Metso

What's New in HSC 7.0

Once the compass gave us a competitive edge when navigating in foggy waters. Today modeling and simulation give us a similar advantage when we navigate oceans of data with hundreds of variables. This is the only way to utilize the current massive information overload. The new HSC Chemistry 7.0 provides us with an easy simulation tool to steer process development and research.

Antti Roine, Pertti Lamberg, Tuukka Kotiranta, Justin Salminen

September 8, 2023

Summary of the new Features

HSC Chemistry 7.0 is not only a process flowsheet simulation software program but it also contains 22 other useful calculation modules and 12 databases with an extensive number of thermochemical, heat transfer and mineralogical data on the same CD. HSC 7 has several new features, for example:

1. Flowsheet Module

- Four different modes (Particles, Reaction, Distribution and Experimental), new Table object, new Page and Layer properties, more robust controls, new Excel Wizards, Mass Balancing and Data Reconciliation routine

2. New Unit Icon Library with 515 Icons

- The unit process icon database was made in cooperation with industrial designers and process engineers. These may be used to visualize process flowsheets.

3. New Add-In Functions

- StreamSM, StreamGM, StreamEQA, StreamXArray, RecoveryXArray, ProgenyStream, ComminutionProductPSD, CubicSpline, ERF.

4. Updated Balance Module

- Automatic entropy (T * S) and Gibbs energy (G) balance calculations were added.

5. Updated Equilibrium Module

- A more robust Gibbs Energy Minimization routine.

6. Updated MW Module with new H, S and Cp Estimates

- Even the original H, S and Cp data sources may contain errors and typos, so the new estimation routine may be used to identify these errors.

7. New Aqueous Solution Property Estimator

- This module estimates non-ideal electrolyte solution properties like activity coefficients and enthalpies. These may be used in Equilibrium module or in process models.

8. Updated H, S and Cp Database

- More than 4000 new species were added and data of 4700 species were updated. The total number of species is now more than 25000.

9. Updated Mineralogical Database

- The number of minerals has been increased from 3581 to 13346 minerals.

10. Updated Help Module

- The new Help module is more robust and has access to unit model help files.

## 11. Windows Vista, Vista 64 and Windows 7 Support

12. Other improvements

- Several new features were added and a large number of small bugs were fixed.

Flowsheet Module

Four different modes for different simulations: 1) Particles (Minerals), 2) Reactions (Hydro), 3) Distribution (Pyro), 4) Experimental. Certain dedicated tools have been developed for this purpose.

Excel wizards have been updated and more commands added to the making of Excel Wizards. **Backups** are now easier to make with the new backup tool. You can also restore old backups.

New Drawing Features:
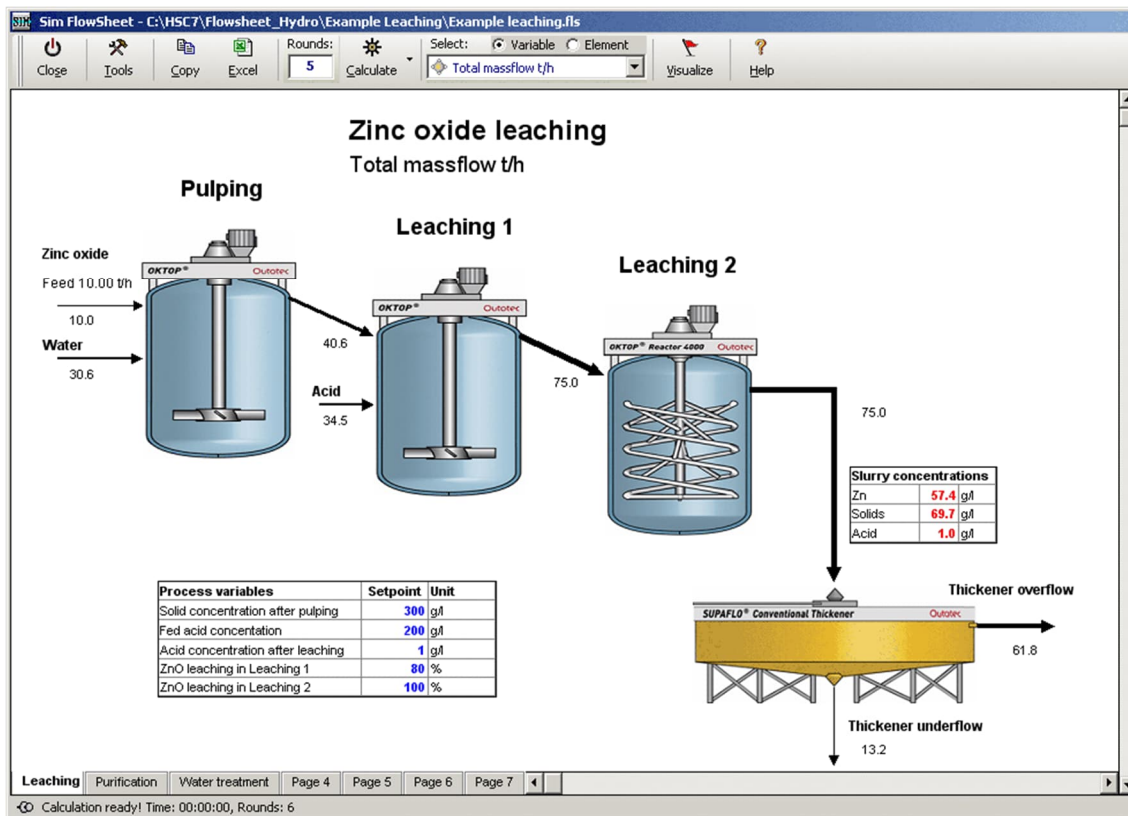
HSC 7 has multiple **new high-resolution icons** for different unit processes. The unit icons are grouped under the following folders: Acid Plan, Analyzers, Experimental, Ferro, Flotation, General, Grinding, H2SO4, Hydro, Iron&Steel, Minerals-Others, Others, Physical Separation, Precious Metals, Pyro, Roasting, Thickeners.

Units may have **default output and input streams**; i.e. when drawing a unit, the defined output streams appear in the flowsheet automatically. This saves time when drawing a flowsheet. Several units have this feature by default.

Unit icons can now be connected to **model wizards**; i.e. HSC Sim loads the defined model wizard when a unit is drawn. It is ready to apply when the drawing and set-ups have been completed.

