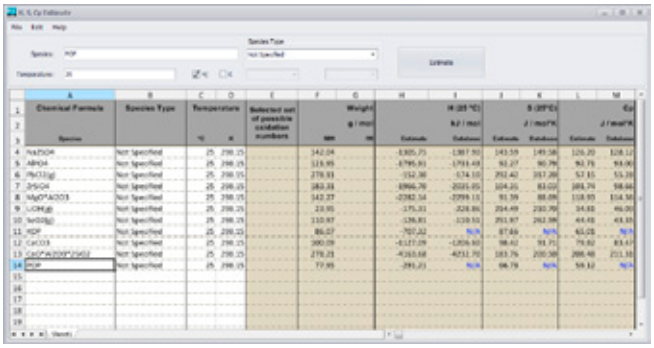
The Diagrams module presents the basic thermochemical data for a given species in graphical format. Eight different diagram types can be drawn as a function of temperature. One of the most useful is the ΔG diagram (Ellingham diagram), which shows the relative stability of various oxides, sulfates, chlorides, and so on as a function of temperature.



Screen capture from the Dia – H, S, Cp, G Diagrams module

Est – H, S Cp Estimation module

The Estimation module gives a rough estimate of the H, S, and Cp values of any chemical species or non-stoichiometric mineral. For those that are included in the HSC database, the module can also give the experimental value. It also gives the oxidation states of the elements in a given chemical compound.

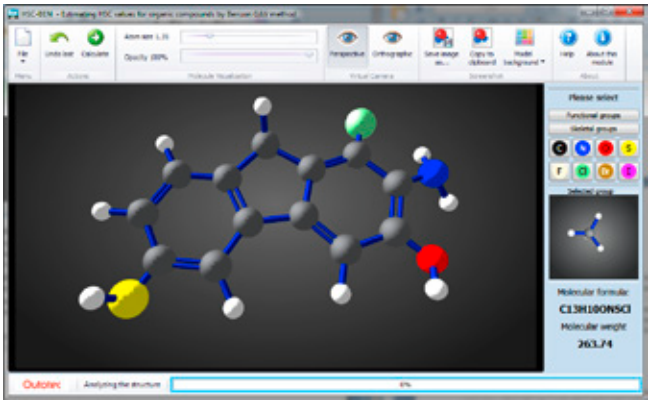


Screen capture from the Est – H, S, Cp Estimations module

Ben – Benson Estimation module

This module estimates the H, S, and Cp values of organic chemical compounds. It is also useful for estimating the properties of complex mixed organic scrap, chemicals, residues, and so on. The number of chemical species is increasing rapidly, with over 90 million identified so far, and estimation routines have an important role because 99.9% of the experimental H, S, and Cp values are missing.

HSC Chemistry's extensive databases and estimation routines form a solid basis for process models.

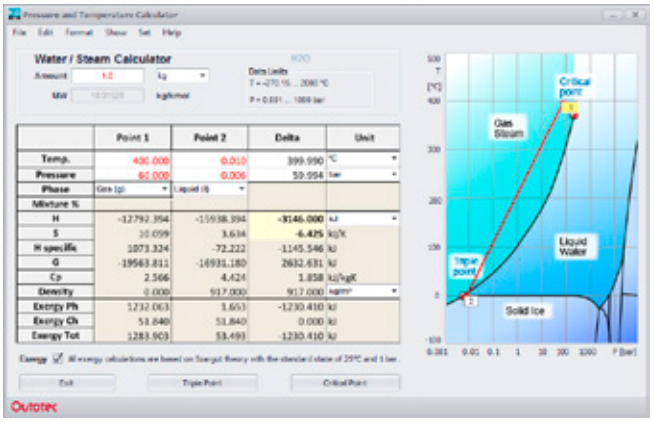


Screen capture from the Ben – Benson Estimation module

HSC CALCULATION MODULES

Wat – Water module

The Water module is a very useful replacement for steam-table books and Mollier diagrams. They also provide enthalpies and other quantities using the same standard states as other HSC modules. The process enthalpy and entropy are calculated along with several other useful thermodynamic data by manually entering the pressure and temperature of the water system, or simply by clicking on the diagram.



