Outotec's HSC 8.0 Chemistry Software

Outotec, the global leader in sustainable minerals and metals processing technology, announces a major update to its HSC Chemistry software. HSC 8.0 – the latest version of the world's most popular thermodynamic calculation software – boasts 18 completely redesigned modules, two new modules, an updated database containing more than 28,000 compounds, and numerous other new features.

HSC 8.0 also introduces significant improvements to the user interface and reporting quality, as well as support for 64-bit Windows 7 and 8 operating systems. The software has been rewritten using the latest Microsoft .NET 4.5 environment, which enables seamless interaction between all modules, and harmonization of formats, settings, and other user-defined functions.

HSC's extensive set of tools and databases can be used to improve existing processes and develop new ones, while uniquely integrating these to quantify the sustainability and resource efficiency of reactors for complete system solutions. 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 – all of which form the basis for Opex and Capex estimation. The software makes it possible to test new process ideas and apply established optimal process conditions for laboratory and pilot-testing campaigns.

The modules and databases are accessed via a new dynamic main menu that can be customized by the user. HSC also brings improved calculation routine accuracy, adds a common chart tool for all modules with 3D features, and expands the capabilities and performance of the built-in Excel emulator. The simpler and more intuitive interface will enable deeper process and sustainability analysis of metallurgical, energy, water, and material-flow systems based on HSC's proven thermochemical modeling capabilities.

HSC now also provides unique new environmental functionalities such as the new Exergy module, which enables easy calculation of material stream exergy to support LCA environmental footprint estimates of complete flowsheets. The updated Sim 8.0 module with improved dialogues and interfaces includes tools such as LCA environmental footprint calculations and interfaces to LCA software.

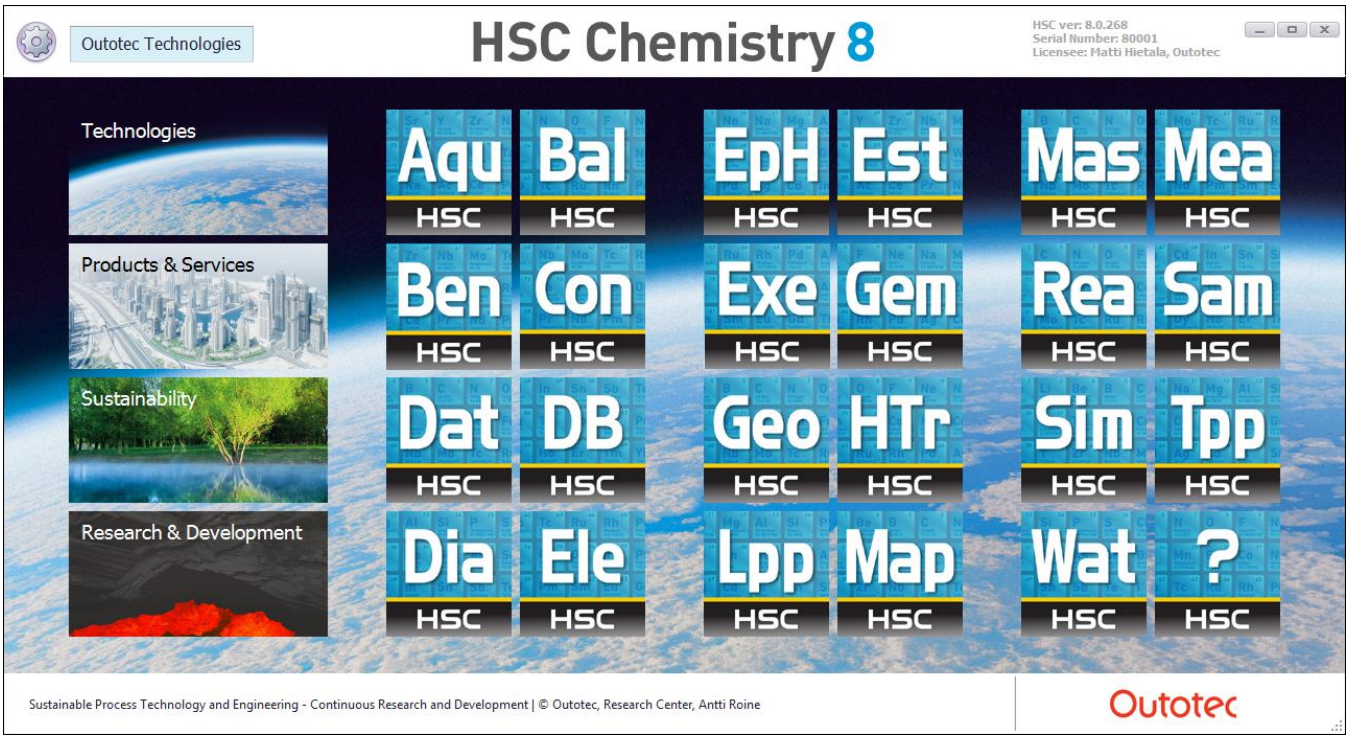
The completely new Benson estimation module makes it possible to estimate the H, S, and Cp values of organic compounds based on the molecular structure using easy graphical user interface.

These are just a few examples of the new and updated functionalities that can be found in HSC 8.0. The new HSC Chemistry will support engineers and scientists with an interest in developing a sustainable, closed-loop infrastructure for the 21st century.

HSC 8.0 will be available October 2014. The HSC 8.0 license also covers HSC 7, which is available now, as well as free update to HSC 8.1. For further information, please contact:

HSC 8.0 New Features

HSC Main Menu (HSC.exe)



HSC 8.0 has been designed to be accessible to scientist and engineer to help quantify the resource efficiency of sustainable solutions for metal production, recycling and residue processing, as well as energy and water and material flow systems. We believe this new menu opens the door of this unique software to a wider community having sustainable engineering and science at heart.

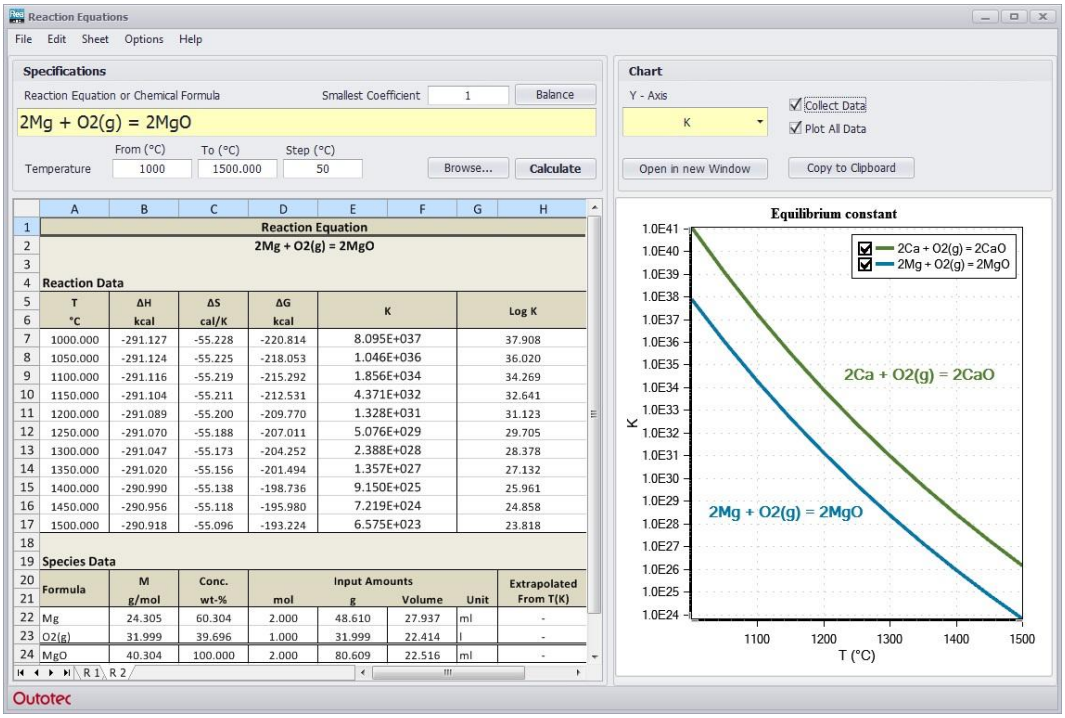
The new dynamic HSC 8.0 main menu permits customization of the menu according to user preferences, for example:

- move the most used calculation module tile rectangles to be the first ones;
- remove and add tile rectangles;
- change images on tile rectangles to user preferences;
- change background images;
- use animation in tile rectangles;
- change image scaling in tile rectangles;
- add new tile rectangles with links to other programs and net pages;
- read HSC and Outotec news feeds in one tile rectangle; and
- provides overview license information.

Summary of HSC 8.0 New Features

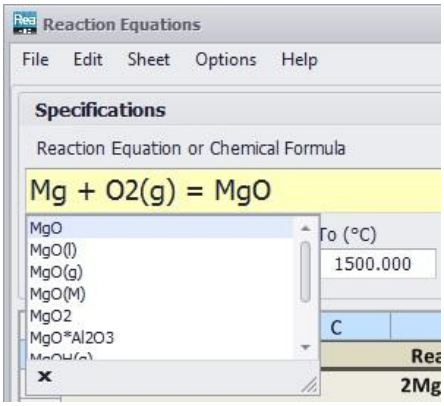
- Most of the HSC 7 calculation modules have been totally rewritten using the latest Microsoft .NET 4.5 environment. This makes it possible to continue HSC development under the latest Windows versions.
- Numerous new features have been added to the updated HSC modules.
- Accuracy of calculation routines has been improved.
- Databases have been expanded from 25,000 to 28,000 chemical species. Data of 1300 species have updated.
- New user interfaces are more ergonomic, intuitive and user-friendly.
- All charting is now done using same charting tool for all the modules.
- The new chart tool also enables 3D charts (with x-, y- and z-axes).
- The new Exergy module enables exergy calculation of material and energy flows easily of unit operations and complete systems.
- The new Sim 8.0 module LCA dialog makes it possible to estimate the ecobalances of processes by exporting data in formats accessible to 3rd party LCA software, thus LCA analyses can now be performed on consistent material and energy balances of process and system models.
- The new Converter module solves a classic problem – conversion of experimental element analysis to chemical compound or mineral analysis.
- The new Benson Estimation module makes it possible to estimate the H, S and Cp values of organic compounds based on the molecular structure using easy graphical user interface.
- Predictive formula typing provides assistance in specifying/selecting species.
- The new HSC 8.0 is designed for 32- and 64-bit Windows 7 and 8 on .NET 4.5 architecture. HSC 7 was designed for 32-bit Windows 2000, XP, and Vista.
- Many HSC modules widely utilize a built in HSC Excel emulator. The new Excel emulator supports Excel versions up to 2010. This means much larger spreadsheets, more functions, xlsx-file support, etc.
- The new Excel emulator runs calculations faster due to multithread recalculation.
- The updated Help module supports Word files up to version 2010.
- Charting options have been added to most modules.
- Multiple figures can be produced on different pages enhance the evaluation and visualization of the produced results of several modules.
- The HSC Main Menu is now dynamic; users can modify according to their current needs, unit and other specific selections
- HSC 7 is composed of different components and separate saving steps were needed to move between these components. Now these components have been integrated into one platform.
- Several new features have been added to Equilibrium module, such as advanced calculations, integrated cell calculations, product removal, 3D diagrams, Cp-filter, DLL-based solution models, etc.
- The new DLL-type unit operation models may be used in Sim 8.0 module along with the HSC 7 Excel-type models. This increases flexibility substantially.

Reaction Module



The **Rea**ction module is used to analyze chemical reaction equilibria and energy requirements. The reaction module also makes it possible to calculate dissolution heats and vapor pressures. The updated module has an attractive new user interface, and new charting tools. The results may be collected on several sheets. The sheets are linked to chart and input data. The sheets also enable creation of charts with several stacked and intersecting curves.

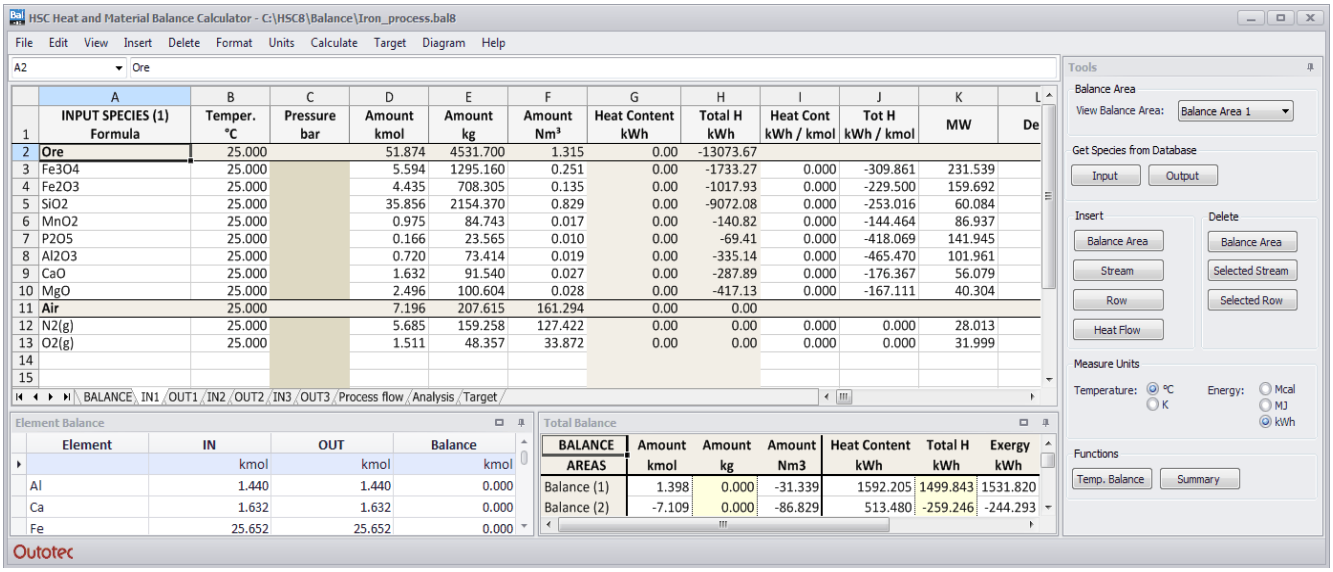
Traditionally researchers have tested their ideas by writing out reaction equations and then calculating equilibrium constants and heats of reaction from standard thermochemical data. HSC does all of the above efficiently – simply type the reaction equations in the input field and HSC gives the heat of the reactions, equilibrium constants at any temperature, and the amount of species etc. and provides useful figures for these. HSC even checks the elemental balance and gives the potential vs. standard hydrogen electrode for electrochemical reactions.