HSC 7 has a new **Table object**. You can draw tables on the flowsheet and display different data on them. The links in the table are two-way links just like on the Control sheet value row. This enables the use of tables to control the process.
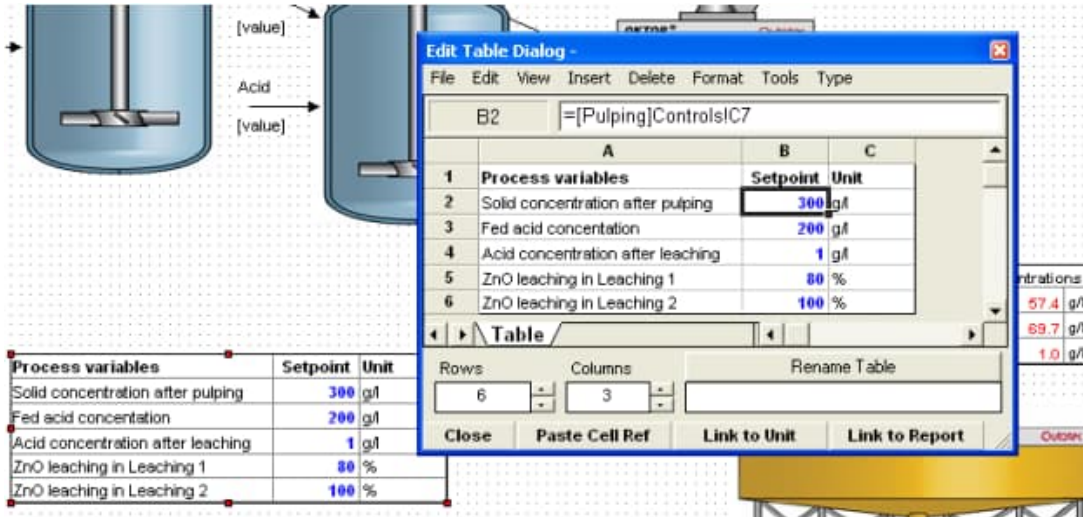

Stream Tables: you can display the values of different variables in different streams by using Stream Tables.
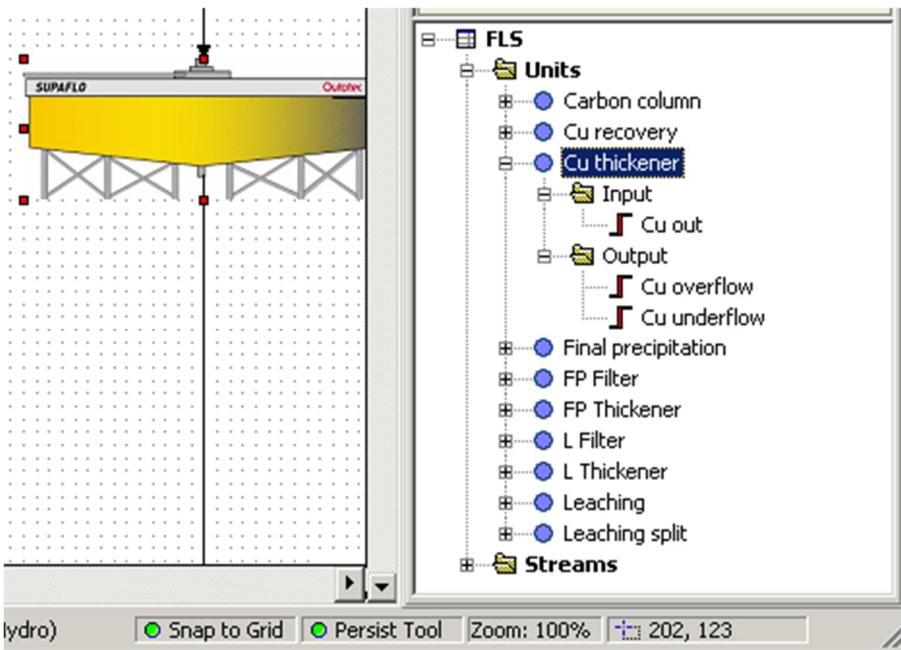

New **Stream and Unit Navigator**: using the navigator will give you better control over how streams are connected. Selecting a unit or a stream in the navigator will also show the selection in the flowsheet and vice versa. If a unit or stream is on a different page, HSC Sim will select and show that page. The navigator has a "Highlight Streams" feature: applying it will highlight the input (colored blue) and output streams (colored red) of the selected unit.

You can distribute your process on several **Pages**. This is a handy way to organize processes especially if they consist of different sections or they are large.

| Leaching | Purification | Water treatment | Page 4 | Page 5 | Page 6 | Page 7 |
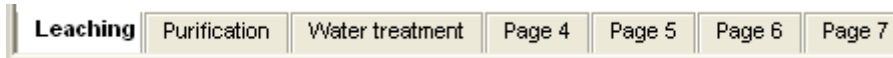
Duplicate Streams is now possible to draw on the flowsheet. These may be utilized, for example, if the stream goes from one page to an other.

New **Layer** property: different drawing objects can be divided into several layers. You can let HSC arrange your drawing objects to different layers by applying "Sort to Layers." You can turn layers on and off and control easily which objects are visible.
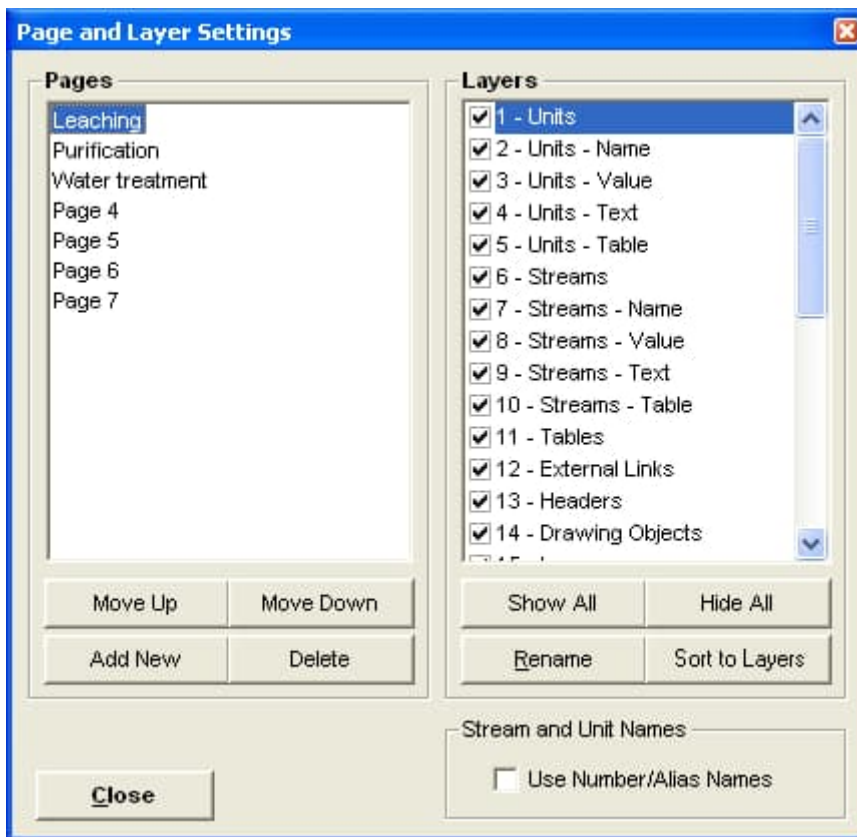
Streams and units can also have **Alias Names**. These are alternative names, which can be displayed on the flowsheet instead of a name label by selecting "Use Number/Alias Names" in the "Page and Layer Setting" window.

File links can now also include **www links**. Double clicking on www link will activate your Internet browser and take you to the linked page.

The editing and scrolling speed of the large flowsheets has been improved considerably.

