Metso's HSC 8.0 Chemistry Software

Metso, 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.

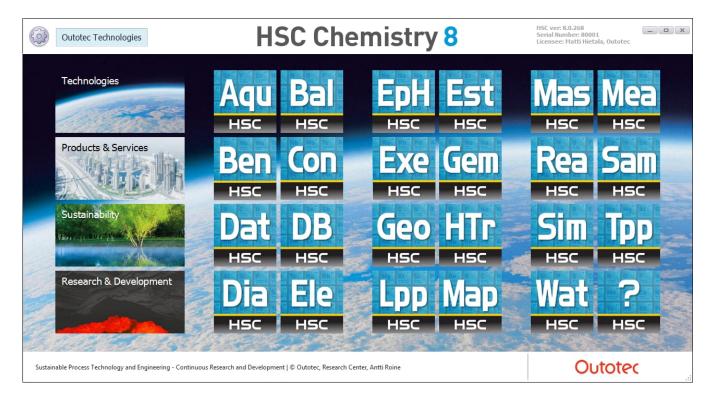
The completely new Benson estimation module makes it possible to estimate the H, S, and Cp values of organic compounds based on the molecular structure using easy graphical user interface.

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.

HSC 8 – New Features 2/27 Antti Roine September 8, 2023

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 Metso 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.

HSC 8 – New Features 4/27 Antti Roine September 8, 2023

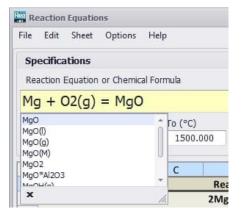
Reaction Module



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8	1050.000	-291.124	-55.225	-218.053	1.046	E+036		36.020	1.0E35 -
9	1100.000	-291.116	-55.219	-215.292	1.856	E+034		34.269	1.0E34 - 2Ca + O2(g) = 2C
10	1150.000	-291.104	-55.211	-212.531	4.371	E+032		32.641	
11	1200.000	-291.089	-55.200	-209.770	1.328	E+031		31.123 ⋿	¥ 1.0E33 -
12	1250.000	-291.070	-55.188	-207.011		E+029		29.705	1.0E32 -
13	1300.000	-291.047	-55.173	-204.252		E+028		28.378	1.0E31 -
14	1350.000	-291.020	-55.156	-201.494		E+027		27.132	1.0E30 -
15	1400.000	-290.990	-55.138	-198.736		E+025		25.961	
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The <u>**Rea**</u>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.

HSC 8 – New Features 5/27 Antti Roine September 8, 2023

Balance Module

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3 Fe3O4	25.00		5.594	1295.160	0.251	0.00	-1733.27	0.000				Input Out	mut
1 Fe2O3	25.00		4.435	708.305	0.135	0.00	-1017.93	0.000					
5 SiO2	25.00		35.856	2154.370	0.829	0.00	-9072.08	0.000				Insert	Delete
6 MnO2	25.00		0.975	84.743	0.017	0.00	-140.82	0.000				Insert	Delete
7 P2O5	25.00		0.166	23.565	0.010	0.00	-69.41	0.000				Balance Area	Balance Area
3 AI2O3	25.00		0.720	73.414	0.019	0.00	-335.14	0.000				Stream	Selected Stream
9 CaO	25.00		1.632	91.540	0.027	0.00	-287.89	0.000				Stream	Selected Stream
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The **<u>Bal</u>** 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



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14 Radiation coefficient (hr)	W/(m ² K)	0.000				0.000
15 Thermal Resistance	°C/kW	5.102	11.613	7.953	0.800	0.833
16 Results						
18 Heat Flow	kW 🔫	45.054	45.054	45.054	45.054	45.054
19 Heat Flux	kW/m² ▼	45.054	45.054	45.054	45.054	45.054
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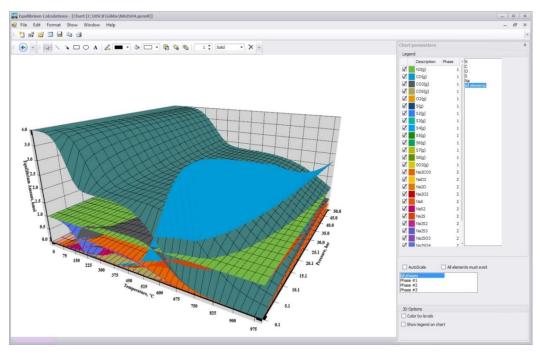
The <u>H</u>eat <u>Tr</u>ansfer module is also called Heat Loss module, because it estimates the heat losses and heat transfer of reactors for various geometries and reactor walls and linings and therefore a useful assistant during thermal design of reactors. The ergonomics and visual appearance of the 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.