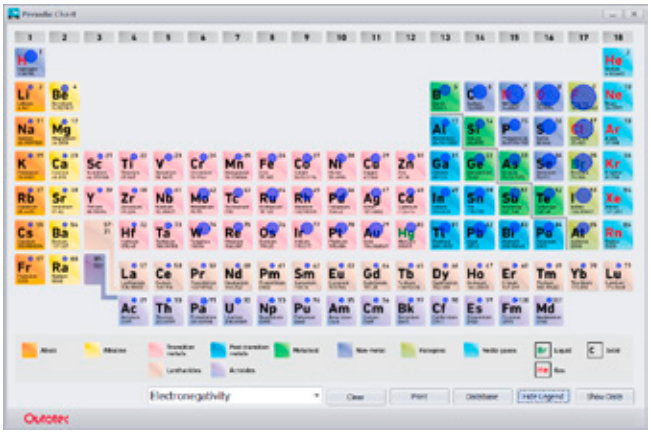
Screen capture from the Wat – Water module

Mea – Measurement Units module

Traditionally, several types of energy, temperature, mass, and volume units have been used in thermochemical calculations, meaning that conversions are needed to compare results from different sources. The Measurement Units module enables quick unit conversions in thermochemistry and in other engineering fields.

Ele – Periodic Chart module

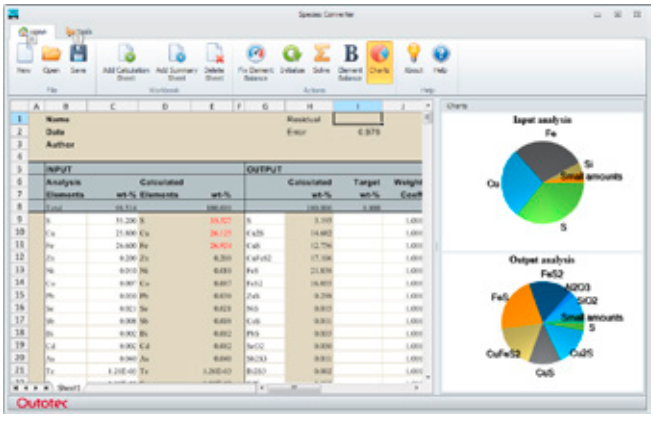
The Periodic Chart module shows the properties of the 56 elements in the database, in both tabular and graphical format. These properties can be easily edited, and new properties and additional data can be added. This module is a dynamic periodic table featuring visual effects and an editable database, and is therefore a very useful tool for visualizing and understanding the properties of elements.



Screen capture from the Ele – Periodic Chart module

Con – Species Converter module

The Species Converter module is a data reconciliation tool that converts elemental analyses into any required species analyses and vice versa. It can also be used to convert elements to non-stoichiometric species. Usually, converting chemical species to elements is easy, but the reverse conversion using inaccurate experimental data is much more challenging.



Screen capture from the Con – Species Converter module

Exe – Exergy Balance module

The Exergy Balance module calculates the exergies of chemical species and energy streams. These calculation routines are used in many other HSC modules. Exergy analysis is used in industrial ecology to measure the amount of usable energy when designing more sustainable processes.books, which give only a limited number of combinations.

DB – H, S, and Cp Database module

The Database module's versatile search and edit functions are integrated into one powerful search dialog. Users can carry out searches based on elements, species, keywords, and so on. The module has a simple and intuitive user interface and includes predictive text entry for chemical formulas. The databases include 28,000 chemical species.

Geo – Mineral Database module

The Mineral Database module contains a collection of tools originally developed for geologists and mineralogists. However, these tools may also be useful for other professionals. This module offers an extensive database with data on over 13,000 minerals. The module has an intuitive user interface and versatile database tools that enable, for example, complex filtering criteria for the mineral database. The mineralogy calculation tool enables complex element/mineral conversions.

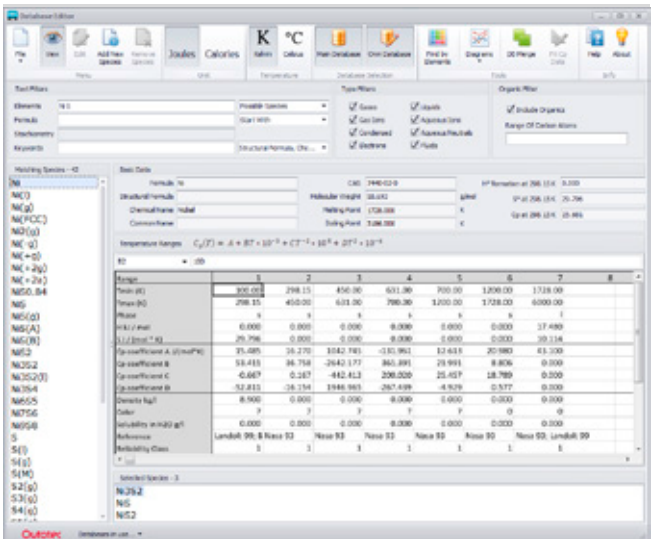
Excel add-in functions

With add-in functions, the HSC database and functions can be used in HSC's built-in spreadsheet editors and in Microsoft Excel, making it possible to carry out thermochemical and mineralogical calculations in Excel spreadsheets. There are more than 100 different add-in functions available.