New Features in Spreadsheets, i.e. Unit files and Report:

Leaching 1

Setpoint	Unit
300	g/l
200	g/l
1	g/l
80	%
100	%

File Edit View Insert Delete Format Tools Wizard Controls Help

Leaching 1

C19   Auto

	A	B	C	D
1		CONTROLS	Run	
2				
3		Number	1	2
4		Y TARGET NAME	Acid conc. after leaching	Fed acid conc.
5		Process Unit	Leaching 2	Leaching 1
6		Measure Unit	g/l	g/l
7		**Set Point**	**1.00**	**200.00**
8		Measured	1.00	199.89
9		Tolerance +/-	0.10	1.00
10				
11		X VARIABLE NAME	H+ feed	Water in acid
12		Process Unit	Leaching 1	Leaching 1
13		Measure Unit	t/h	t/h
14		Value	0.13	28.23
15		X Min Limit	0.00	0.00
16		X Max Limit	1.00	50.00
17		X Max Step		
18				
19		CONTROL METHOD	Auto	Auto
20		Active		
21		Iterations Max Limit	5	5
22		Iterations Min Limit		
23		Operation		

\ Input / Output / Dist \ Controls / Model / Wizar

Vis   Sync   Temperature: °C

Named ranges: you can add name-defined ranges to the spreadsheet. These may be used within the controls and models.

You can use **cell comments** in the spreadsheets.

Protection in spreadsheets: you can easily protect the unit models from changes. After protection, only cells with a blue font can be changed.

Copy Cell Reference and Paste Cell Reference for quick and easy formula references between the units and streams. The old "Set Link Source Cell" – "Set Link" is still usable but the new name describes the operation better.

Formula Navigator has been added for easier checking of cell formulas.

Upper or lower case characters can be used in **g/l measurement units** (g/L, G/l, etc) when the concentration is calculated automatically.

Improved and More Robust Controls:
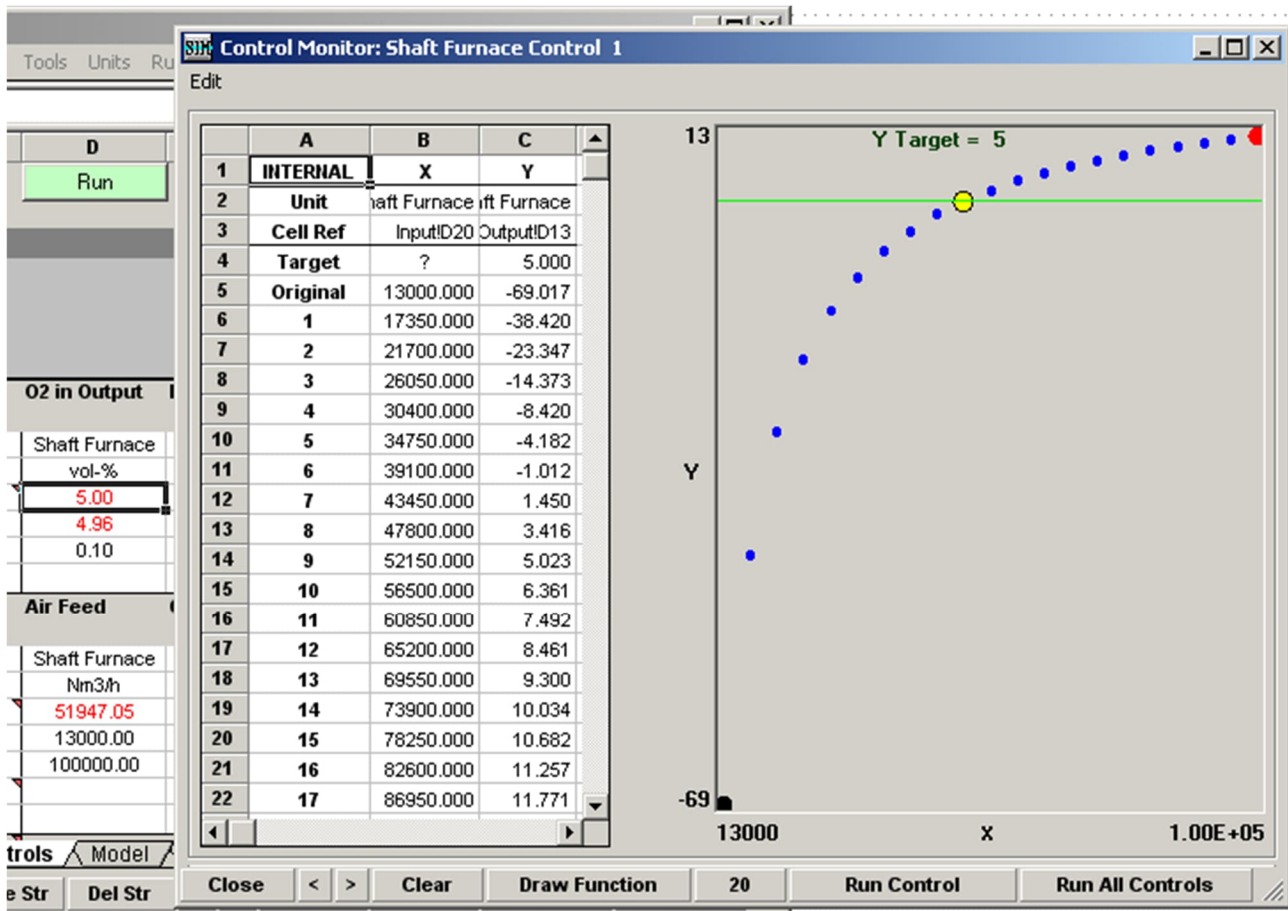
The control calculation routines have been improved. The problems with values close to the minimum or maximum limit has been fixed and the controls can now calculate more complex cases. Also, simple direct/reverse control has been added.

The improved Control Monitor dialog makes it easier to find, for example, the feasible X Min and Max limits for the variable. The new "Draw Function" button may be used to illustrate and identify the shape and discontinuity points of the control function.

New Features in Running the Simulation:
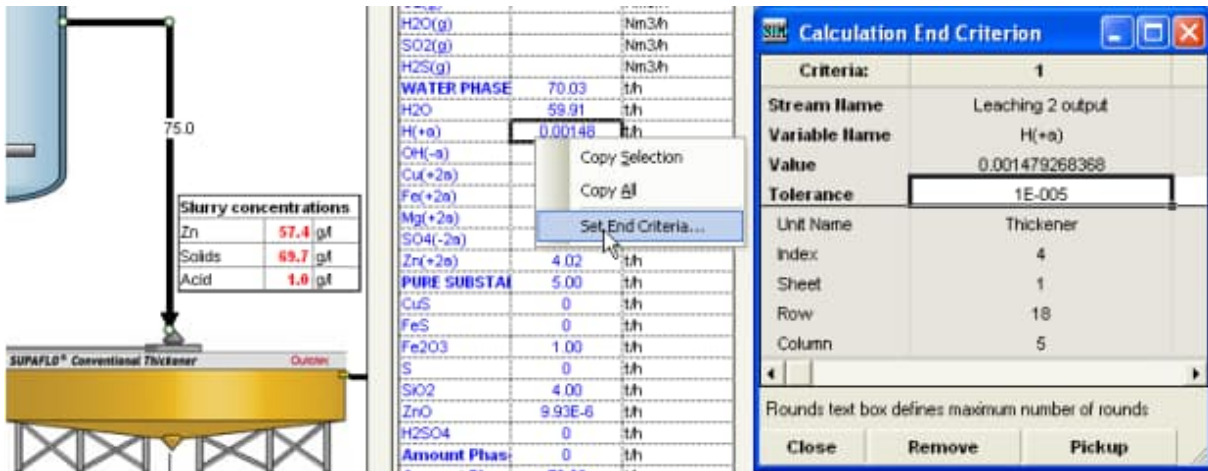
Calculation stop criteria to ensure that the simulation has reached steady state