HSC 8 – New Features 7/27 Antti Roine September 8, 2023

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. <u>**G**</u>ibbs <u>**E**</u>nergy <u>**M**</u>inimization (<u>**Gem**</u>) 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.

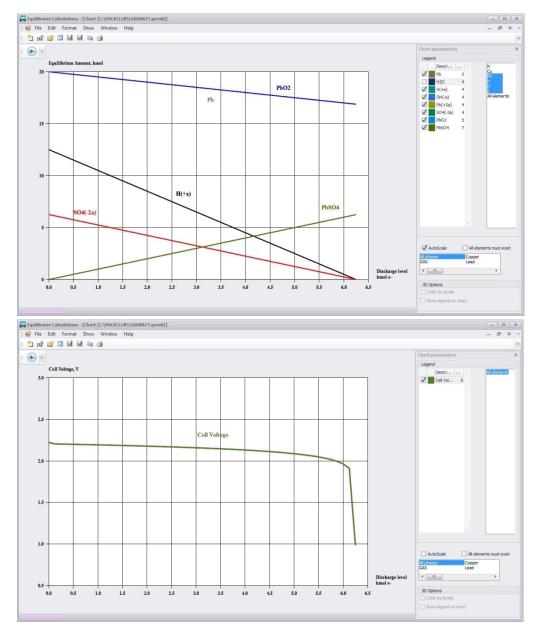
The new Gibbs 8.0 module has a long list of new features, the important ones including:

- 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.

HSC 8 – New Features 8/27 Antti Roine September 8, 2023

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

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1 2	Water Phase Data	Temp.	Amount	Amount	Amount	H Ideal	H Estimate	Cp Ideal	Cp Estimate	H Ideal	H Estimate	Cp Ideal
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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
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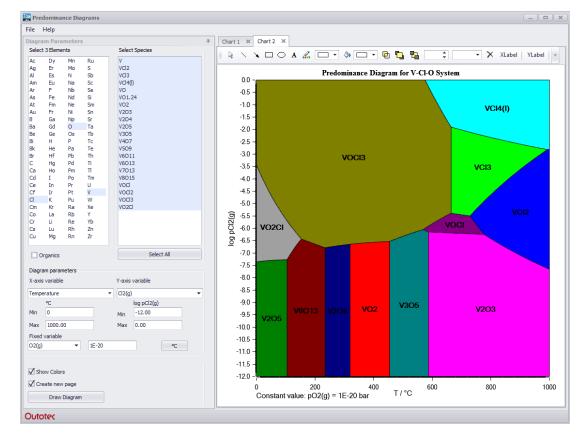
The <u>Aqu</u>a module contains non-ideal aqueous electrolyte models and databases. This module also includes a large number of standard state data for neutral components and ionic species. The Aqua module works as a standalone tool to calculate water solution properties, but it may also be utilized 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.

HSC 8 – New Features 10/27 Antti Roine September 8, 2023



Stability Diagrams Module

The **<u>Tpp</u>** 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.

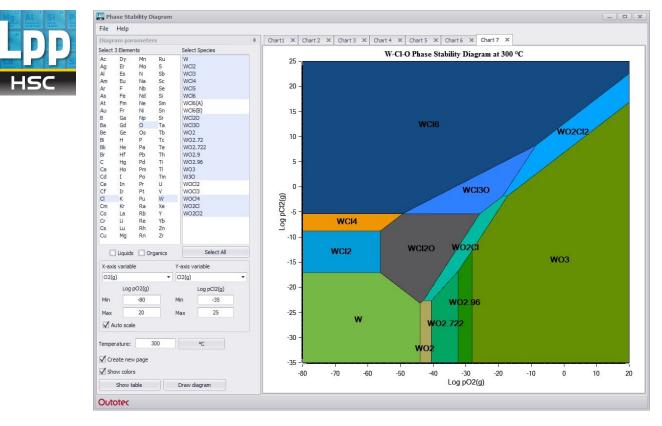
These diagrams may be used, for example, to review the kinds of chemical species that exist in the process gas line when there is a change in process conditions and temperatures. The diagrams are also useful when estimating roasting conditions or high temperature corrosion problems.