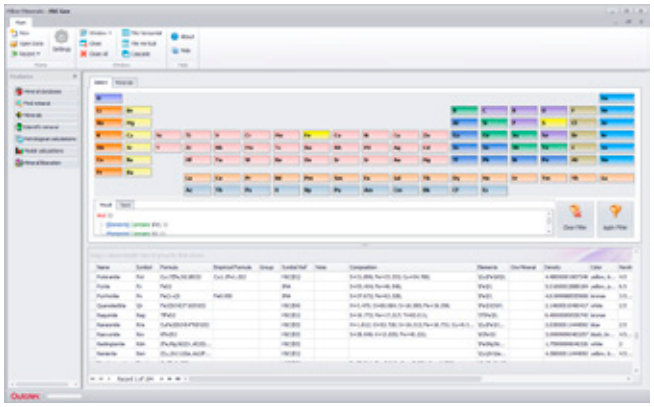
In the Sim module these functions turn unit models into small "HSC engines". For example, the StreamEQ function calculates the equilibrium composition for given raw materials and temperature. Similar HSC internal functions may be called from your own .NET applications.

Help module

The Help module contains manuals for all HSC modules and databases. Keyword searches can be carried out in all manuals.



Screen capture from the DB – H, S, and Cp Database module



Screen capture from the Geo – Mineral Database module

HSC Chemistry's modules are designed to help you find solutions to practical questions in process R&D.

SIM – FLOWSHEET SIMULATION MODULE

The Sim module is a versatile flowsheet simulation platform for many different types of process models. Users can easily create Excel- or DLL-type customizable unit operation (reactor) models and connect them using a flowsheet. The module can be used to create process models for hydrometallurgical and pyrometallurgical systems, as well as for minerals processing and physical recycling systems.

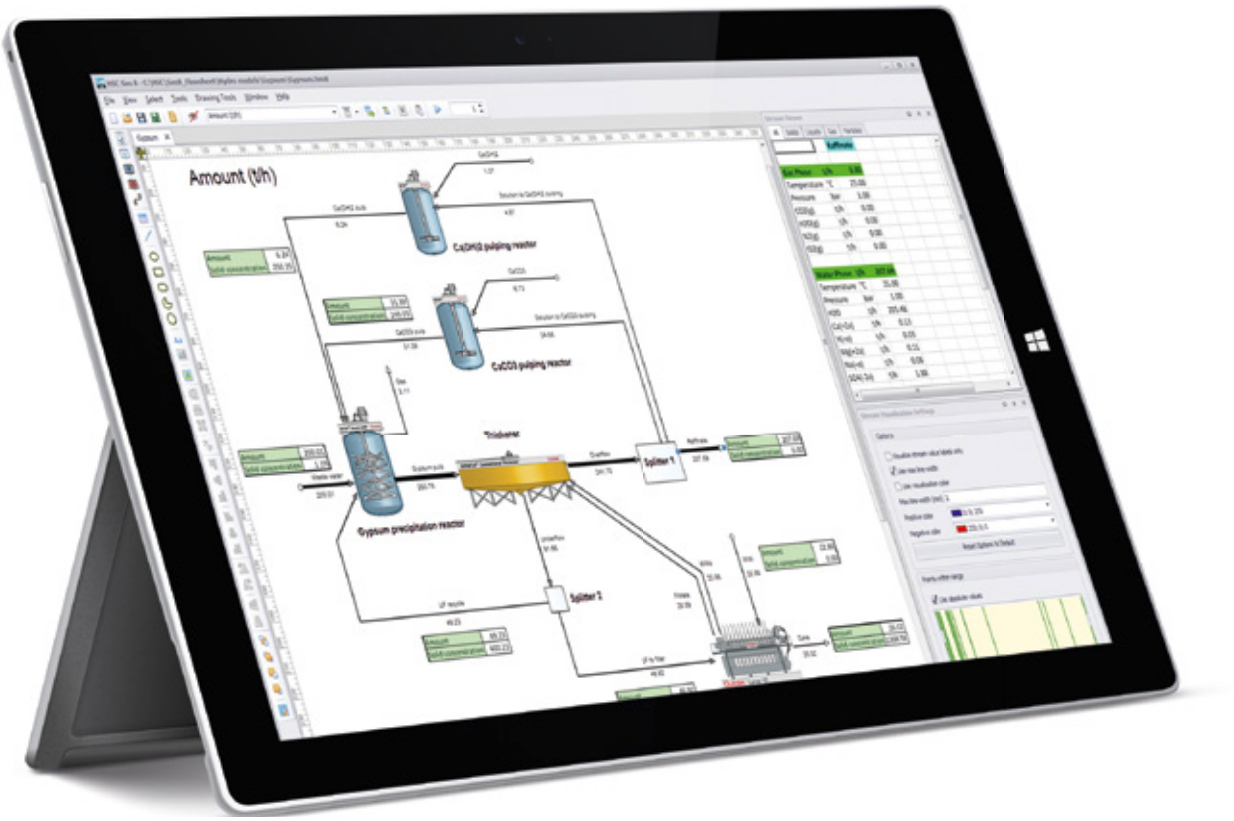
Most HSC Chemistry modules enable simulation of chemical reactions in a single process unit. The Sim module extends this capability to a whole process consisting of multiple units. Modeling and simulation are the most important tools when developing new processes and improving existing ones. The process calculations derived from these tools are the basis for the design, dimensioning, and engineering of reactors, plants, and systems.