A new **Find Error** routine has been developed. With this routine you can test your drawing before processing further and easily locate errors to fix them. Find Error checks the streams and units e.g. for correct connections. You can find this tool from Run Mode, Tools, Find Errors… This routine checks the control, materials amount, sync. area and element balance errors of all the units. With a single double click you can move to the error cell.
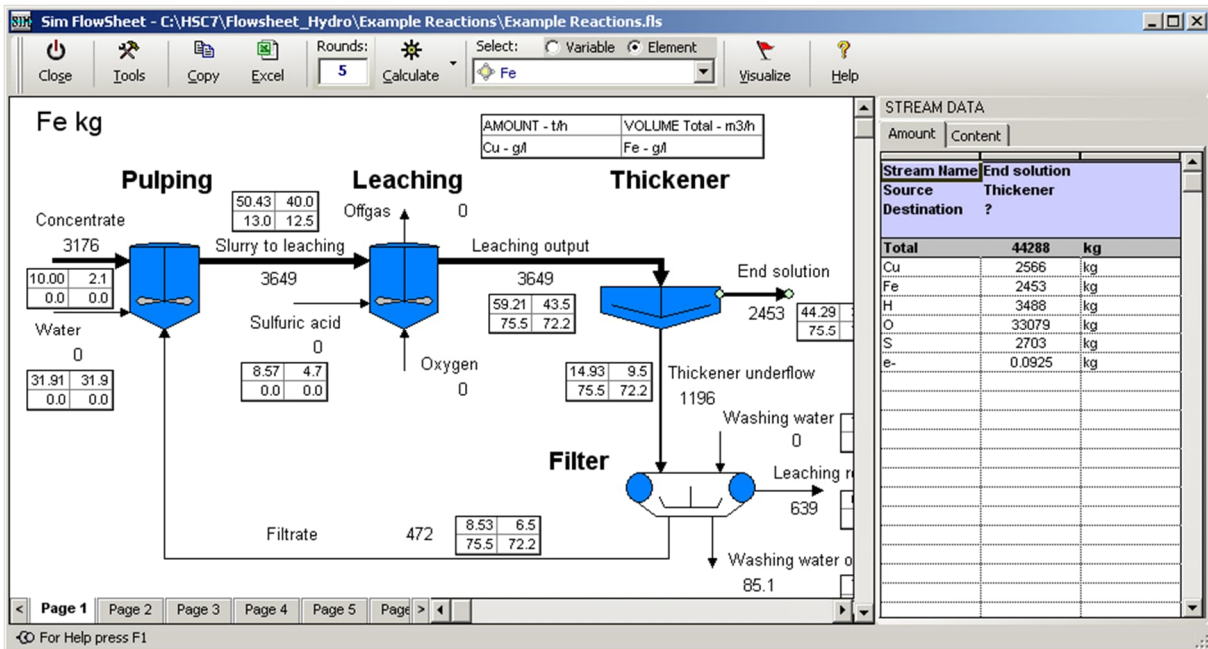
Visualization of elements in the Run Mode is possible with Reaction and Distribution Models. The visualization works in the same way as the visualization of variables.

New Features in Particles (Mineral) Mode:

When defining the mineralogy of the process (mineral setup) you have **direct access to the HSC Mineral Database** with **13346 records of different mineral analyses**. When selecting an appropriate mineral you can browse the database and compare available minerals in the XY and Line charts (see below). The **New Mineral Database Browser** makes it easy to add new minerals to the Database.
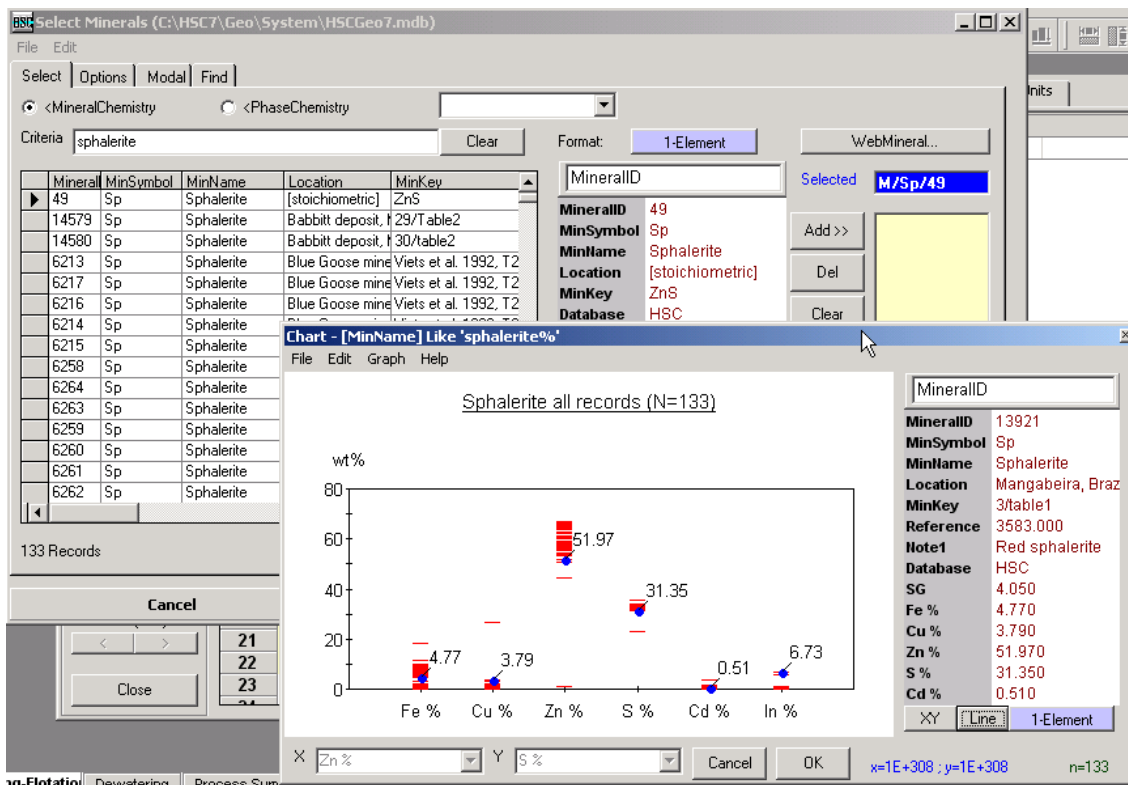
You can store your feed streams definition files in the new **Stream Database** and use them later.