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.

HSC 8 – New Features 11/27 Antti Roine September 8, 2023

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.

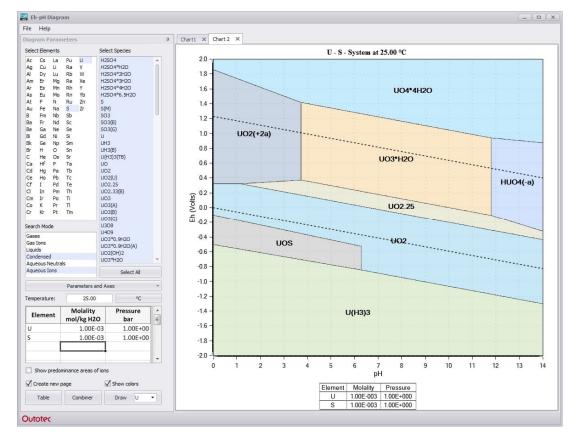
The new Lpp 8 module integrates the previous Lpp 7 input and calculation modules. This makes testing different systems much easier.

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.

HSC 8 – New Features 12/27 Antti Roine September 8, 2023

EpH Module





<u>E</u>h-<u>pH</u>-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.

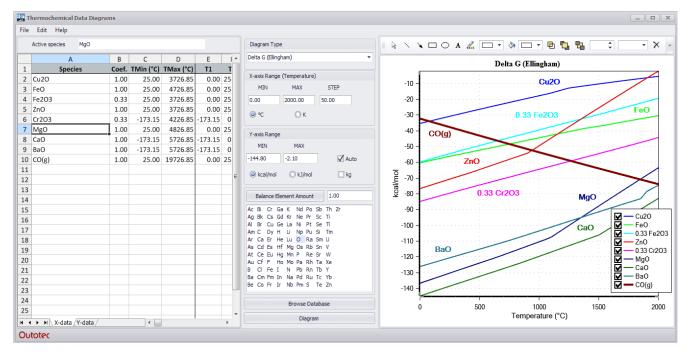
These diagrams may widely be applied in leaching, precipitation and corrosion studies. These diagrams give a quick view of the behavior of elements and species in water solutions as functions of pH and potential.

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.

HSC 8 – New Features 13/27 Antti Roine September 8, 2023

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

						Species Type								
	Species: KOP					Not Specified		•		- e				
Ter	nperature: 25]	№ «с	Пк	Ţ	-		E	istimate				
	A		В	С	D	E	F	G	н	1	1	К	L	M
1	Chemical Fo	rmula	Species Type	Tempe	rature	Selected set	Wei	ight	H (2	5 °C)	S (2	5°C)	0	р)
2	112 112					of possible oxidation	g / 1	mol	kJ /	mol	J/m	nol*K	J / n	nol*K
3	Species			°C	к	numbers	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	AIPO4		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
	KOP		Not Specified	25	298.15		86.07		-707.32	N/A	87.66	N/A	65.01	N/A



The HSC <u>Est</u>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.

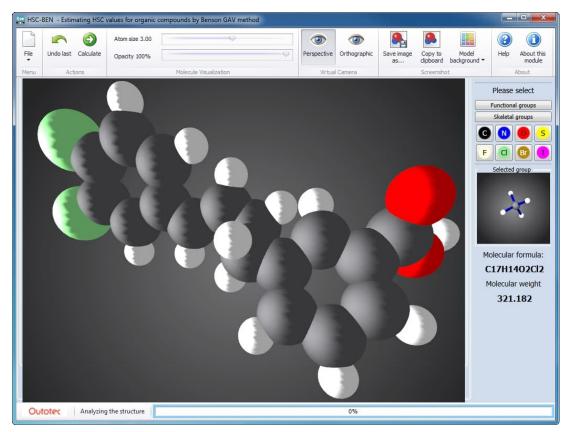
The quality of this data is essential in process modeling and simulation. The module may be used to identify errors in experimental data and estimate the missing data needed in calculations. It has also been applied to check for errors in the HSC database.