The new predictive formula input helps find the available species from the database.

Predictive formula input is also available in many other modules.

Balance Module



1	INPUT SPECIES (1) Formula	Temper. °C	Pressure bar	Amount kmol	Amount kg	Amount Nm³	Heat Content kWh	Total H kWh	Heat Cont kWh / kmol	Tot H kWh / kmol	MW
2	Ore	25.000		51.874	4531.700	1.315	0.00	-13073.67			
3	Fe3O4	25.000		5.594	1295.160	0.251	0.00	-1733.27	0.000	-309.861	231.539
4	Fe2O3	25.000		4.435	708.305	0.135	0.00	-1017.93	0.000	-229.500	159.692
5	SiO2	25.000		35.856	2154.370	0.829	0.00	-9072.08	0.000	-253.016	60.084
6	MnO2	25.000		0.975	84.743	0.017	0.00	-140.82	0.000	-144.464	86.937
7	P2O5	25.000		0.166	23.565	0.010	0.00	-69.41	0.000	-418.069	141.945
8	Al2O3	25.000		0.720	73.414	0.019	0.00	-335.14	0.000	-465.470	101.961
9	CaO	25.000		1.632	91.540	0.027	0.00	-287.89	0.000	-176.367	56.079
10	MgO	25.000		2.496	100.604	0.028	0.00	-417.13	0.000	-167.111	40.304
11	**Air**	25.000		7.196	207.615	161.294	0.00	0.00			
12	N2(g)	25.000		5.685	159.258	127.422	0.00	0.00	0.000	0.000	28.013
13	O2(g)	25.000		1.511	48.357	33.872	0.00	0.00	0.000	0.000	31.999
14											
15											

BALANCE | IN1 | OUT1 | IN2 | OUT2 | IN3 | OUT3 | Process flow | Analysis | Target

Element Balance

Element	IN	OUT	Balance
	kmol	kmol	kmol
Al	1.440	1.440	0.000
Ca	1.632	1.632	0.000
Fe	25.652	25.652	0.000

Total Balance

BALANCE AREAS	Amount kmol	Amount kg	Amount Nm3	Heat Content kWh	Total H kWh	Exergy kWh
Balance (1)	1.398	0.000	-31.339	1592.205	1499.843	1531.820
Balance (2)	-7.109	0.000	-86.829	513.480	-259.246	-244.293

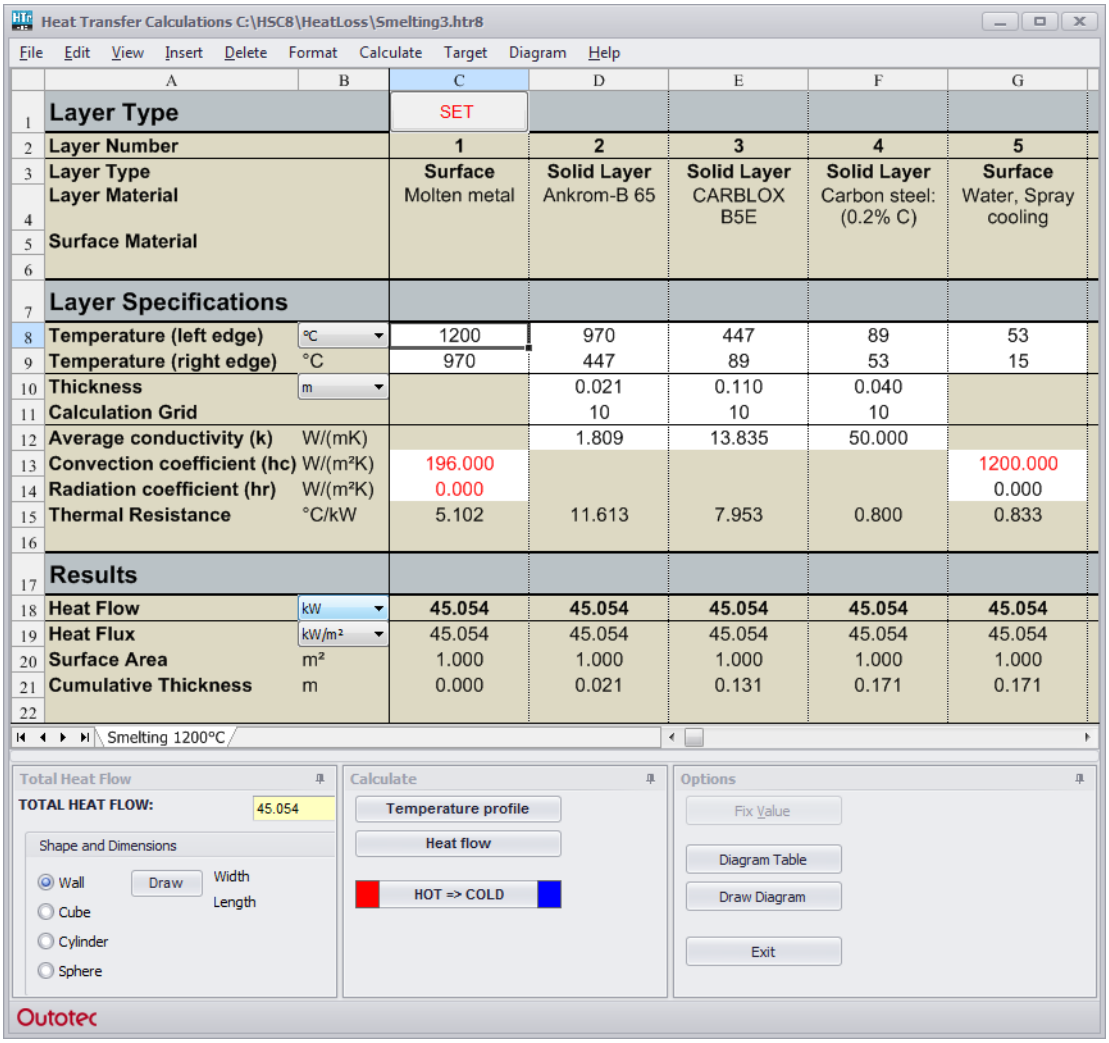
The **Bal**ance module is used to estimate the heat and material balances of one to as many linked unit processes as required. The new module has an improved user interface and charting tools, as well as new predictive chemical formula typing.

Users can modify the user interface according to their own requirements. The new updated module calculates also exergy balances.

Heat balance calculations are usually carried out when developing new chemical processes and/or improving older ones. This module calculates the real or constrained heat balances, with given mass balances as the boundary conditions, but not the theoretical balances at equilibrium conditions.

This tools is excellently suited also for undergraduate mass and energy balance teaching while also quantifying sustainability.

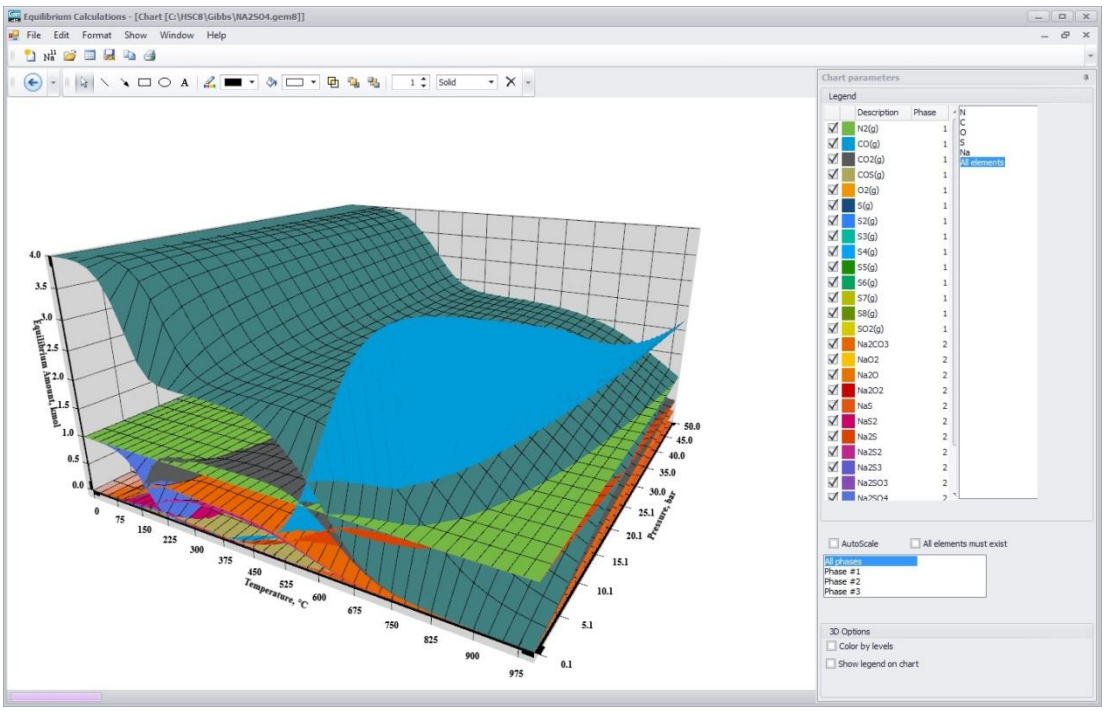
Heat Transfer Module



The **H**eat **Tr**ansfer module is also called Heat Loss module, because it estimates the heat losses and heat transfer of reactors for various geometries and reactor walls and linings and therefore a useful assistant during thermal design of reactors. The ergonomics and visual appearance of the user interface have been improved. The databases have been updated, expanded and references have been added to the data. The new “Specify Layer Type” dialog makes the specification of layer properties much easier than earlier. Measurement unit changes have also been made easier.

The main purpose of this module is to estimate total heat loss or draw the temperature profile of a wall or reactor. However, it can also be used to compare different materials and different set-ups, for example the use of insulation when a material has a critical maximum temperature or when the outside air cannot exceed a certain temperature. The conduction, convection and radiation databases also provide a resource such as simple reference tables for material properties. This also makes it an excellent tool for teaching heat transfer and losses from reactors.

Equilibrium Module



Gibbs equilibrium calculations offer a practical way to investigate and study the effect of raw materials and process variables on the products of a chemical reactor and systems to estimate recoveries, opportunities and limits of sustainability. **G**ibbs **E**nergy **M**inimization (**Gem**) method is utilized in the calculations.

With this HSC module calculation of the equilibrium composition and amounts of prevailing phases in any reactor is made easy. One needs to specify the quantity of raw materials, temperatures, and the species of the system. These can be specified by selecting the elements of the system, or providing the compounds selected from HSC's unique database, or by editing an old file.

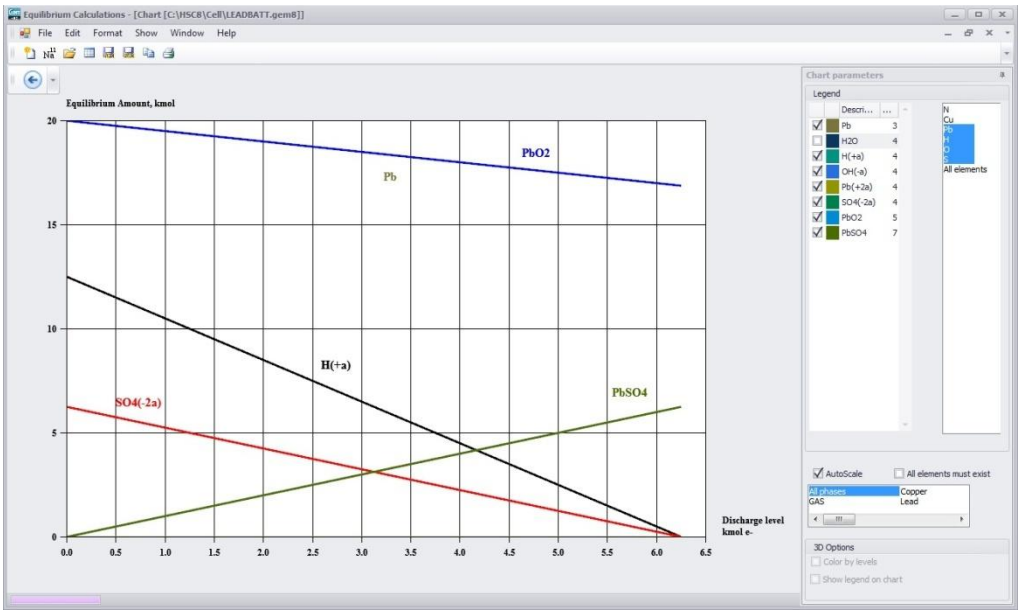
Activity coefficients can be defined, if required, as constants or as a function of temperature and composition. The module can also use separate .NET4.5 class libraries (DLLs) as the source of the activity coefficient models.