You can have several input streams and some of them can be **Solid Streams** and some **Liquid Streams**, but the latter lack mineralogical characterization.

The particle mode uses **new Add-in functions**, which have improved the calculation speed significantly, HSC 7 uses about one tenth of the time used by HSC 6. The new recovery calculation updates the recovery values immediately (compared to HSC 6 where the update for recoveries happened only after the last simulation round).

New model wizards have been developed for mineral processing unit operations, including: crusher, mill, screen, hydrocyclone, conditioner (for changing floatability component parameters), flotation cell, and thickener.

Using Liberation Data in Simulating Mineral Processes:

A unique feature of HSC Sim is that you can use true measured particles in your simulations. You can read data also from the database of the JK Mineral Liberation Analyzer (MLA). **Improved liberation data processing tools** can handle the following tasks to define the mineral setup and feed stream mineralogy: 1) Reading raw MLA data files, 2) Combining minerals, 3) Rebalancing the MLA data to match with chemical assays, 4) Packing the liberation data to create uniform particle classes.

The unit models have been improved to handle particle data. **Improved crushers and mills models** (and other units reducing particle sizes) can now process multiphase particle data to produce a desired particle size distribution and simultaneously keep the material balance and forecast the liberation distribution of the product stream.

Improved separation unit models (like flotation, cyclone, magnetic separator) can separate multiphase particles based on their size, density, and composition.

The stream Properties window displays a deep analysis of each stream in the process.
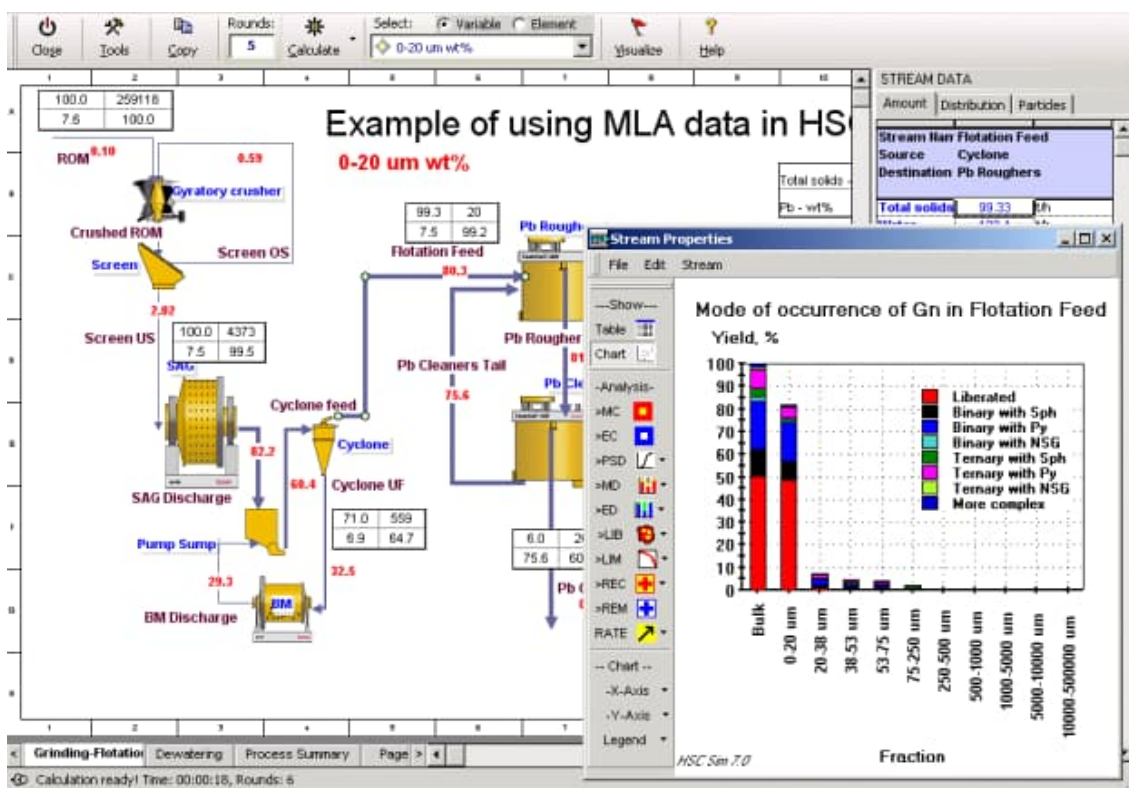
Experimental Mode:

HSC Sim has a **New Experimental Mode** in addition to the simulation mode. This has been designed so that you can collect your experimental data, visualize your measurements in the flowsheet and enter into the mass balancing and data reconciliation.

You can visualize stream properties, e.g. assays, such as **Stream Labels** and **Stream Tables**.

You can collect several tests or surveys on separate sheets in the **Experimental Data Tables**.

You can paste stream data, for example chemical assays, into the Experimental Data tables easily because in the assay the tables samples (streams) can be in any order; HSC looks for the stream name and makes the connection according to the name, not the order.

Once the experimental data is ready, you can mass balance and do the data reconciliation in the Mass Balance module (see following page).
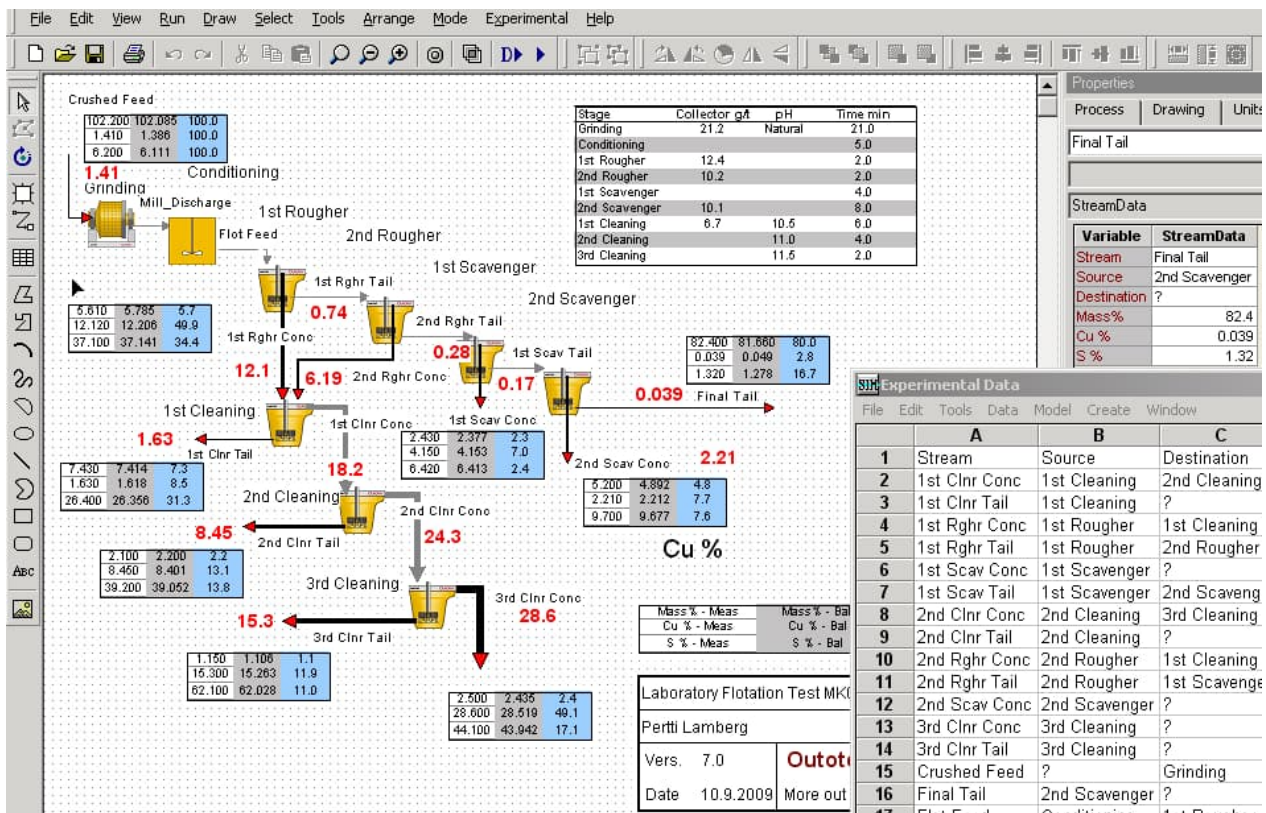
Mass Balancing and Data Reconciliation:

The Mass Balance and Data Reconciliation module has been recreated. You can solve six types of problems:

1) Reconcile measured or estimated component flow rates (1D components).
2) Mass balance and reconcile chemical analyses (1D assays),
3) Mass balance minerals in a minerals processing circuit (1D Minerals),
4) Mass balance size distribution and water balance (1.5D),
5) Mass balance assays and components in 2- or 3-phase systems where the bulk composition is not analyzed (2D Components),
6) Mass balance minerals or chemical assays size-by-size (2D Assays).

The Mass Balance and Data Reconciliation module works together with the flowsheet; different mass balancing values can be displayed as labels or tables on the flowsheet.

You don't have to draw a separate mass balance flowsheet; HSC creates the mass balancing nodes automatically from the flowsheet and if some streams have not been analyzed, HSC increases the mass balance node size accordingly.

The step-by-step Mass Balancing Wizard guides you through: 1) selection of components to be balanced, 2) selection of streams to be included in the mass balancing, 3) defining the error models, 4) defining reference (feed) streams, 5) checking of mass balance nodes and erroneous assays.
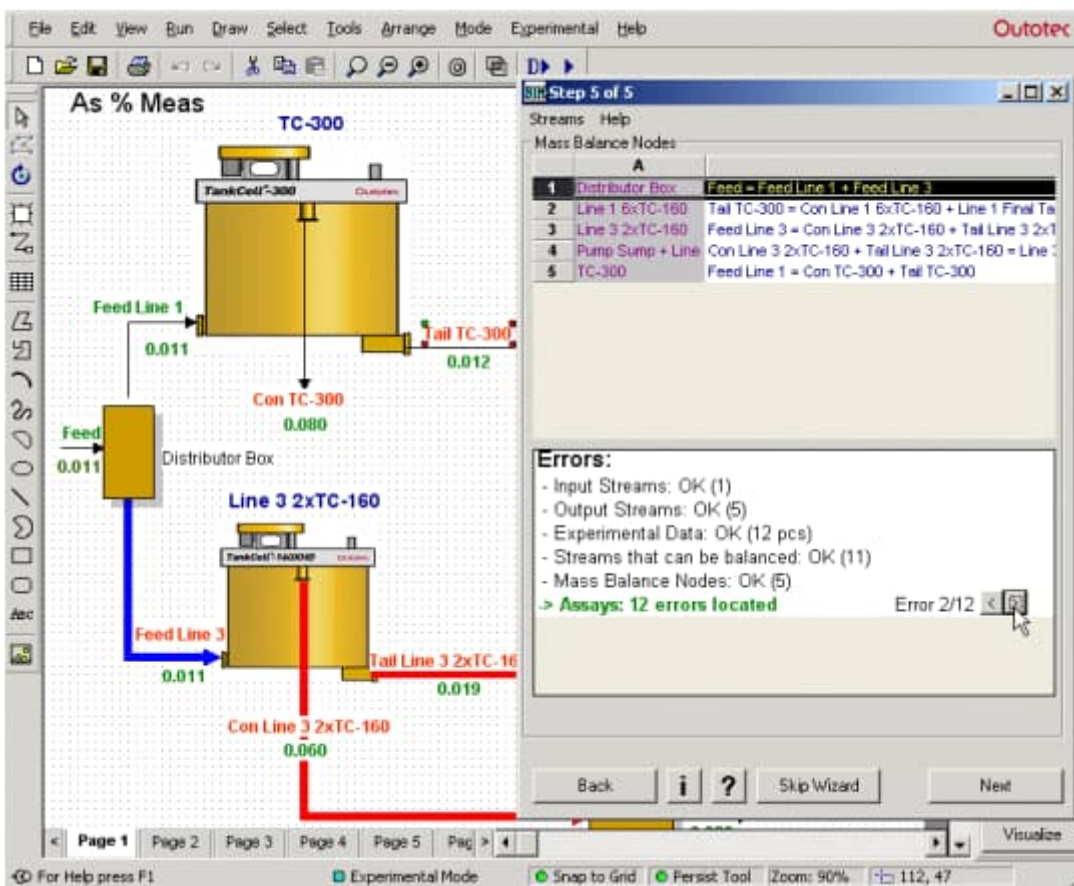
The error models available enable you to set the detection limit, relative error and maximum standard deviation individually for each component. In addition, you can give a sampling error for each stream.

HSC has four different mathematical routines for mass balancing and data reconciliation: 1) Least Squares method (LS), 2) MinMax (minimizes the maximum difference), 3) Non-negative least squares method (NNLS) and 4) Constrained least squares method (CLS). In the latter, you can set minimum and maximum values for each component to be mass balanced. Besides, there is a separate constraint for the condition: Component sum = 100; this is often used in minerals processing if the sum of mass balancing minerals is 100%.
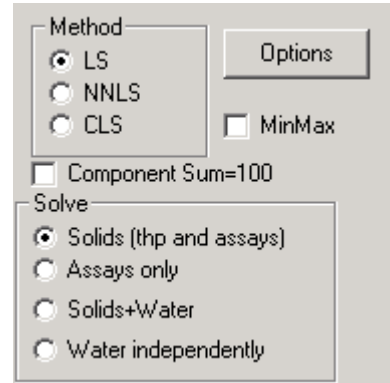
Different graphical methods are available for the user to evaluate and report the mass balancing result: Shankey diagram, parity chart, difference chart, weighed least square sum graph.

Once you have defined the mass balancing conditions for one data set you can mass balance several hundreds of similar cases with a single press of the button. The mass balancing module will use the same error model and same conditions for all data sets.