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

HSC 8 – New Features 15/27 Antti Roine September 8, 2023

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.

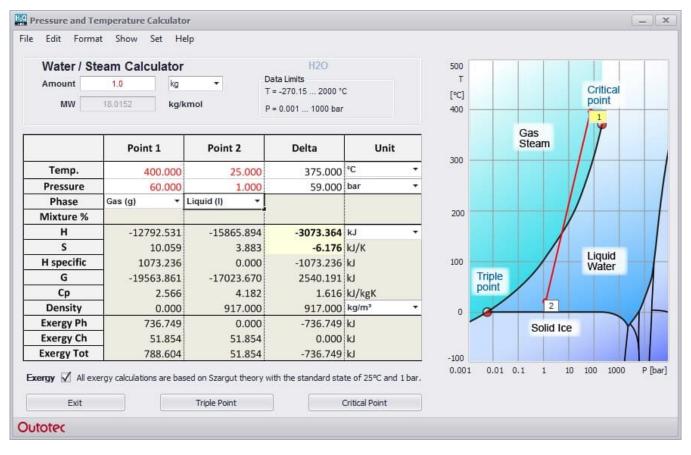
This module enables more accurate H, S, and Cp estimates for organic species than those given by the Est estimation module, which suits inorganic species better.

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.

HSC 8 – New Features 16/27 Antti Roine September 8, 2023

Water Module





The <u>Wat</u>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



11111	no segura			10	4000
Unit Con	version			Sampler and Gra	phs
Mass			•		
	▼ t	•	✓ ton(long)	Samp	ler
Class	Sheet			Water	in air
Clear	Sheet				
A9	•				
			_		-
	A	В	С	D	E
1	Data 1	Units 1	Data 2	Units 2	
2	37.2	1	8.8851828	cal, gm.(IST.)	
3	1	J	0.238849	cal, gm.(IST.)	
4	4.186745601	J	1	cal, gm.(IST.)	
5	1	I	0.26417205	gal(US)	
6	3.785411818	1	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 <u>Mea</u>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.