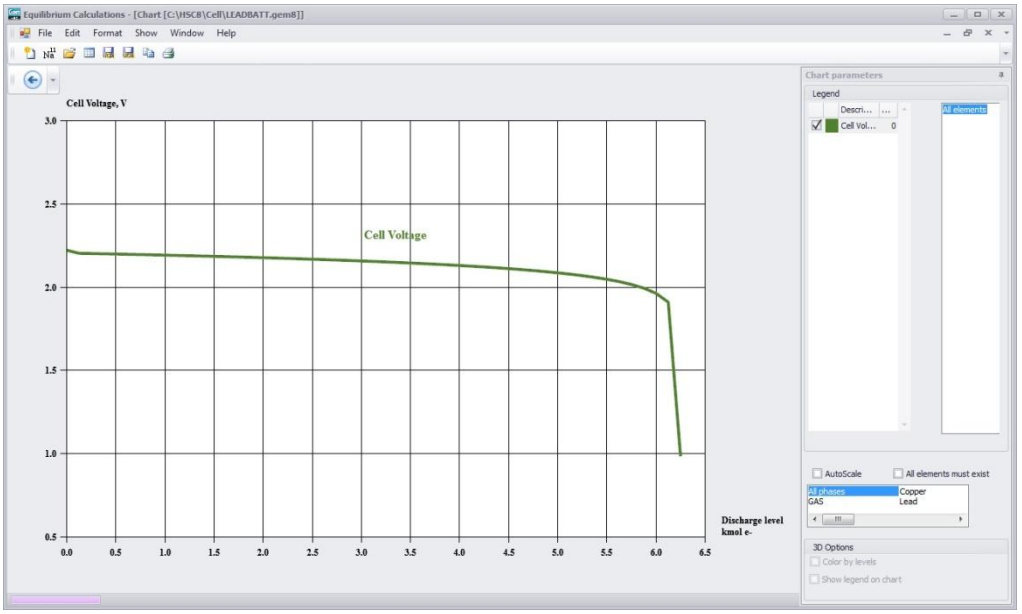
Calculations can be repeated at stepwise intervals over any entered range of raw material quantities or reaction temperatures in order to visualize the effect of these process variables.

The new Gibbs 8.0 module has a long list of new features, the important ones including:

- New charting tools and 3D graphics have been added with two independent variable calculation modes.
- The new Gibbs 8.0 is easier to use, as all the separate Gibbs 7 components have been integrated into one module.
- More advanced calculation options have been added, such as Constant volume, and Adiabatic calculations. Target calculations make it possible to search for conditions that lead to the desired species concentration.
- The Removal of Products option makes it possible to calculate, for example, transitory evaporation. New Open Atmosphere/Fixed Activity calculation options allow the modeling of open systems.
- Intelligent restricted Cp extrapolation decreases Cp estimation errors.

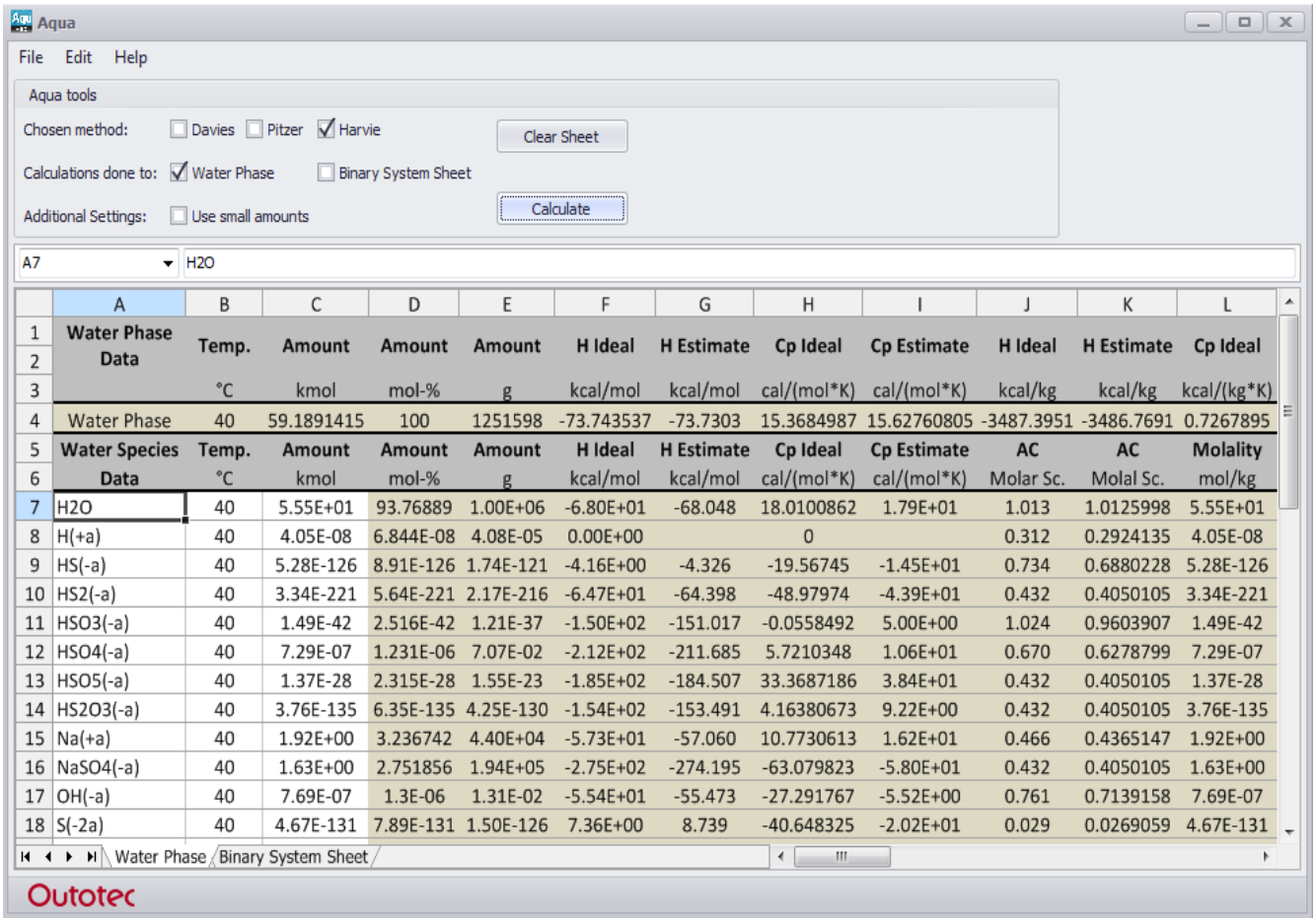
Cell / Equilibrium Module





The Cell module calculations have been integrated into Gibbs 8.0. Now it uses the same Gibbs Energy Minimization routine than the main equilibrium module. Cell module make it possible to calculate phase compositions and cell voltages of electrochemical cells. This integration also enables plotting of 2D and 3D charts in electrochemical systems (discharge level can be a chart axis).

Aqua Module



	A	B	C	D	E	F	G	H	I	J	K	L
1	Water Phase Data	Temp.	Amount	Amount	Amount	H Ideal	H Estimate	Cp Ideal	Cp Estimate	H Ideal	H Estimate	Cp Ideal
2												
3		°C	kmol	mol-%	g	kcal/mol	kcal/mol	cal/(mol*K)	cal/(mol*K)	kcal/kg	kcal/kg	kcal/(kg*K)
4	Water Phase	40	59.1891415	100	1251598	-73.743537	-73.7303	15.3684987	15.62760805	-3487.3951	-3486.7691	0.7267895
5	Water Species	Temp.	Amount	Amount	Amount	H Ideal	H Estimate	Cp Ideal	Cp Estimate	AC	AC	Molality
6	Data	°C	kmol	mol-%	g	kcal/mol	kcal/mol	cal/(mol*K)	cal/(mol*K)	Molar Sc.	Molal Sc.	mol/kg
7	H2O	40	5.55E+01	93.76889	1.00E+06	-6.80E+01	-68.048	18.0100862	1.79E+01	1.013	1.0125998	5.55E+01
8	H(+a)	40	4.05E-08	6.844E-08	4.08E-05	0.00E+00		0		0.312	0.2924135	4.05E-08
9	HS(-a)	40	5.28E-126	8.91E-126	1.74E-121	-4.16E+00	-4.326	-19.56745	-1.45E+01	0.734	0.6880228	5.28E-126
10	HS2(-a)	40	3.34E-221	5.64E-221	2.17E-216	-6.47E+01	-64.398	-48.97974	-4.39E+01	0.432	0.4050105	3.34E-221
11	HSO3(-a)	40	1.49E-42	2.516E-42	1.21E-37	-1.50E+02	-151.017	-0.0558492	5.00E+00	1.024	0.9603907	1.49E-42
12	HSO4(-a)	40	7.29E-07	1.231E-06	7.07E-02	-2.12E+02	-211.685	5.7210348	1.06E+01	0.670	0.6278799	7.29E-07
13	HSO5(-a)	40	1.37E-28	2.315E-28	1.55E-23	-1.85E+02	-184.507	33.3687186	3.84E+01	0.432	0.4050105	1.37E-28
14	HS2O3(-a)	40	3.76E-135	6.35E-135	4.25E-130	-1.54E+02	-153.491	4.16380673	9.22E+00	0.432	0.4050105	3.76E-135
15	Na(+a)	40	1.92E+00	3.236742	4.40E+04	-5.73E+01	-57.060	10.7730613	1.62E+01	0.466	0.4365147	1.92E+00
16	NaSO4(-a)	40	1.63E+00	2.751856	1.94E+05	-2.75E+02	-274.195	-63.079823	-5.80E+01	0.432	0.4050105	1.63E+00
17	OH(-a)	40	7.69E-07	1.3E-06	1.31E-02	-5.54E+01	-55.473	-27.291767	-5.52E+00	0.761	0.7139158	7.69E-07
18	S(-2a)	40	4.67E-131	7.89E-131	1.50E-126	7.36E+00	8.739	-40.648325	-2.02E+01	0.029	0.0269059	4.67E-131

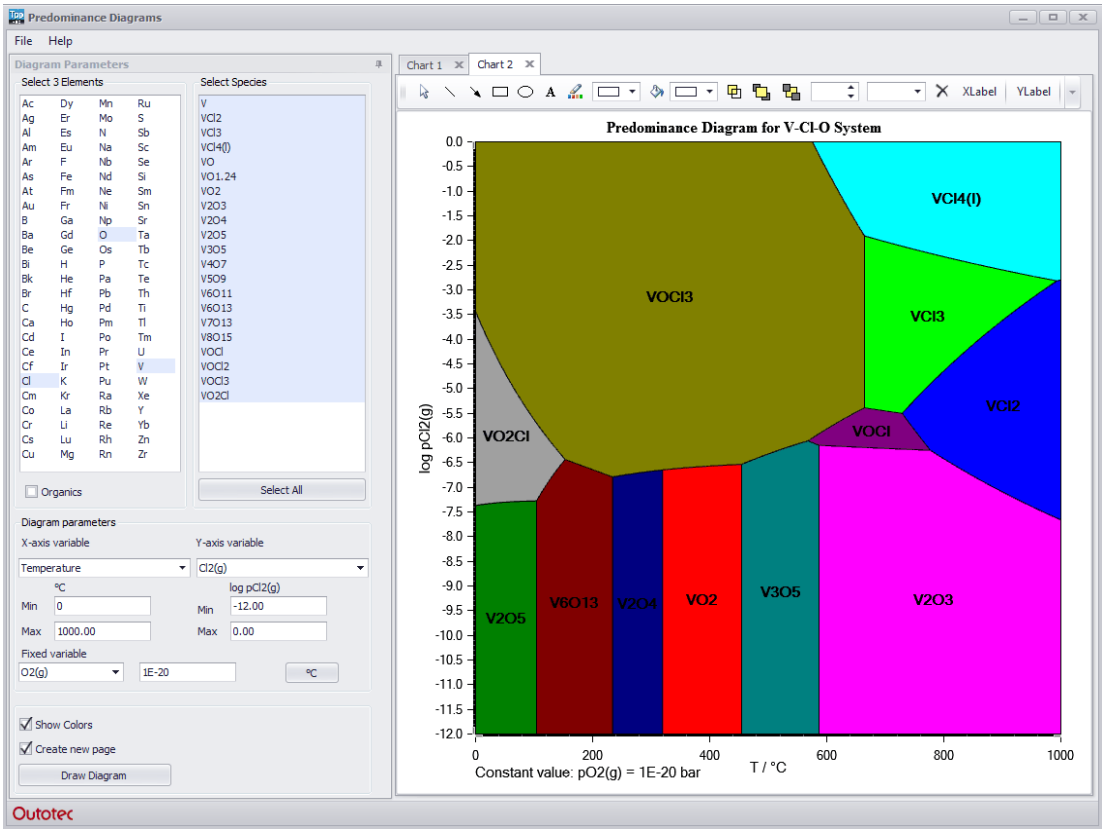
The **Aqu**a module contains non-ideal aqueous electrolyte models and databases. This module also includes a large number of standard state data for neutral components and ionic species. The Aqua module works as a standalone tool to calculate water solution properties, but it may also be utilized directly in the equilibrium module for water solutions.

The Aqua module calculates ionic activities, mean activity coefficients, osmotic coefficients, solution enthalpies, heat capacities, etc. Three different water solution models are available: the Davies model (extended Debye-Hückel), the semi-empirical Pitzer model (with binary interactions only), and Harvie's modification of the Pitzer model (binary and ternary parameters). The Pitzer parameter database can be used for binary electrolyte systems as well as for multicomponent solutions.

An extensive database has been collected including temperature-dependent Pitzer binary and ternary ion interaction parameters. The total number of Pitzer parameters in the HSC Aqua database is currently 1031. This includes 425 cation-anion pairs, 114 cation-cation and anion-anion pairs, 199 ternary coefficients, and 293 ion-neutral pairs.

The module has been totally rewritten and the user interface has been updated. The Titration routine, Binary System Sheet and user database will be available later on in HSC 8.1.