New Distribution (Pyro) Mode of the Sim Module
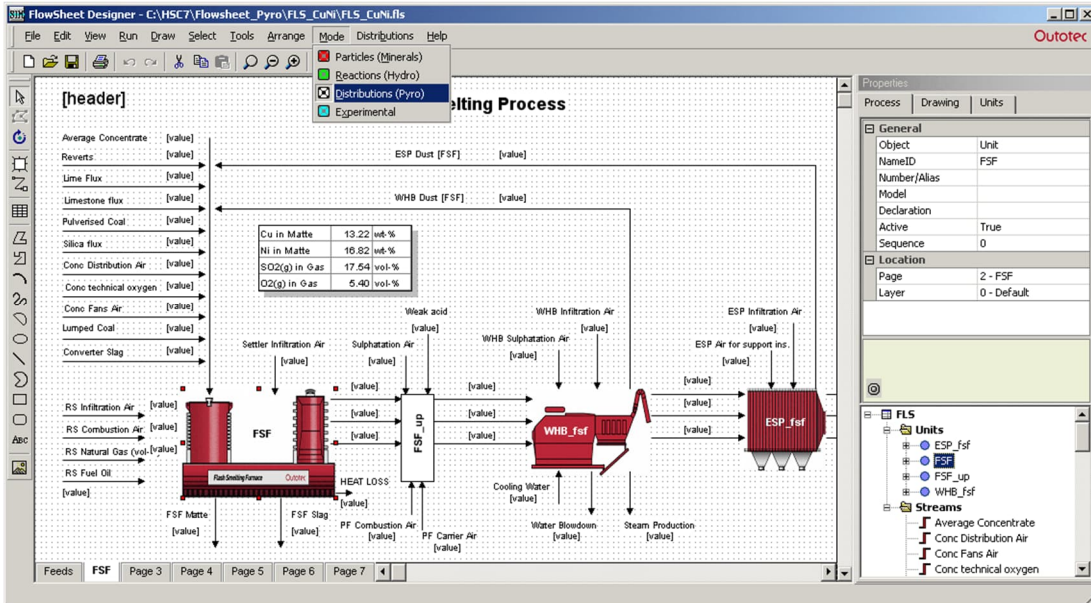
The Sim flowsheet module was originally made for the simulations of chemical reactions and mineral processing. The new Distribution (Pyro) mode also makes it more feasible for high temperature process models, which are based on the distributions of elements.

The distribution mode handles streams as rows unlike the Reaction and Particle modes, where each stream reserves one column. These streams may be saved to the stream database and reused in some other process model. The lack of a fixed variable list makes Distribution mode streams and units easier to reuse in the other process models. The Distribution mode behaves more like the old HSC Balance module.

The balance module automatically calculates H, T*S and G balances on the Dist sheet. The Sim module also automatically calculates the total input amounts of the elements. The Dist sheet is used to divide the input elements into output streams and species. These distribution values may be constants, which may be regulated with controls or Excel type formulas. The Distribution mode uses the same improved control tools as the Reaction and Particle modes.

The old HSC Balance module models may be imported into the Sim Flowsheet Distribution mode using the Balance Import dialog.

New Unit Icon Library with 515 Icons
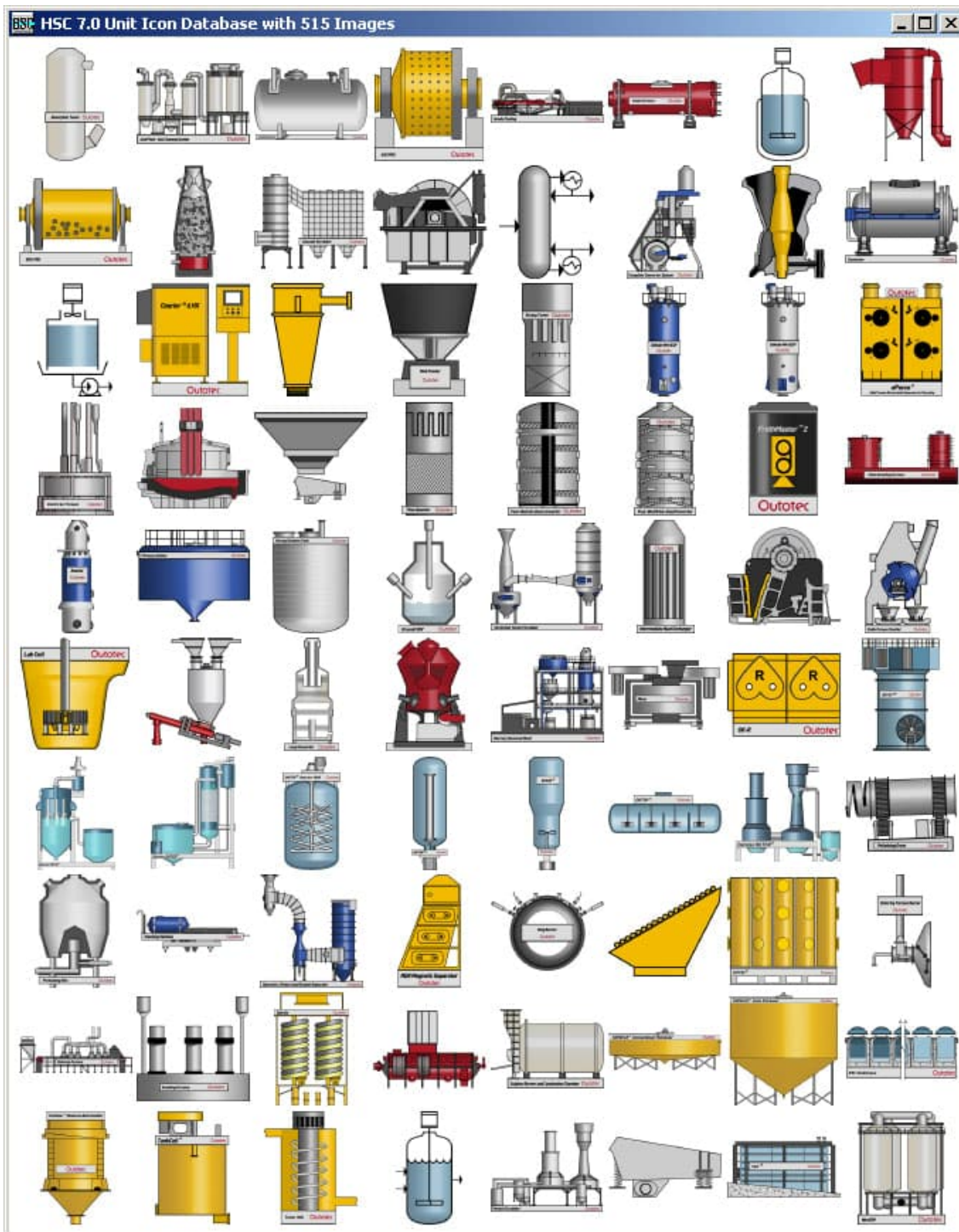
High-quality unit icons help you draw more illustrative flowsheet models. This library was created in cooperation with process engineers and industrial designers.