HSC 8 – New Features 18/27 Antti Roine September 8, 2023

Elements Module

Periodi	c Chart																
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Hydrogan 1.00794																	Helium A002602
Lilhium 4,941	Beryllium 9.0121831											Bersn 10,811	Carton 12.0107	Nitrogen 14.0067	02197774 15.77774	Ta Trend Ta 3	Nee 10 Neon 20.1797
© 11 Na Sodium 22.9897928	Megnesium 24.3050											Aluminium 24.9915385	SILCON 28.0855	Phosphorus 36,973761998	5016 Suther 32.066	Chierine 35.453	Argan Argan 37,948
Putansium 39.0903	Calsium 40.079	Scandium L4.955900	Ti Titanium 47.847	V ²³ Vanadium 50.9415	Cr Chromium 51.9961	Manganese S4.738044	Fe 26	Coball 58.733194	Nichal 58.4934	Cu Copper 63.546	Zn 200 30	Ga 31 Gallum 49.723	Germanium 77.63	Arsenie 74,921595	Selanium 78.971	35 Bromine 79.904	Kr Krypten 83.798
Rubidium 85.4678	³⁸ Sr Strentlum 87.62	♥ 39 Yitirium 88,90584	O 40 Zr Directium 91.224	Nichlum 92.90637	Mo Hulybdenum 95.95	Tc ⁴³ Technetium (78)	Ruthenium 101.07	Rhodium 102.90550	Palladium 106.42	Ag 47 Silver 107.8682	Cadmium 112.414	114.818 49	Sn Tin 118.718	SD Antimarty 121.740	Tellurium 127.60	126.90447	Xe 54
© 55 Cs Caesium 132,905451%	© 56 Ba Barlum 137.327	57- 71	72 Hf Hatnium 178.49	Ta Ta Tantalum 180.94788	Tungslen 182.84	Ree 75 Rhanium 186.207	0576 Osmium 190.23	177 Iridium 192.217	Platinum 195.084	AU 79 Gold 196.966569	Hg 80 Marcury 200.59	Thelium 204.3833	PB Lead 207.2	83 Bismuth 208,98040	Polasium (209)	Astatine (210)	Raden (222) 86
© 87 Fr Francium (223)	e BB Ra Radium (224)	89- 101	© 57 La Lathanum 138,90547	© 58 Ce Certum 140.116	• 59 Pr Prassodymian 140.90766	Neodynium 144.242	Promotihium	© 62 Sm Samarium 150.36	© 63 Eu Europium 151.764	Gd Gd Gadetinium 157.25	65 Tb Terbiam 158,92535	Dy Dysbrosium 142,500	67 Ho Holmium 164,93033	© 68 Er Erbium 167.259	69 Tm Thuthum 168,93422	70 Yb Yttartolam 173.054	© 71 Lu Lutatium 174.7568
			AC Actinium (227)	90 Th Thorizm 232,0377	Pa Protactinium 231.03586	92 U Uranium 230.02891	93 Np Nuptinium (237)	Pu Pu Putonium (244)	Amaritium Amaritium	Cm Curium (247)	97 Bk Berkellium (247)	Cf Californium (251)	99 Es Einsteinium (252)	Fm Fremium (257)			
Aik	cati	Aika	üne	Transit metals Lantha		Post-tran metals Actinides	-	Metalloid		Non-metal	Ha	logens	Nobi	e gases	Br Liqu] Solid
				Electroi	negativi	ity		•	Cle	ar	Print		Database	e Hi	de Legend	Sho	w Data
Outo	otec																



The <u>Ele</u>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.



HSC 8 – New Features 19/27 Antti Roine September 8, 2023

Converter Module

6	3						Species Con	verter				X
w.	2	Home	Tools									
)	i - E	¢	¢		9						
Nev	N	Open Save	Add Calcula Sheet	ation Add Summ Sheet	ary Delete Sheet	About He	lp					
		File		Workbook		Help						
	A	В	С	D	E	FG	н	L	J	K	Output Analysis	'n
1 2 3		Name Date Author					Residual Error	0.003			Output an	alysis
4		INPUT				OUTPU	r					(- (-)
6	_	Analysis		Calculated		OUTPO	Calculated	Target	Weight	Туре		FeS2
7		Elements	wt-%	Elements	wt-%		wt-%	wt-%	Coeff	.,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		
8		Total	100.000		100.000	6	100.000	70.000				SiO2
9		Cu	28.000	Cu	28.000	Cu2S	0.00E+00		1.000			
10		Fe	27.000	Fe	27.001	CuS	6.500		1.000			Small am
11		Ni	1.000	Ni	1.000	CuFeS2	68,385	70.000	10.000			CuS
12		Co	0.500	Co	0.500	CuSO4	0.00E+00		1.000			
13		S	34.000	S	33.999	FeS	0.00E+00		1.000		CuFeS2	
14		SiO2	9.500	Si	4.440	FeS2	13.297		1.000			
15				0	5.059	NiS	1.547		1.000			
16				Н	0.000	CoS	0.773		1.000			
17				[Others]	-1.52E-04	SiO2	9,499		1.000			
18						[Others]	0.00E+00		0.001			
19												
20	-	u) charte /					1.1				Input Analysis Output	Analysis
-		H Sheet1					<					
0	Ut	otec	_			_						



The <u>**Con</u>**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.</u>

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.