Stability Diagrams Module



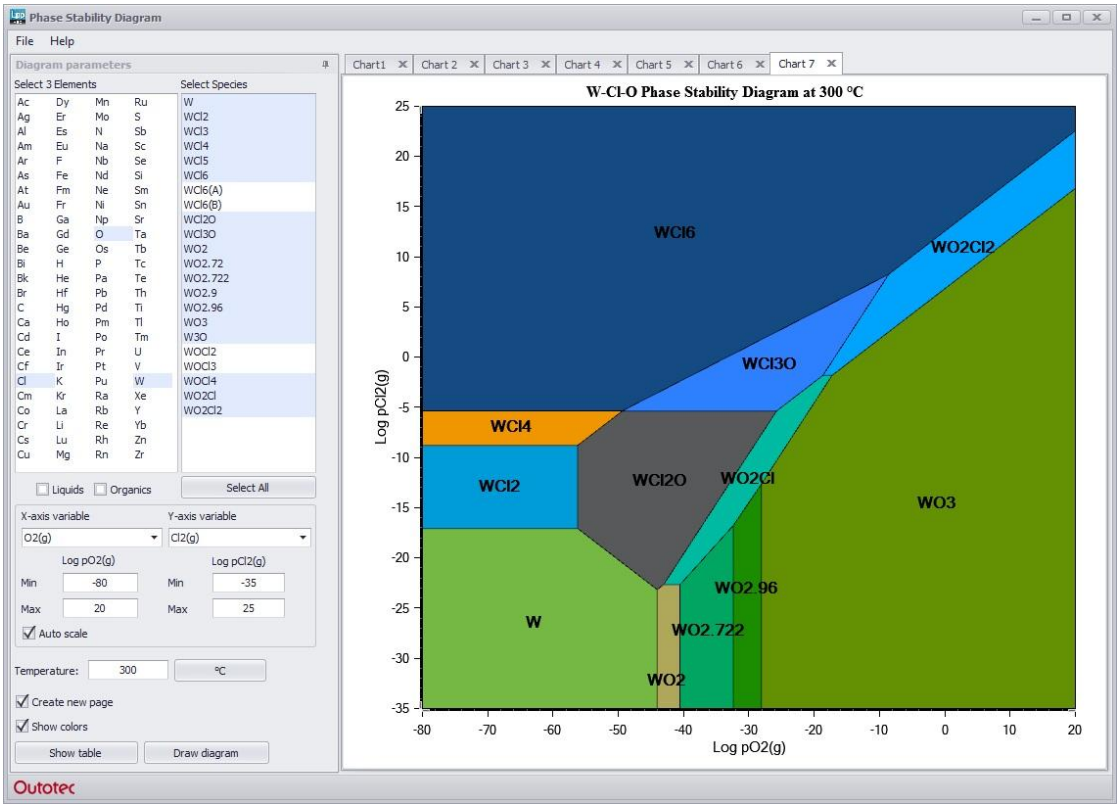
The **Tpp** Diagram module calculates phase stability diagrams using partial pressures on both axes or with temperature on the x-axis and partial pressure on the y-axis. This module calculates the diagram on the basis of minimum Gibbs energy. However, it does not check each x and y point in order to decrease the calculation time. The calculation is made using a preset resolution grid and a specific algorithm that builds the graph of phase boundaries.

These diagrams may be used, for example, to review the kinds of chemical species that exist in the process gas line when there is a change in process conditions and temperatures. The diagrams are also useful when estimating roasting conditions or high temperature corrosion problems.

The new Tpp 8 module integrates the old Tpp 7 input and calculation modules, this makes testing different systems much easier than with previous Tpp module. The ergonomics and visual appearance have been greatly improved. The new charting tool improves the visual quality of the results. The Chart page option makes comparison of different diagrams easy for detailed analysis.

The calculation routine has been rewritten, and now the routine is much more robust, accurate and faster.

Lpp Module



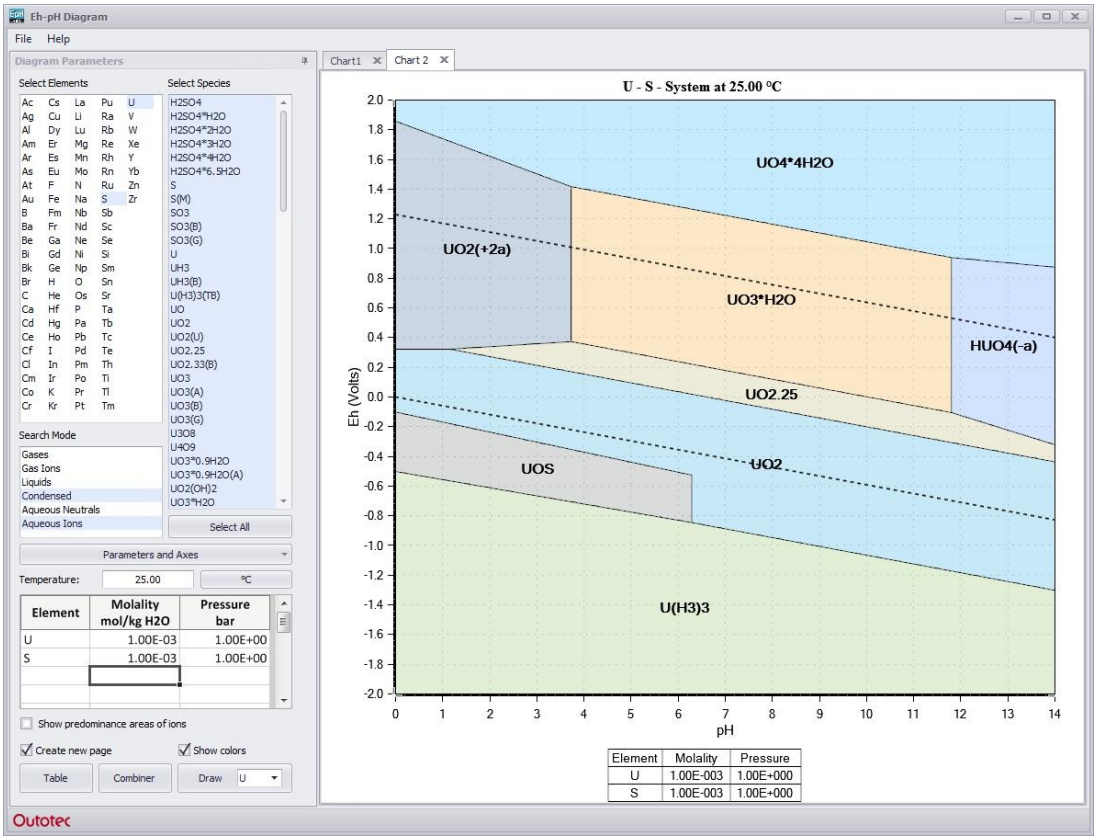
The **Lpp** phase stability diagrams show the stability (predominance) areas of condensed phases in a ternary system in isothermal conditions, with the remaining constraints as the other axis. The Lpp Diagram module draws isothermal phase stability diagrams of three element systems. These diagrams are also known as predominance area diagrams or Kellogg diagrams.

These diagrams are very useful when a quick estimate of the prevailing phases is required. It is assumed that all phases are pure substances. Mixture phases are not taken into account in basic phase stability diagrams. Lpp diagrams may be used, for example, to estimate which species are stable as a function of oxygen and sulfur pressure in the process gas line.

The new Lpp 8 module integrates the previous Lpp 7 input and calculation modules. This makes testing different systems much easier.

The ergonomics and visual appearance have been greatly improved. The new charting tool improves the visual quality of the results. The Chart page option makes comparison of different diagrams easier for detailed analysis.

EpH Module



Eh-**pH**-diagrams, also known as Pourbaix diagrams, show the thermodynamic stability areas of different species in a water solution. Stability areas are presented as a function of pH and electrochemical potential scales. Usually the upper and lower stability limits of water are also shown in the diagrams by dotted lines. Traditionally, these diagrams have been taken from different handbooks. However, in most handbooks these diagrams are available only for a limited number of temperatures, concentrations, and element combinations.

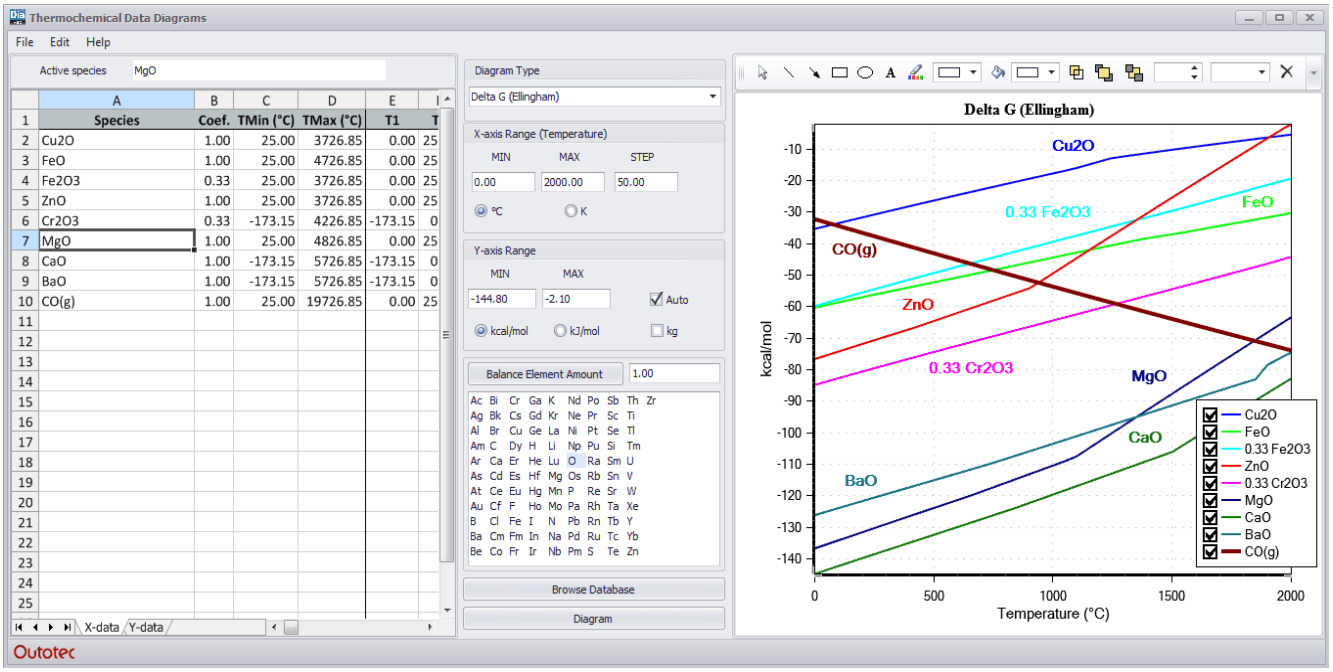
The Eh-pH module of HSC Chemistry allows the construction of diagrams in a highly flexible and fast way, because the user can draw the diagrams exactly at the selected temperature and concentration.

These diagrams may widely be applied in leaching, precipitation and corrosion studies. These diagrams give a quick view of the behavior of elements and species in water solutions as functions of pH and potential.

The new EpH 8 module integrates the previous EpH 7 input and calculation modules.

The ergonomics and visual appearance have been greatly improved. The new charting tool improves the visual quality of the results. The Chart page option makes comparison of different diagrams easier for detailed analysis and comparison of different systems.

Diagrams Module



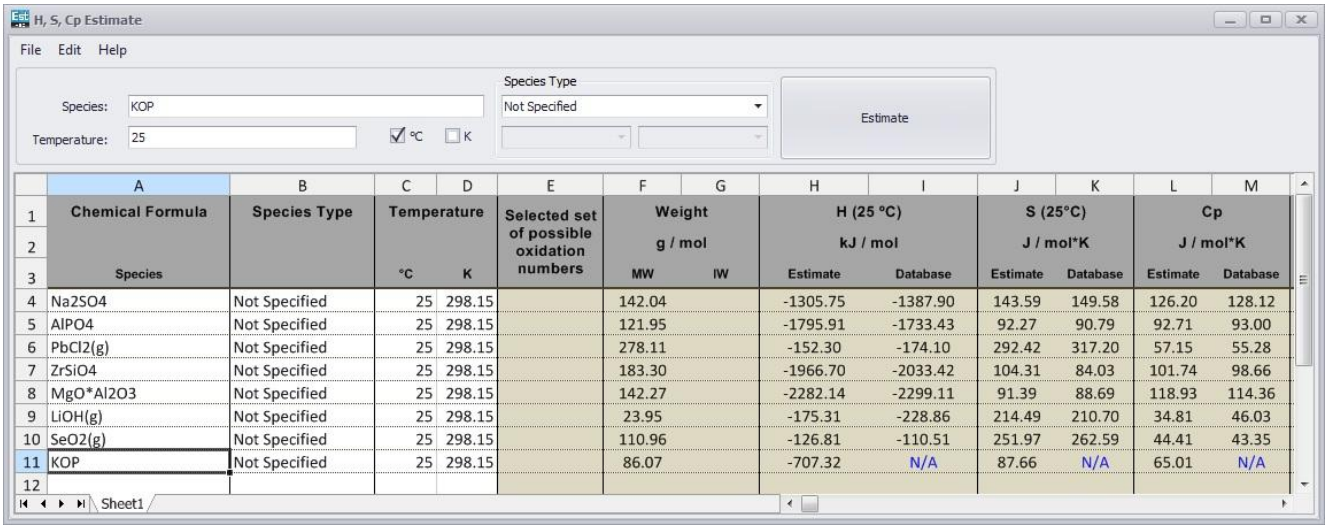
The **Dia**gram module presents the basic thermochemical data for a given species in graphical format. Eight different diagram types can be drawn as a function of temperature. One of the most useful diagrams is the DG diagram (Ellingham diagram). It shows the relative stability of various oxides, sulfates, chlorides, etc. as a function of temperature.

The user interface and graphics quality have been greatly improved compared to the old Diagram 7 module. The same chart tool has been applied as used in the new Tpp, Lpp, and EpH modules.

Predictive formula typing provides great help in specifying species.

The Diagram module is utilized, for example, by the HSC Database module to draw H, S, Cp and G diagrams as a function of temperature.