CAPEX, OPEX, and LCA

The cost, energy efficiency, and environmental impact of a process – which determine the CAPEX and OPEX – are established in the modeling stage. This stage also harmonizes the various different procedures to enable realistic environmental footprint calculations with valid material and energy balances.

The module has many useful features, including tools for LCA (Life Cycle Assessment) environmental footprint calculations, exergy calculations, and distribution specifications. The LCA tool makes it possible to estimate the eco-balances of processes by exporting data in formats compatible with third-party LCA software.

The sophisticated Mass Balance module uses experimental data to calibrate the theoretical process models, while the converter module makes it possible to convert mineralogical materials streams to the stoichiometric chemical species needed in chemical process models.



UNIT OPERATION MODELS

With the Sim platform the user can create Excel or DLL-type unit operation models. Predefined templates are divided into four categories (modes): Reaction, Distribution, Particle, and Other. The unit models and types share several common features.

Particle mode

Unit operation calculations are based on particle distributions. This mode is often used in minerals processing and physical recycling. Typical unit operations are crushing, grinding, flotation, gravity separation, and screening.

Reaction mode

Reaction mode unit operation calculations are based on chemical reactions, i.e. the process models are described by a relevant selection of chemical-reaction equations. The Reaction mode unit editor contains wizards to make model development easier. This mode is typically used in hydrometallurgical processes.

Distribution mode

Distribution unit operation models are based on element distributions. This makes it possible to calibrate theoretical mass and energy-balance models with experimental distribution data. This mode is typically used in pyrometallurgical processes.

Mass Balance module

Experimental process data usually requires harmonization by data reconciliation. Such data is often incomplete and contains errors, leading to problems when applying the data to process models.

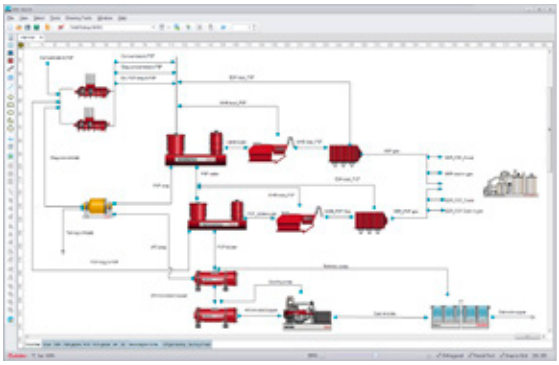
The Mass Balance module uses complex data reconciliation techniques to convert incomplete experimental process data to balanced data. This makes it possible to calibrate theoretical process models or simply to create consistent analyses for yield and efficiency estimates for complete energy and material-flow systems. This module is connected to the Sim module. The Sim Model Fit tool enables the conversion of balanced experimental data into model parameters.