HSC 8 – New Features 20/27 Antti Roine September 8, 2023

Exergy Module

Broy	vse database Insert stream	Input •	Normal stream	-	Mass Bala	ance (ka)	Heat	Balance (kJ)	Exergy Bala	ance (kJ)	All exercy calculati	ons are based on s	Szarout theory y	with the standard state	being 25°C and 1 b
	lete stream Delete sp			ulate)	-12			8353.66	-5705		Normal stream acce	pts any species.		fect of pressure to ent	
	A	В	С	D	E	F	G	н	1	J	к	L	M	N	0
1	Streams and	Mass	Amount	Molfraction	т	P	S	н	ΔG_f (25°C)	Ex_element	al 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														
.0	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
.1	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		
2	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														
L4															
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
6	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		
.7	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		
.8	Insert/paste species here														
9	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
0	*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		
4	SO3(g)	0.00	0.00		1100.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
5	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		
6	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														

Outotec



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

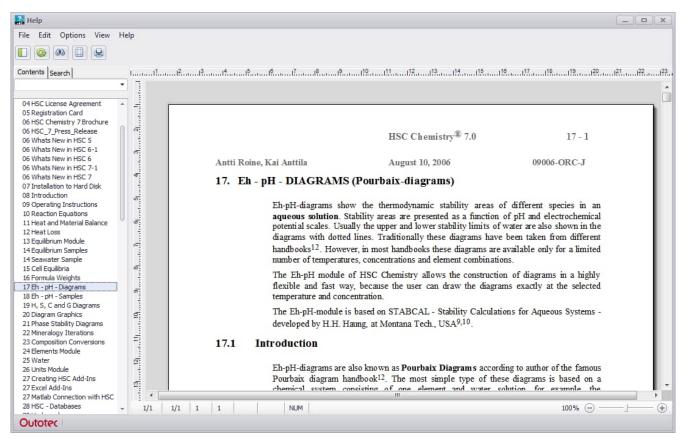
File View Edit	Joules Calories	Kelvin	°C Celsius Ma	in Database O	wn Database		agrams DB M	erge	Fit Cp Data	Help At	pout					
Menu	Unit	Tem	perature	Database Se	lection		Tools			Info						
Text Filters					Type Filters			Organ	nic Filter							
Elements Ni S		-1	Possible Species	-	Gases		ds		Include Or							
Formula			Start With	-	Gas Ions		ous Ions			÷.						
Stoichiometry					Condense		ous Neutrals	Rar	nge Of Cart	oon Atoms						
Keywords			Structural Formul	cha a	V Electrons											
Reywords			Structural Formul	a, crie •												
Matching Species - 28	Basic Data															
li	Formula	Ni				Molecular We	sight 58	.700			g/mol					
Ni(I)	Structural Formula	-			-	Melting Point	17	28.000			к					
Ni(g)	Chemical Name	Nickel				Boiling Point	31	86.000			к					
Ni(FCC)	Common Name	-				H ^o formation	at 298.15 K 0.	000			kJ/mol					
Ni2(g)		7440-02-0	12			S° at 298, 15		,796			J/(mol*K)					
viS0.84	0.84										1.544.555.54					
NiS NiS(a)	Temperature Rang	es C _p (T) = A + BT *	$10^{-3} + CT^{-2}$	$*10^{5} + DT^{2}$	* 10 ⁻⁶										
NiS(A)	Range		1	2	3	4	5		6	7						
NiS(B)	Tmin (K)		100	298,15	450	631	. 700		1200	1728						
vis2	Tmax (K)		298.15						1728	6000						
li352	Phase		Solid						Solid	Liquid						
li352(l)	H kJ/mol S J/(mol*K)		0.000 29.796	0.000					0.000	17,480						
1354	Cp coefficient A	1/(moi*K)	15.485						0.980	43.100						
li6S5	Cp coefficient B	5701151 119	53.411						8.806	0.000						
1756	Cp coefficient C		-0.667	0.167	-442.412	200.020	25.457	1	8.789	0.000						
1958	Cp coefficient D		-52.811	-16, 154	1946.962	-267.439	-4.929		0.577	0.000						
	Density kg/l		8.900	0.000					0.000	0.000						
5(I)	Color		White	White	White	White	White	N/A	N/A							
	Solubility in H2O	g/l	0.000						0.000	0.000						
	Reference Reliability Class		Landolt 99, B		Nasa 93	Nasa 93	Nasa 93	Nasa 93	Nasa 1	a 93, Lan						
6(g)	Reliability Class		1	-	1	1			1	1						
6(g) 6(M)																
6(g) 6(M) 62(g)	Selected Species -	3														
5(g) 5(M) 52(g) 53(g)	Selected Species - Ni3S2	3														
5(g) 52(g) 53(g) 54(g) 55(g)		3														
5(g) 5(M) 52(g) 53(g) 54(g)	Ni3S2	3														



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 <u>Help</u> 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.