Estimation Module



	Chemical Formula	Species Type	Temperature		Selected set of possible oxidation numbers	Weight g / mol		H (25 °C) kJ / mol		S (25°C) J / mol*K		Cp J / mol*K	
	Species		°C	K		MW	IW	Estimate	Database	Estimate	Database	Estimate	Database
4	Na2SO4	Not Specified	25	298.15		142.04		-1305.75	-1387.90	143.59	149.58	126.20	128.12
5	AlPO4	Not Specified	25	298.15		121.95		-1795.91	-1733.43	92.27	90.79	92.71	93.00
6	PbCl2(g)	Not Specified	25	298.15		278.11		-152.30	-174.10	292.42	317.20	57.15	55.28
7	ZrSiO4	Not Specified	25	298.15		183.30		-1966.70	-2033.42	104.31	84.03	101.74	98.66
8	MgO*Al2O3	Not Specified	25	298.15		142.27		-2282.14	-2299.11	91.39	88.69	118.93	114.36
9	LiOH(g)	Not Specified	25	298.15		23.95		-175.31	-228.86	214.49	210.70	34.81	46.03
10	SeO2(g)	Not Specified	25	298.15		110.96		-126.81	-110.51	251.97	262.59	44.41	43.35
11	KOP	Not Specified	25	298.15		86.07		-707.32	N/A	87.66	N/A	65.01	N/A
12													

Sheet1

The HSC **Est**imation module gives a rough estimate of the H, S, and Cp values for the chemical species and non-stoichiometric minerals that exist in the HSC database, and also for those that do not exist in the HSC database. The Estimation module also gives the oxidation states of the elements in a given chemical compound.

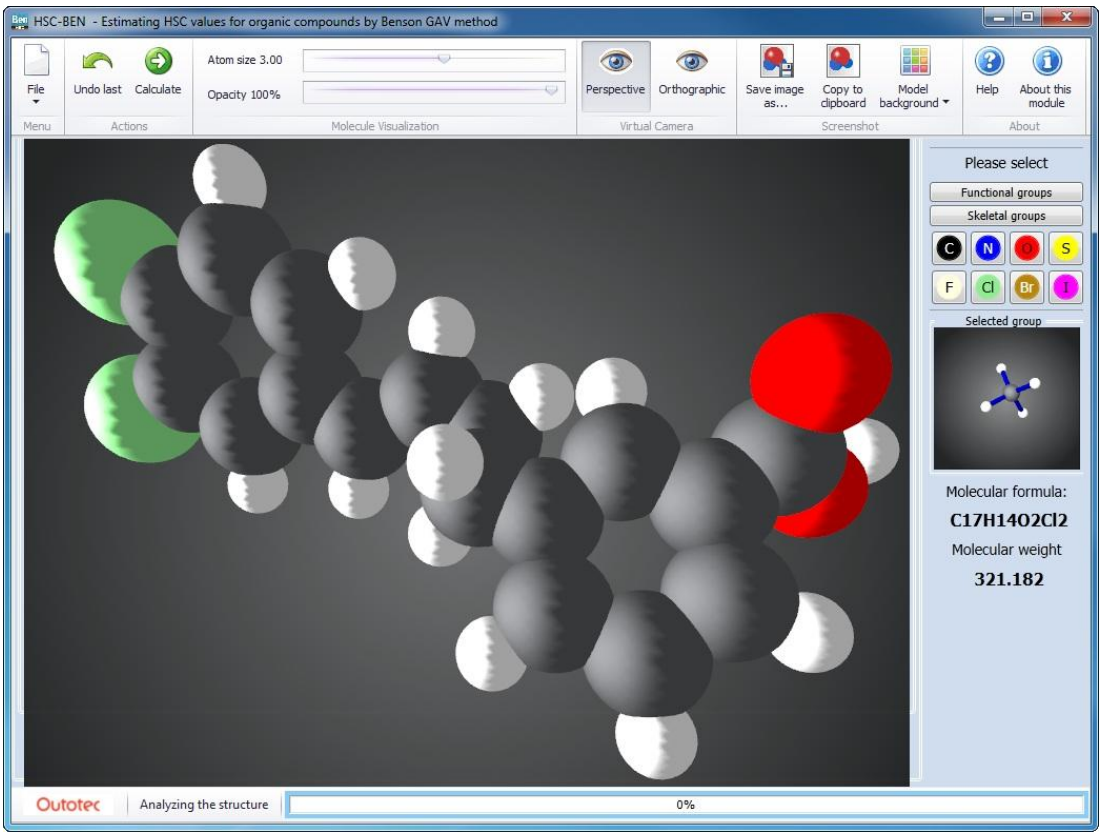
HSC estimates are based on statistical data mining methods, which utilize stoichiometric element amounts, oxidation states, element interactions, etc., which may be calculated automatically from the chemical formula.

This module is easy to use: the user types in the formula and the program gives the formula weight, oxidation states, and H, S, and Cp estimates.

The quality of this data is essential in process modeling and simulation. The module may be used to identify errors in experimental data and estimate the missing data needed in calculations. It has also been applied to check for errors in the HSC database.

Small improvements have also been made to the estimation calculation routines; the new Inorganic/Organic option may be used to improve the estimates.

Benson Estimation Module



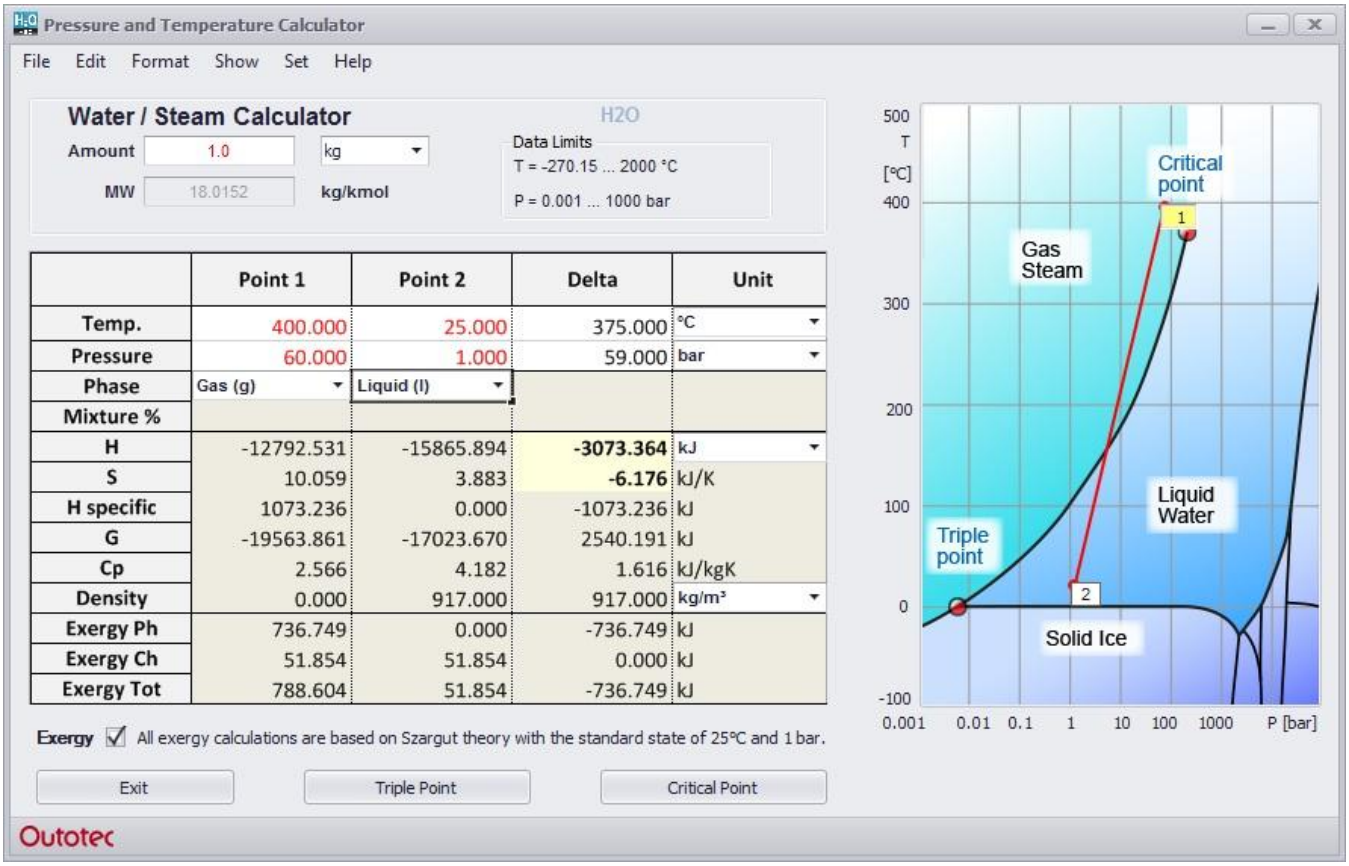
Benson estimation is a new module which estimates the H, S and Cp data of organic chemical compounds especially also useful to estimate properties for complex mixed organic scarp, residues etc. The number of organic compounds is obviously large and quite often the H, S and Cp data are missing.

This module enables more accurate H, S, and Cp estimates for organic species than those given by the Est estimation module, which suits inorganic species better.

The new module has an easy to use 3D molecular graphics user interface to construct molecules, effective calculation routines and a large Benson parameter database.

The results may easily be saved in the HSC database, which makes them available to other HSC modules.

Water Module



The **Wat**er calculator module is a very useful replacement for steam table books and Mollier diagrams. However, water module gives the enthalpies and other quantities using the same standard states as other HSC modules.

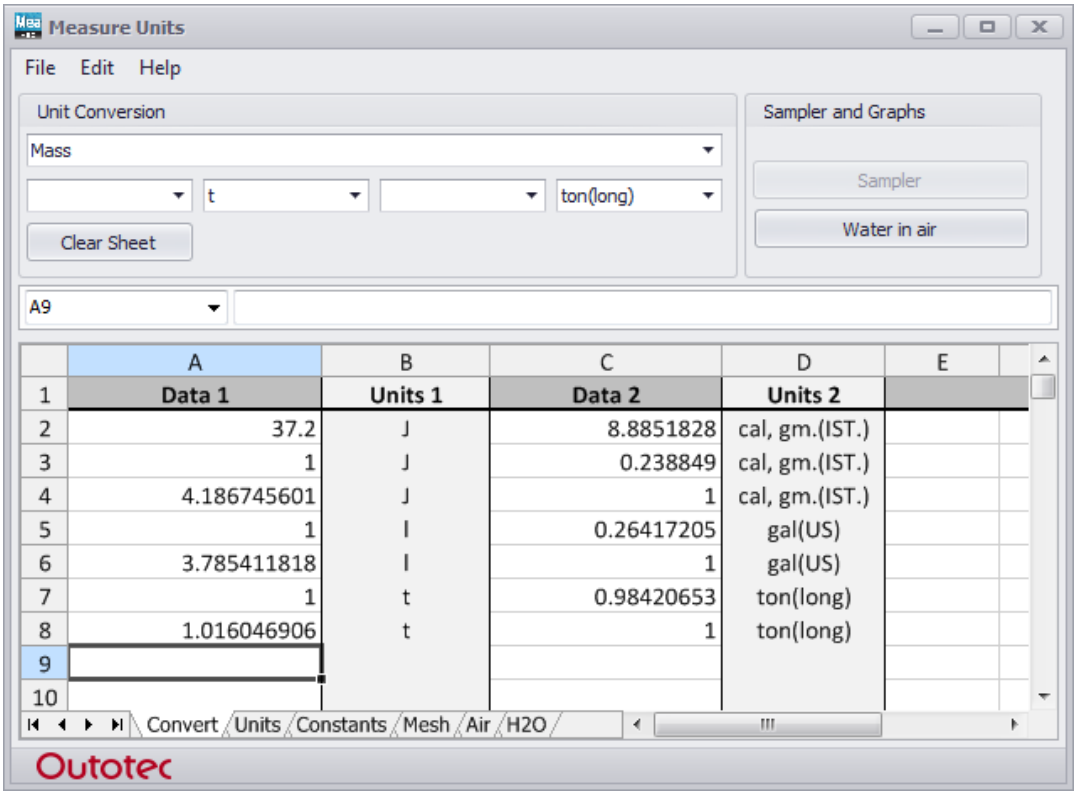
By directly typing the pressure and temperature of the process points, or by simply clicking on the diagram, the process enthalpy and entropy are calculated along with several other useful thermodynamic data.

The Water module may be used, for example, to estimate energy balances of steam boilers and power plants.

The calculation code and user interface have been updated, and new exergy calculations have been added.

This will be expanded to other fluids (liquids) in HSC 8.1.