Screen capture from the Mass Balance module

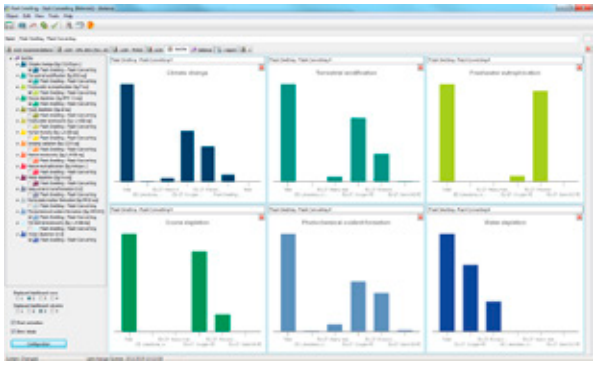
Unit operation models provide unique flexibility when creating process models. Scaling and pricing calculations, as well as other post-processing tasks, can be carried out using the built-in Excel emulator.

ASSESSING ENVIRONMENTAL IMPACT WITH THE SIM MODULE

Best available technologies, flowsheets, and recycling system maximizing resource efficiency – benchmarks



Environmental indicators based on industry benchmarks



Examples of SIM module calculation outputs

- Mass and energy balances
- $US/t product (CAPEX and OPEX)
- Recyclability index (based on system simulation of whole cycle)
- Energy: GJ and MWh/t product (source specific)
- Exergy: GJ and MWh/t product
- kg CO_2/t product
- kg SO_x/t product
- g NO_x/t Product
- m^3 water/t product (including ions in solution)
- kg residue/t product (including composition)
- kg Fugitive Emissions / t product
- kg Particulate Emissions / t Product

Examples of environmental impact software outputs

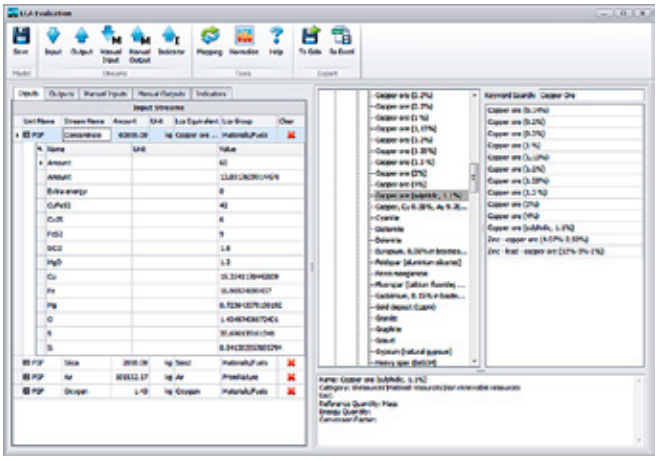
- ReCiPe (and similar) – endpoint estimation
- Global Warming Potential (GWP)
- Acidification Potential (AP)
- Eutrophication Potential (EP)
- Human Toxicity Potential (HTP)
- Ozone Layer Depletion Potential (ODP)
- Photochemical Ozone Creation Potential (POCP)
- Aquatic Ecotoxicity Potential (AETP)
- Abiotic Depletion (ADP)
- Water Footprint (Green, Blue, Gray)

The LCA tool is integrated into the Sim module, enabling real life-cycle analysis of the process. The tool automatically collects process input and output streams and calculates a few key indicators such as carbon dioxide emissions.

Sim process models are based on material and energy balances; this automatically leads to thermodynamically accurate eco-balances. This is the main advantage of simulation-based eco-balances over conventional LCA methods, which often do not meet critical element and energy-balance boundary conditions.

For environmental impact assessment, the Sim module combines process simulation functionality with the LCA functionality of third-party software such as GaBi. This provides a rigorous mass and energy balance as well as a techno-economic basis for LCA, and thus links environmental impact analysis to technology.

The LCA tool makes it possible to optimize the whole process not only from the technical and economic point of view, but also from the perspective of its environmental impact. It is critical to do this at the process design stage as it is difficult and expensive, or even impossible, to make changes during the engineering, construction, and start-up stages.



Screen capture of the LCA tool

For more information please visit www.outotec.com/HSC

Finland, August, 2016

Outotec provides leading technologies and services for the sustainable use of Earth's natural resources. As the global leader in minerals and metals processing technology, we have developed many breakthrough technologies over the decades for our customers in metals and mining industry. We also provide innovative solutions for industrial water treatment, the utilization of alternative energy sources and the chemical industry. Outotec shares are listed on NASDAQ OMX Helsinki. **www.outotec.com**

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