HSC 8 – New Features 23/27 Antti Roine September 8, 2023

Mass Balance Module

Dpen Save Save As Import	HSC7 Data	Import ReX D	lata Errors	Σ = 100 Me	ethod: LS Data	to Bala	nce PSD E	<u>∫^</u> Balance	Backcald	culate Calculate	
Balancing Navigator 🛛 🛱 🗙				Dataset 🔺						Properties	ц. :
				Dataset1					_ 0	Stream	
Experimental Data ^	St 🔺	Vari 🔺	Fraction +	Value	Balanced Value	Diff	RelDiff I	Min Max	PSD.	Name	CC1
Units	- CC1	+ Cu %	Bulk	11.30	11.74			MILL MOX	KSD	Source	1st Cleaner
Streams	+ ttr	+ Cu %	74-106 um	13.05	8.73					Destination	2nd Cleaner
Variables			1.	10000000						Туре	Solids/Slurry
Size Fractions			37-74 um	11.91	12.74					Stream Goodness Σ WSSQ (χ2)	883,441173299179
Data Sets			20-37 um	9.92	11.23					Σ Difference	52.24085022895289
Measurement Data			106-250 um	14.21	13.39						€ 7.003509037355645
			0-20 um	11.60	11.45						€ 0.01616170377778.
Data Status ^		+ Fe %	Bulk	38.80	42.11					Stream Flow by Eq	
Stream View			74-106 um	48.90	49.13					Reference Strea	a
Variable View			37-74 um	44.10	43.59					Multiplier	0
Valiable view			20-37 um	38.50	42.84	4.3	0.10				
Standard Deviations			106-250 um	47.40	40.46	6.9	0.17				
SD - Stream View SD - Variable View Balancing ^ © <u>Calculate</u>	9.0	004 - 102 -		· · · · ·	Parity Chart anpa Parity Chart Appa 200 - 0 -			•	л х		
Compare Reporting	Balance A	1.0 1.	5 2.0 2. Round	5 3.0	Ba		200 Value		78.00		1000



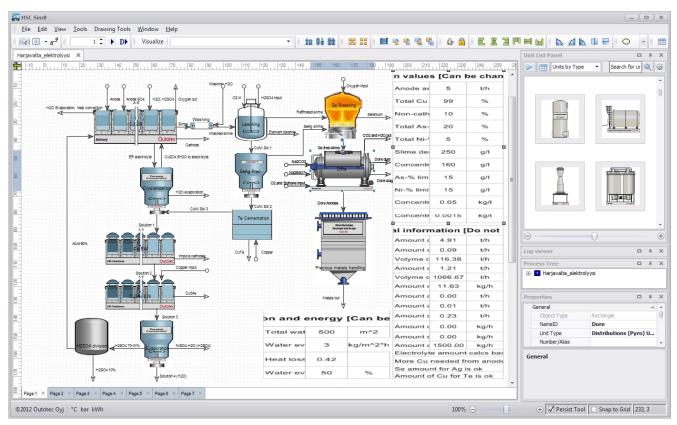
The <u>Mas</u>s Balance module uses data reconciliation techniques to convert incomplete experimental process data to balanced data, which may be used to calibrate theoretical process models or simply to create consistent analyses for yield and efficiency estimates for complete energy and material flow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

HSC 8 – New Features 24/27 Antti Roine September 8, 2023

Sim Flowsheet Module





The <u>Sim</u> 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.

HSC 8 – New Features 25/27 Antti Roine September 8, 2023

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. Mineralbased 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. Water Density database have been updated with 49 new species.

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.

<u>The DLL Type</u> 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.

HSC 8 – New Features 26/27 Antti Roine September 8, 2023

Life Cycle Assessment (LCA)

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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.

HSC 8 – New Features 27/27 Antti Roine September 8, 2023

Geo Module

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HSC <u>Geo</u> 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.