Measure Units Module

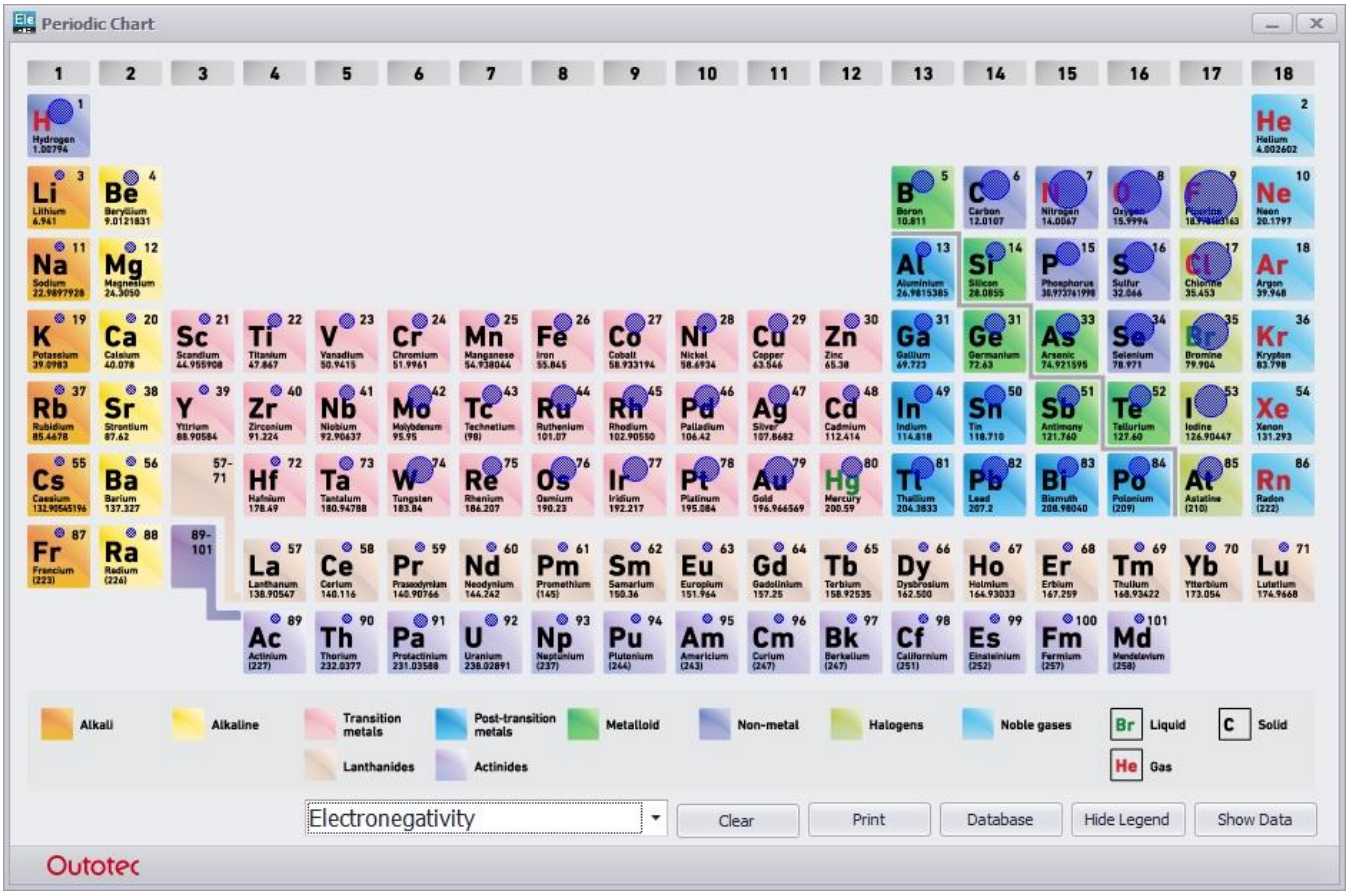


	A	B	C	D	E
1	**Data 1**	**Units 1**	**Data 2**	**Units 2**	
2	37.2	J	8.8851828	cal, gm.(IST.)	
3	1	J	0.238849	cal, gm.(IST.)	
4	4.186745601	J	1	cal, gm.(IST.)	
5	1	l	0.26417205	gal(US)	
6	3.785411818	l	1	gal(US)	
7	1	t	0.98420653	ton(long)	
8	1.016046906	t	1	ton(long)	
9					
10					

Traditionally, several types of energy, temperature, mass, and volume units have been used in thermochemical calculations. Therefore, conversions are needed to compare results from different sources. The **Mea**sure Units Conversion module is an easy tool for fast unit conversions in thermochemistry as well as in other engineering fields.

This module carries out an extensive number of measure unit conversions. The user interface has been updated. The databases have been expanded and also references have been added to the new version. This module gives also several other often used constants and water and air properties.

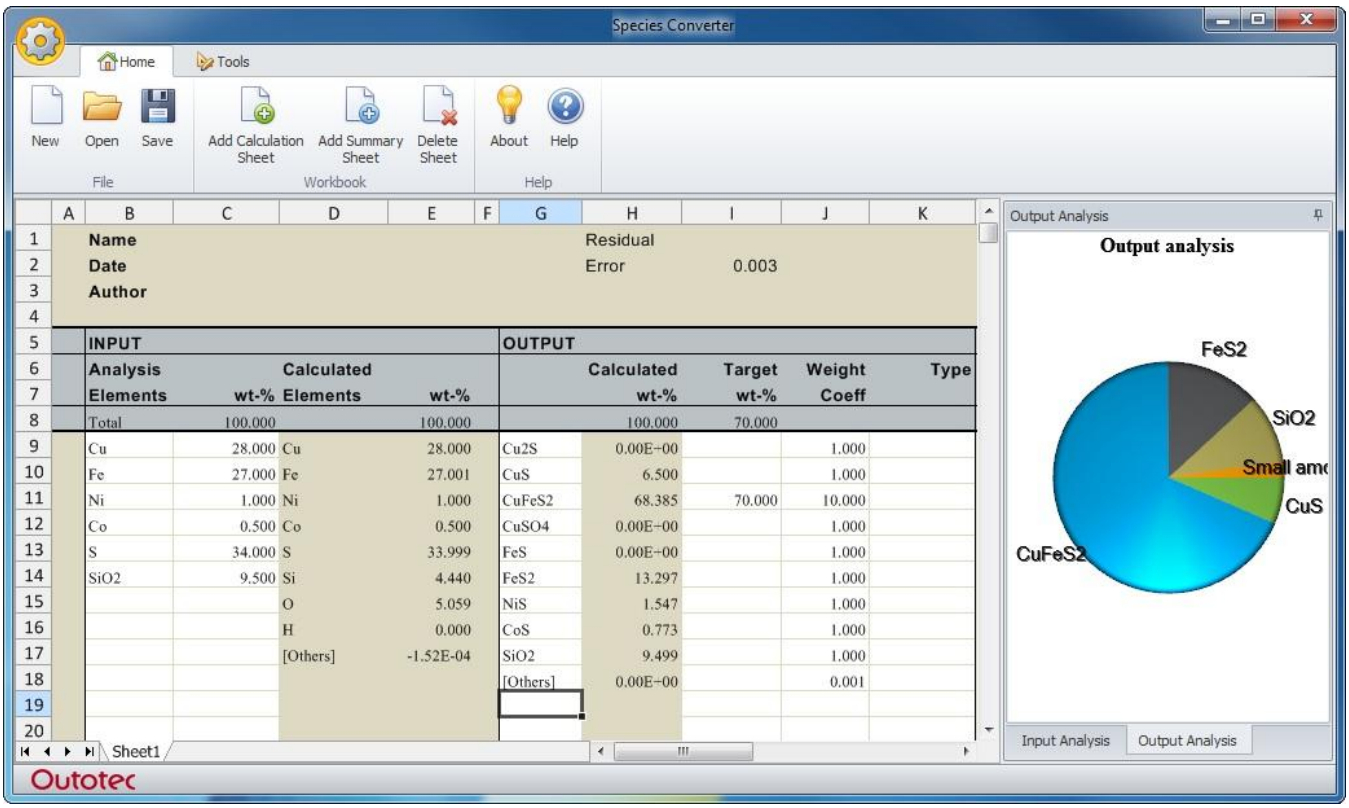
Elements Module



The **Ele**ments module shows the 56 properties of the elements in the database in numbers and in graphical format. These properties can be easily edited, while new properties and additional data can be added.

The user interface and visual effects of the Periodic Chart module have been improved significantly. The Element module is thus not a static Periodic Table, but a dynamic one with visual effects and an editable database very useful to visualize and understand the properties of elements.

Converter Module



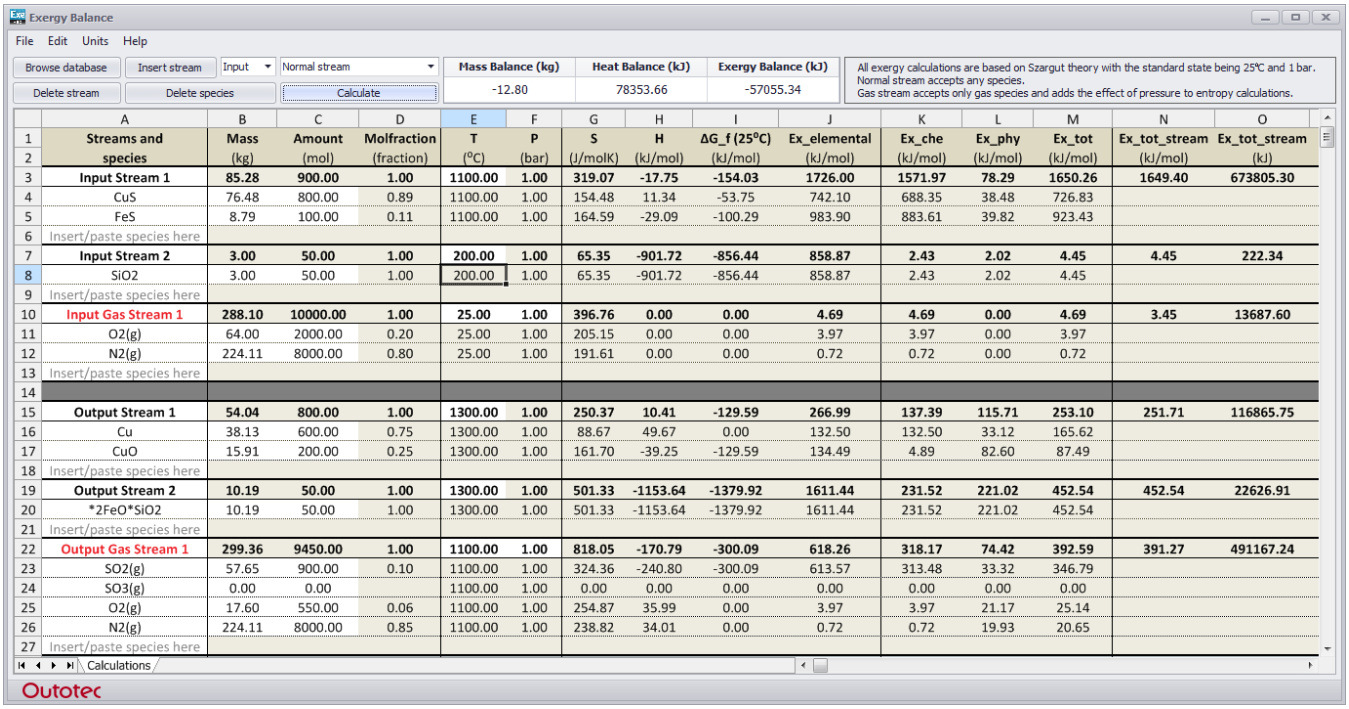
The **Con**vert module is new, data reconciliation tool converting elemental analyses into any required species analyses and *vice versa*. It may also be applied to convert elements to non-stoichiometric species. Usually chemical species are easy to convert to elements, but the reverse conversion from inaccurate experimental data is a much more challenging task. Three different solution methods are available.

Often measured or experimental element and mineralogical analyses contain errors. However, before the raw materials can be applied in process models, the inaccurate experimental analyses must be converted into stoichiometric chemical species, as thermochemical data is required for species to be able to understand the thermodynamics of systems.

The new module makes it possible to use inaccurate experimental element analysis (e.g. XRF, ICP etc.) as a starting value and modify the output species using the mineralogical analysis (e.g. XRD). This is done using the Target values for the species.

The new Converter module replaces the HSC 7 Convert and Mineralogy Iteration modules, and also the Sim 7 Mineralogy Calculator.

Exergy Module



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	Streams and	Mass	Amount	Molfraction	T	P	S	H	ΔG_f (25°C)	Ex_elemental	Ex_che	Ex_phy	Ex_tot	Ex_tot_stream	Ex_tot_stream
2	species	(kg)	(mol)	(fraction)	(°C)	(bar)	(J/molK)	(kJ/mol)	(kJ/mol)	(kJ/mol)	(kJ/mol)	(kJ/mol)	(kJ/mol)	(kJ/mol)	(kJ)
3	**Input Stream 1**	**85.28**	**900.00**	**1.00**	**1100.00**	**1.00**	**319.07**	**-17.75**	**-154.03**	**1726.00**	**1571.97**	**78.29**	**1650.26**	**1649.40**	**673805.30**
4	CuS	76.48	800.00	0.89	1100.00	1.00	154.48	11.34	-53.75	742.10	688.35	38.48	726.83		
5	FeS	8.79	100.00	0.11	1100.00	1.00	164.59	-29.09	-100.29	983.90	883.61	39.82	923.43		
6	Insert/paste species here														
7	**Input Stream 2**	**3.00**	**50.00**	**1.00**	**200.00**	**1.00**	**65.35**	**-901.72**	**-856.44**	**858.87**	**2.43**	**2.02**	**4.45**	**4.45**	**222.34**
8	SiO2	3.00	50.00	1.00	200.00	1.00	65.35	-901.72	-856.44	858.87	2.43	2.02	4.45		
9	Insert/paste species here														
10	**Input Gas Stream 1**	**288.10**	**10000.00**	**1.00**	**25.00**	**1.00**	**396.76**	**0.00**	**0.00**	**4.69**	**4.69**	**0.00**	**4.69**	**3.45**	**13687.60**
11	O2(g)	64.00	2000.00	0.20	25.00	1.00	205.15	0.00	0.00	3.97	3.97	0.00	3.97		
12	N2(g)	224.11	8000.00	0.80	25.00	1.00	191.61	0.00	0.00	0.72	0.72	0.00	0.72		
13	Insert/paste species here														
14															
15	**Output Stream 1**	**54.04**	**800.00**	**1.00**	**1300.00**	**1.00**	**250.37**	**10.41**	**-129.59**	**266.99**	**137.39**	**115.71**	**253.10**	**251.71**	**116865.75**
16	Cu	38.13	600.00	0.75	1300.00	1.00	88.67	49.67	0.00	132.50	132.50	33.12	165.62		
17	CuO	15.91	200.00	0.25	1300.00	1.00	161.70	-39.25	-129.59	134.49	4.89	82.60	87.49		
18	Insert/paste species here														
19	**Output Stream 2**	**10.19**	**50.00**	**1.00**	**1300.00**	**1.00**	**501.33**	**-1153.64**	**-1379.92**	**1611.44**	**231.52**	**221.02**	**452.54**	**452.54**	**22626.91**
20	*2FeO*SiO2	10.19	50.00	1.00	1300.00	1.00	501.33	-1153.64	-1379.92	1611.44	231.52	221.02	452.54		
21	Insert/paste species here														
22	**Output Gas Stream 1**	**299.36**	**9450.00**	**1.00**	**1100.00**	**1.00**	**818.05**	**-170.79**	**-300.09**	**618.26**	**318.17**	**74.42**	**392.59**	**391.27**	**491167.24**
23	SO2(g)	57.65	900.00	0.10	1100.00	1.00	324.36	-240.80	-300.09	613.57	313.48	33.32	346.79		
24	SO3(g)	0.00	0.00		1100.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
25	O2(g)	17.60	550.00	0.06	1100.00	1.00	254.87	35.99	0.00	3.97	3.97	21.17	25.14		
26	N2(g)	224.11	8000.00	0.85	1100.00	1.00	238.82	34.01	0.00	0.72	0.72	19.93	20.65		
27	Insert/paste species here														

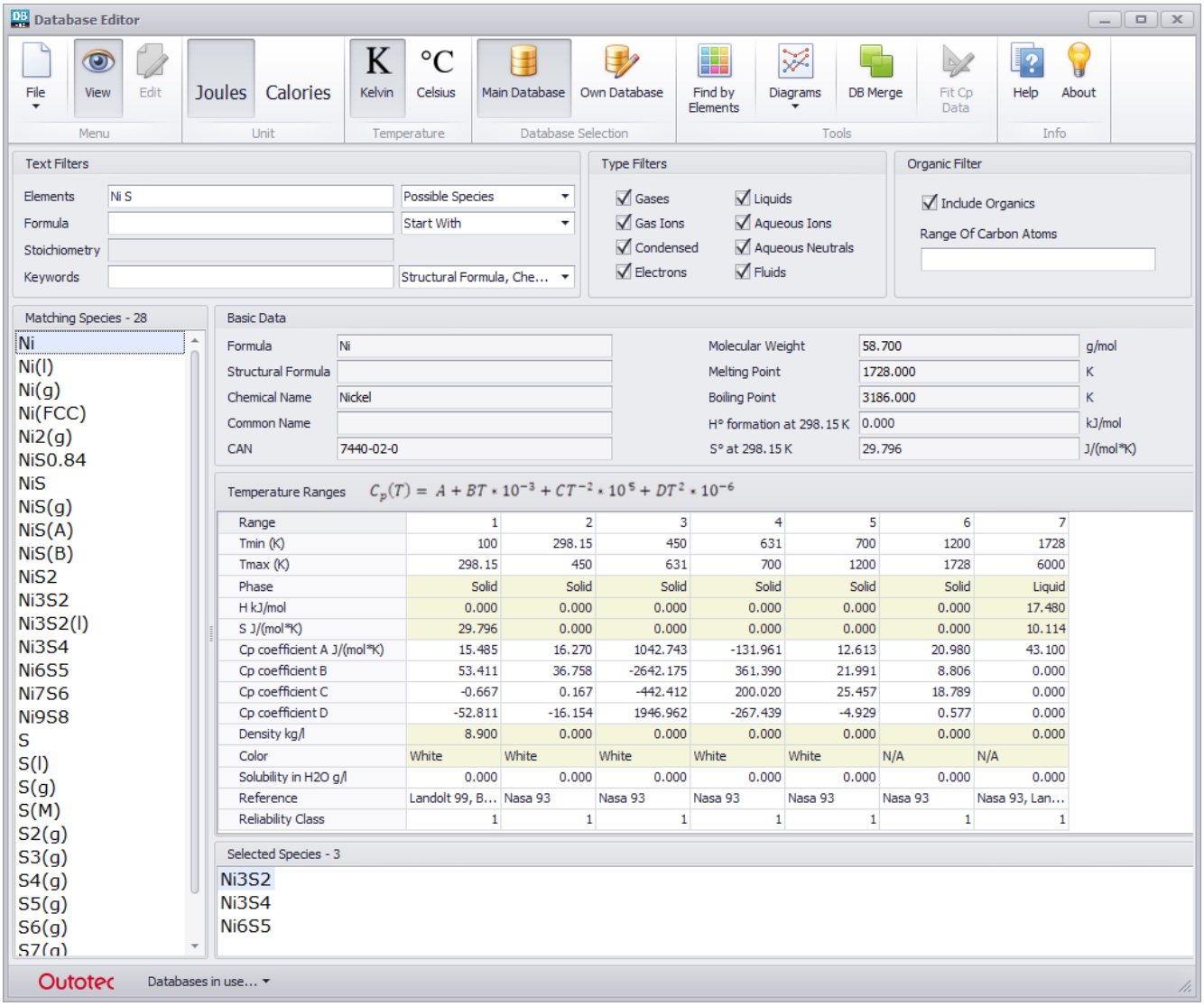
This new HSC 8.0 **Exe**rgy module calculates the exergies of chemical species and streams. These same calculation routines are utilized in many other HSC modules. Exergy calculations support LCA environmental footprint estimates to quantify sustainability. Exergy analysis may also help to use energy more efficiently.

This module allows the user to calculate exergy, mass and heat balance for a system where there can be multiple input and output streams (inclusive of energy losses) with multiple species. Exergy calculations can be performed for three different types of streams and user can see the results for physical, chemical and total exergy.

The three different types of streams are explained in the upper right corner of the screen where the exergy calculation standard state is also mentioned. The type of stream can be recognized from the color of the stream title: the normal stream is black, the ideal gas stream is red and the energy stream is green.

Normal stream accepts any species and is usable for any stream and the ideal gas stream accepts gaseous species. It should also be noted that the ideal gas stream uses pressure for entropy calculations. Energy stream in and output types allow the user to enter also heat and electricity amounts for the system.

HSC Database Module



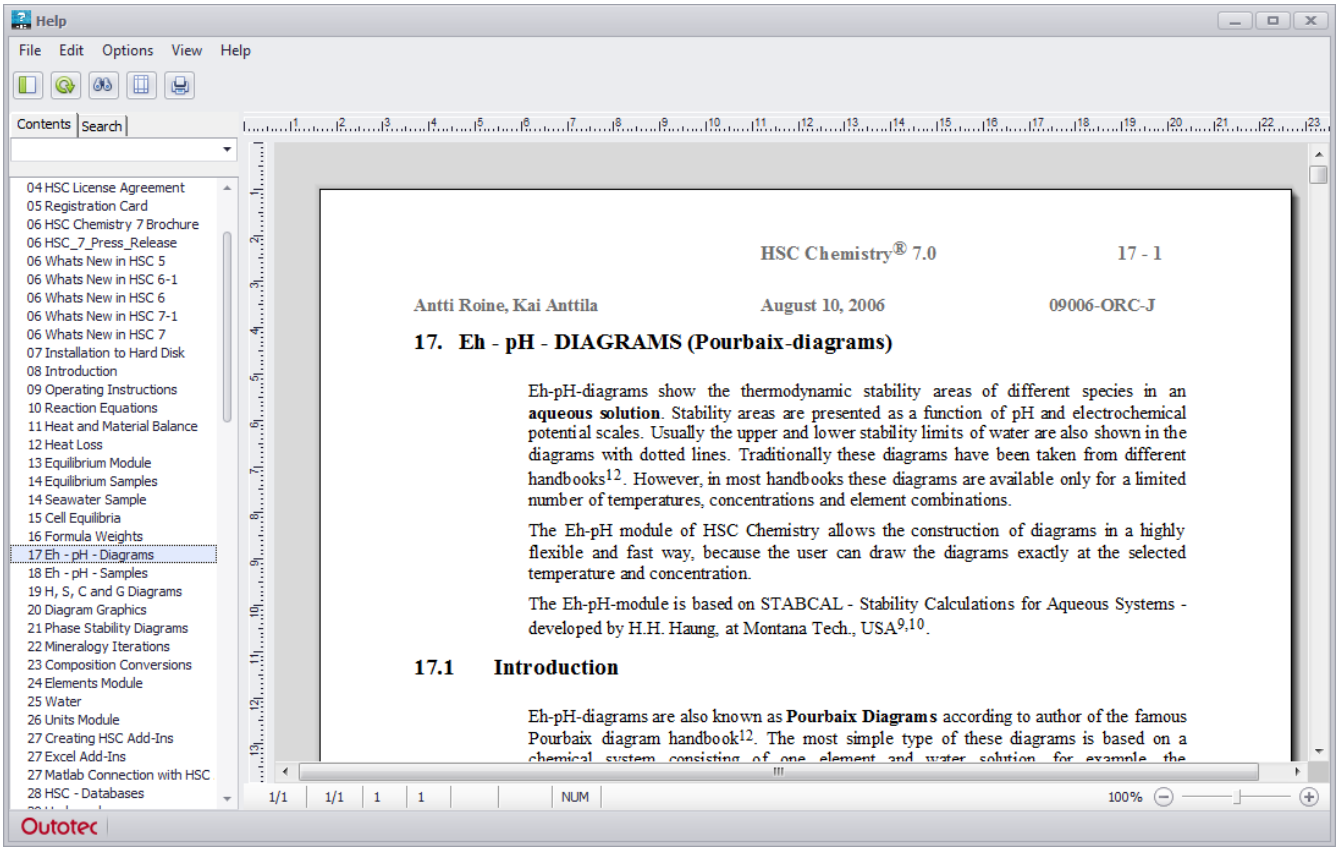
The HSC **D**ata**b**ase search and edit dialogs have been totally redesigned. HSC 7 dialogs have been integrated into one powerful search dialog, and a large number of new search options have also been added to this same dialog.

The HSC database architecture has also been updated. The new database also contains fields for comments and references without character space limitations.

A new predictive chemical formula typing system has been included. The ergonomics and visual appearance of the user interface have been improved.

Databases have been expanded from 25,000 to 28,000 chemical species. Data of 1300 species have updated.

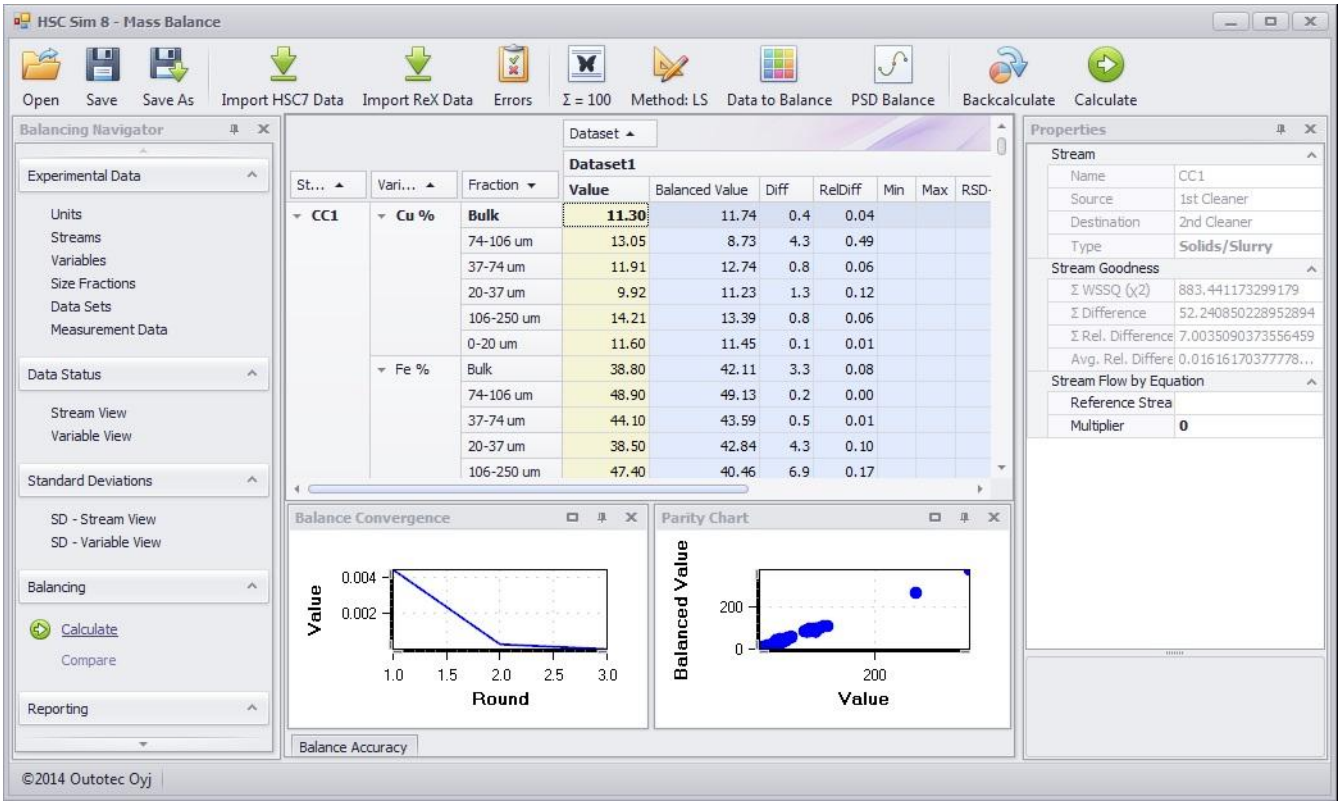
Help Module



The **Help** module has been completely rewritten. It contains manuals for all HSC modules and databases; search is possible to carry out for all the manuals using different key words.

The new Help module supports now supports Word files up to version 2010.

Mass Balance Module

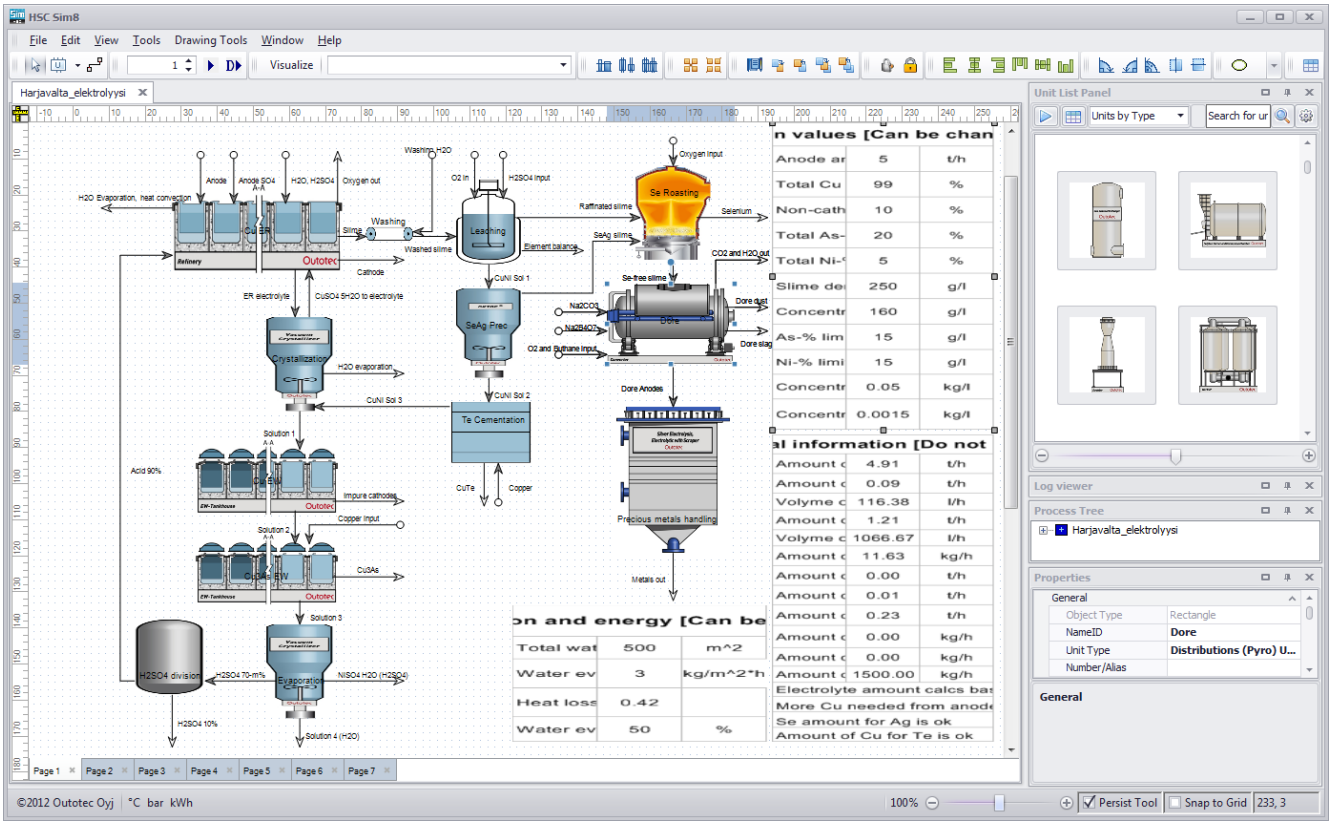


The **Mas**s Balance module uses data reconciliation techniques to convert incomplete experimental process data to balanced data, which may be used to calibrate theoretical process models or simply to create consistent analyses for yield and efficiency estimates for complete energy and material flow systems.

The Mass Balance module is connected to the Sim module. The first new version is tuned for mineral processing models, but the Mass Balance module will be expanded to other Sim modes for HSC 8.1.

New features include: Much easier and a more ergonomic user interface than used in HSC 7, with improved and more robust calculation routines. Partial balance areas, new charting options, new error models for measurements, data status preview, back calculations, dynamic tables, stream functions with multipliers, imports previous Mass Balance files, stream type definitions, etc.

Sim Flowsheet Module



The **Sim** module may be used to create flowsheet-based process models for hydrometallurgical and pyrometallurgical flowsheets as well as minerals processing systems also including physical recycling. The user interface and calculation routines have been completely revised and numerous features have been added.

Modeling and simulation are the most important tools required when developing new processes and improving previous ones. Process calculations are the basis of the design, dimensioning, and sizing of reactors, plants and systems.

The economy, energy efficiency, environmental impact, and sustainable effects of the process are established in the modeling stage and therefore establish CAPEX and OPEX. This stage also integrates disciplines, while it also harmonizes practices and enables realistic environmental footprinting with valid material and energy balances.

The Sim 8.0 module has four basic unit operation modes: Particle (Mineral Processing), Reaction (Hydrometallurgy), Distribution (Pyrometallurgy), and Experimental. Each unit operation model may be an Excel- or DLL-type file. Drawing and many other features are similar in all unit modes and types.

The Sim 8.0 has many new features including tools for LCA environmental footprint calculations, exergy calculations, improved distribution dialog, etc.

Particle Mode

Unit operation calculations are based on particle distributions. This mode is often used in minerals processing and physical recycling with crushing, grinding, flotation, gravity separation, or screening unit operations. HSC Sim has a special mineral stream set-up dialog for processes where minerals are treated. Mineral-based models treat particles, which have at least the following properties:

- size (diameter)
- mineral composition by wt.% including liberation details-

In addition, the models may have other parameters like composition by volume%, mineral composition by surface area%, whiteness, and hardness. Globally, minerals have a certain chemical composition and specific gravity and therefore HSC calculates these properties for each particle and also for each stream.

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. Processes can either be small single-unit processes or complete plants with all recycle streams. The Reaction Mode unit editor contains Wizards to ease the development of the models.

This mode may be used in chemistry, hydrometallurgy, etc. for leaching, precipitation, evaporation, liquid – liquid extraction processes, and liquid purification processes - just to mention a few. The Reaction progress rate parameters make it possible to calibrate theoretical mass and energy balance models using experimental reaction rate data.

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 may be used for applications where elements can be split into different streams with distributions. This is a common practice in pyrometallurgical calculations, but may also easily be applied to many other areas like chemistry, energy technology, recycling, etc.

Experimental / MassBalance Mode

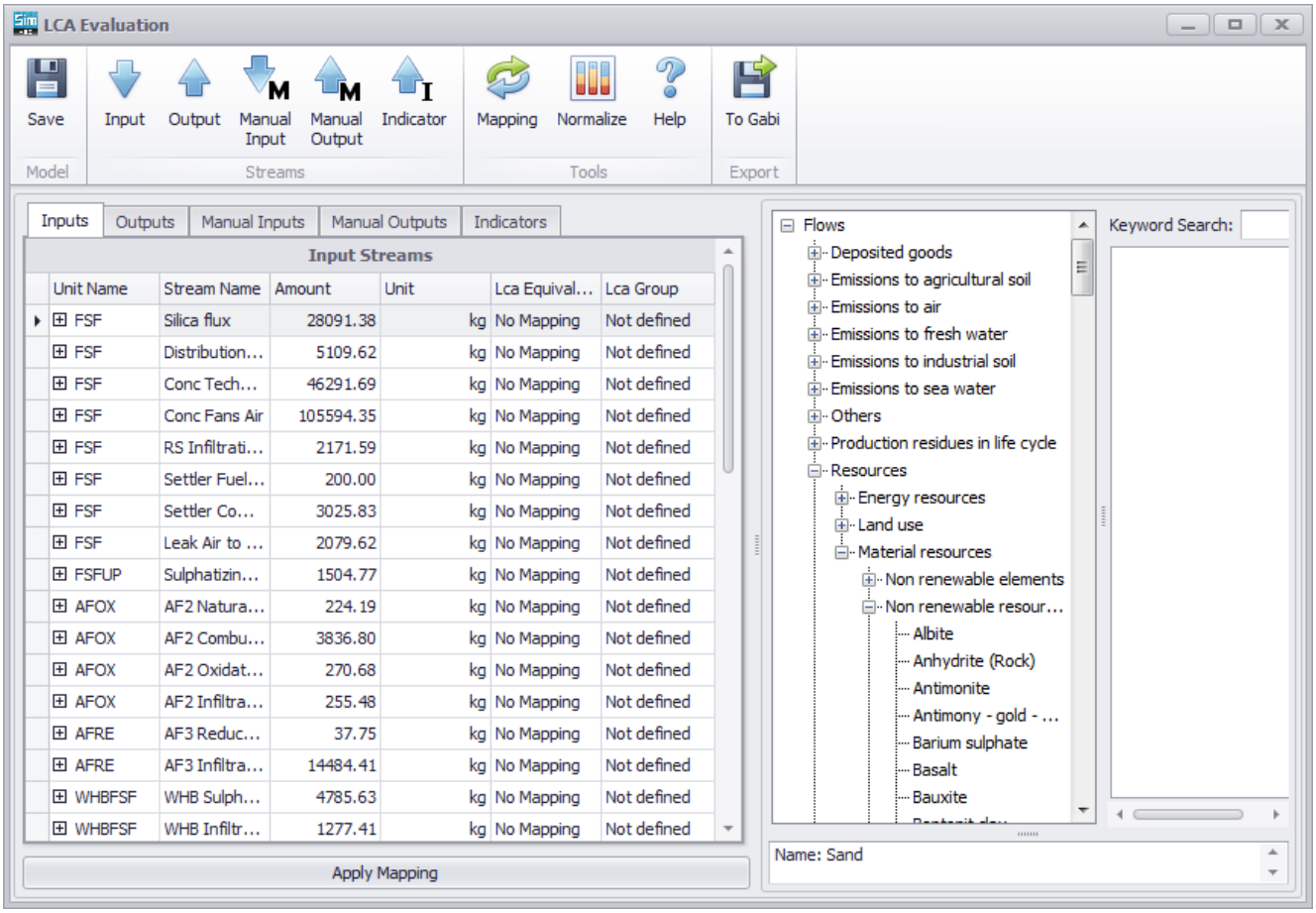
The Experimental mode is made for experimental process data harmonization by data reconciliation. Usually such data is incomplete and contains errors, which leads to problems when balance values are required. Please see details from the MassBalance Module.

Unit Types

Excel type unit models are based on an Excel-style unit editor with different wizards. The unit files are Excel-compatible files. This same unit type is also used in Sim 7.

The DLL Type unit models can be developed using compilers like VB.NET, C#.NET, etc. providing a large degree of flexibility. The Unit Editor has Input and Output sheets and a sheet for the unit parameters. Please note that this new unit type is not compatible with old Sim 7.

Life Cycle Assessment (LCA)



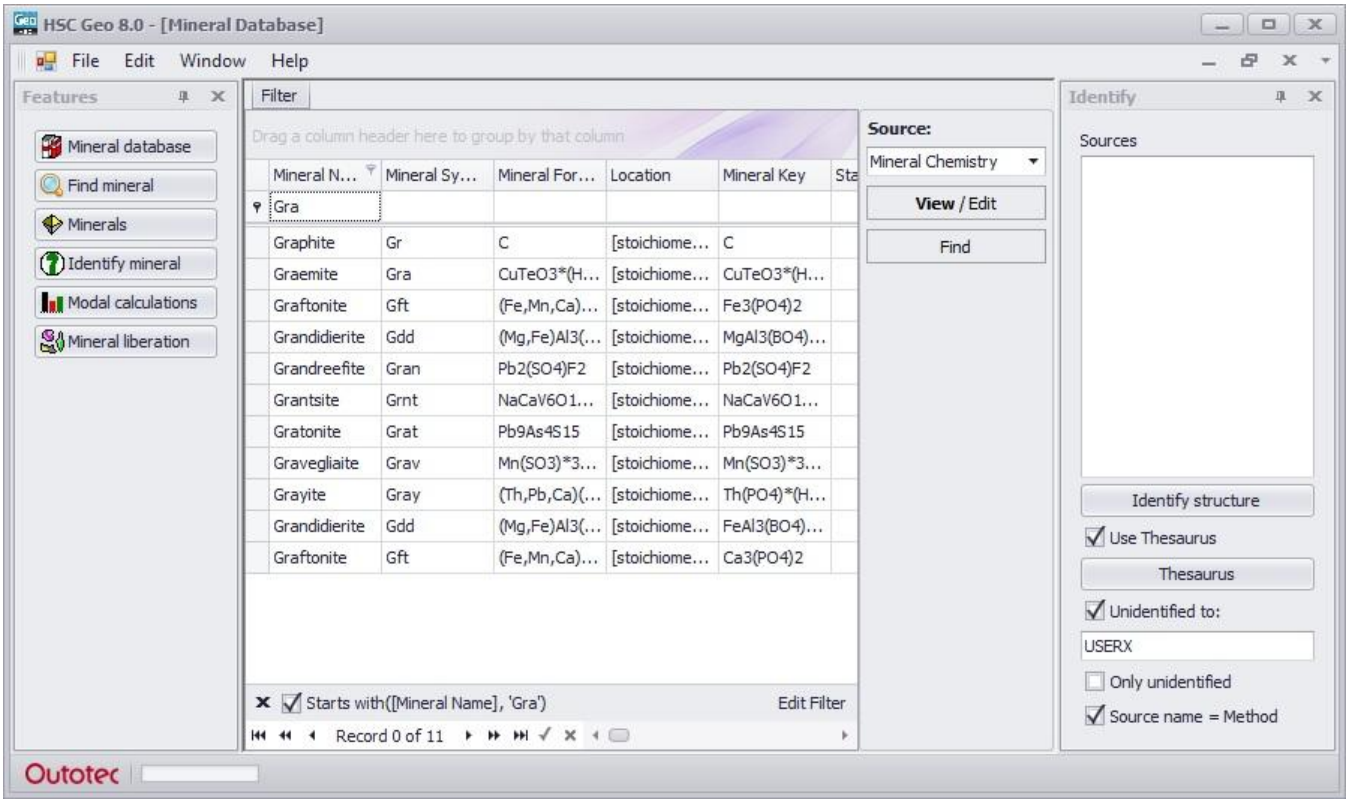
The new **LCA** tool has been integrated into the HSC Sim module. This enables the real life-cycle analysis of the process. Sim process models are based on material and energy balances; this leads to thermodynamically accurate ecobalances thus augmenting conventional LCA methods, which quite often do not meet critical element and energy balance boundary conditions.

The Sim LCA tool automatically collects process input and output streams and calculates few key indicators like carbon dioxide emissions. LCA dialog enables the user to map the stream materials from different LCA databases like GaBi®, OpenLCA, etc.

LCA dialog enables to specify also additional information not given in the process model like transporting costs, auxiliary equipment energy consumptions, etc.

Mapped process data may be exported to other programs using the Ecospold XML file format. Data extracted from flowsheets for LCA analysis can also be exported to Excel for further use in any relevant tool for environmental impact assessment.

Geo Module



HSC **Geo** is a collection of tools developed originally for geologists and mineralogists. However, these tools may also be useful for other professionals. HSC Geo offers an extensive database with data on 13,346 minerals.

The most critical Mineral Database tools and routines have been rewritten, the new user interface is more logical than in HSC 7. The new user interface enables, for example, complex filtering criteria for the mineral database.

The Microsoft Access database has been replaced with the new SQLite database, database structure has been reorganized with less duplicate information.