Metso
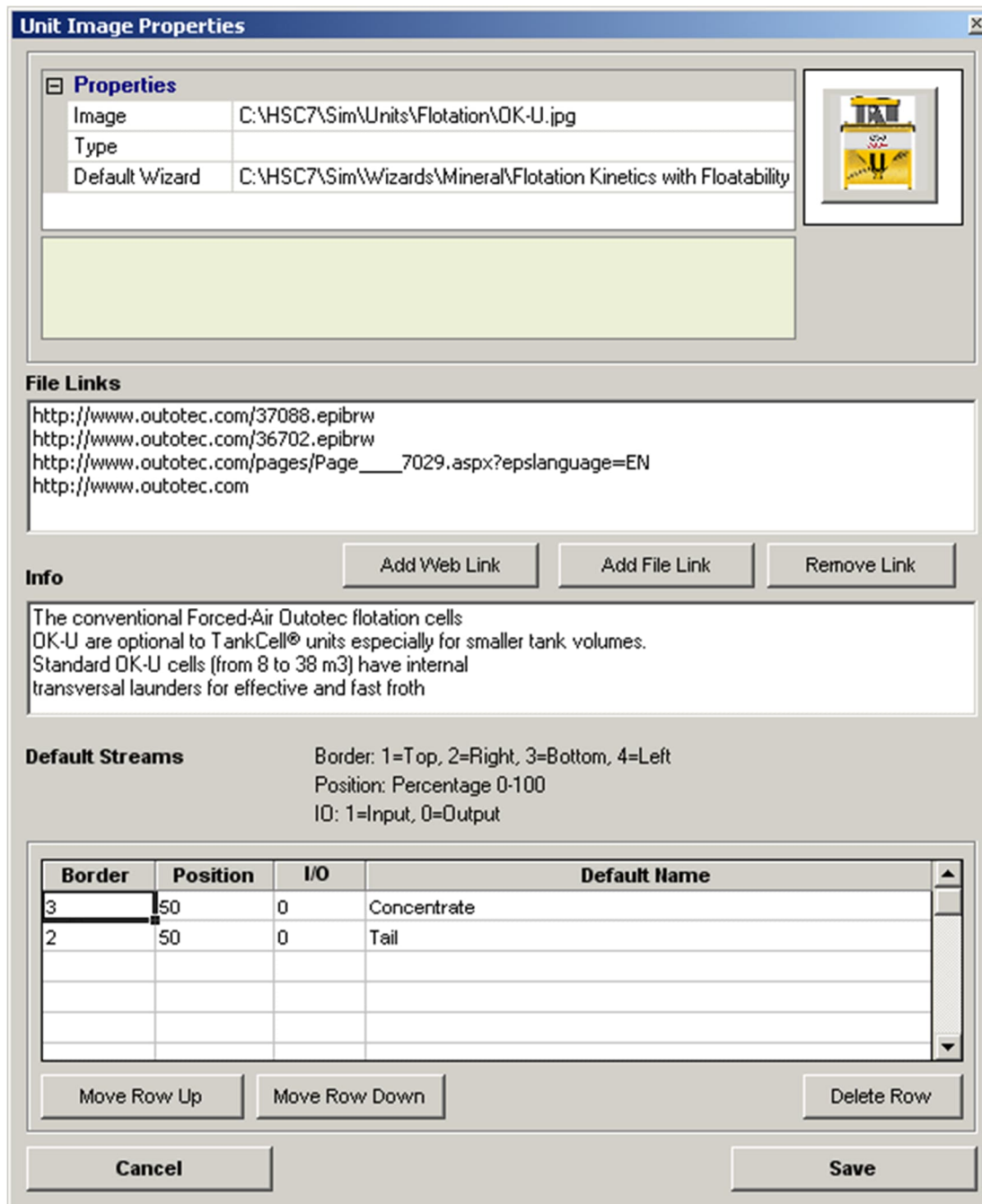
The unit icons may be connected with Model Wizards (Particle and Reaction mode), unit models (Distribution mode), Internet and file links. These file links may be used to give more information of the process units. These file links are also available in the flowsheet behind the unit icons.

Some other data like streams and descriptions may easily be added to the unit icons using the updated Unit Image Properties dialog.

New Add-In Functions

						Old		New	Old		New
						Add-In	Definition	Add-In	Add-In	Definition	Add-In
	StreamSM and StreamGM			R =	1.9870	cal/(K*mol)					
	HSC 7.0 Addin function samples					StreamS()	-Rn(xLn(x))	StreamSM()	StreamG()	RnT(xLn(x))	StreamGM()
	GAS STREAM	T	Content	Amount		S	S Mix	S + S Mix	G	G Mix	G + G Mix
		°C	mol-%	mol		kcal/K	kcal/K	kcal/K	kcal	kcal	kcal
						28.20		28.46	-29316.49		-29515.53
			100.00	500.00		28.20	0.26	28.46	-29316.21	-199.04	-29515.25
	N2(g)	500	68.00	340.00		17.87	0.18	18.05	-12664.36	-136.98	-12801.33
	O2(g)	500	5.00	25.00		1.40	0.01	1.41	-995.35	-5.75	-1001.10
	H2O(g)	500	5.00	25.00		1.33	0.01	1.34	-2371.48	-5.75	-2377.23
	SO2(g)	500	20.00	100.00		6.99	0.06	7.05	-11958.88	-49.45	-12008.33
	CO(g)	500	0.10	0.50		0.03	0.00	0.03	-32.41	-0.01	-32.41
	CO2(g)	500	1.90	9.50		0.58	0.00	0.58	-1293.74	-1.10	-1294.84

O9 = =0.001*StreamSM(B11:B16;F11:F16;C11)

HSC Add-In functions may be used in Sim module models or in MS Excel. Several new Add-In functions have been added to HSC 7.0:

- **StreamSM**: Stream entropy with mixing effect, this may be used if the stream consists of one solution only.
- **StreamGM**: Stream Gibbs energy with mixing effect.
- **StreamEQA**: Calculates equilibrium composition of the stream like StreamEQ, but it has an activity coefficient array as an additional argument.
- **StreamXArray**: Calculates the properties of the stream (such as composition by element and by mineral, size distribution) for the stream based on particles. StreamXArray is significantly faster and replaces the StreamX function of HSC 6.
- **RecoveryXArray**: Calculates the recoveries of elements and minerals in the stream based on particle data. RecoveryXArray is significantly faster and replaces the old RecoveryX function of HSC 6.
- **ProgenyStream**: Calculates the flow rates of each particle type after grinding according to given particle size distribution. Is capable of keeping the mass balance over size reducing units even with liberation data (true multiphase particles).
- **ComminutionProductPSD**: Calculates the particle size distribution of a mill or crusher according to appearance function, breakage function, and discharge function (or optionally if the breakage/discharge ratio is given).
- **CubicSpline**: Calculates the expected Y values for counterpart X values based on observed X' and Y' values.
- **ERF**: Error function

- Three old functions have been renamed to improve Excel 2007 compatibility:
  HNM3 -> H_NM3, **K -> K_MOL**, **S -> S_MOL**
- A new Measurement Unit menu option is available in Excel.
- The calculation speed of the Add-In functions has been increased.

Updated Balance Module

The old traditional HSC Balance module calculates enthalpy and material balances of the process units. Now, the HSC 7.0 balance module also automatically calculates the entropy (S * T) and Gibbs energy (G) balances in columns T and U, which may be used to estimate entropy and Gibbs energy changes in the process.

Updated Equilibrium Module
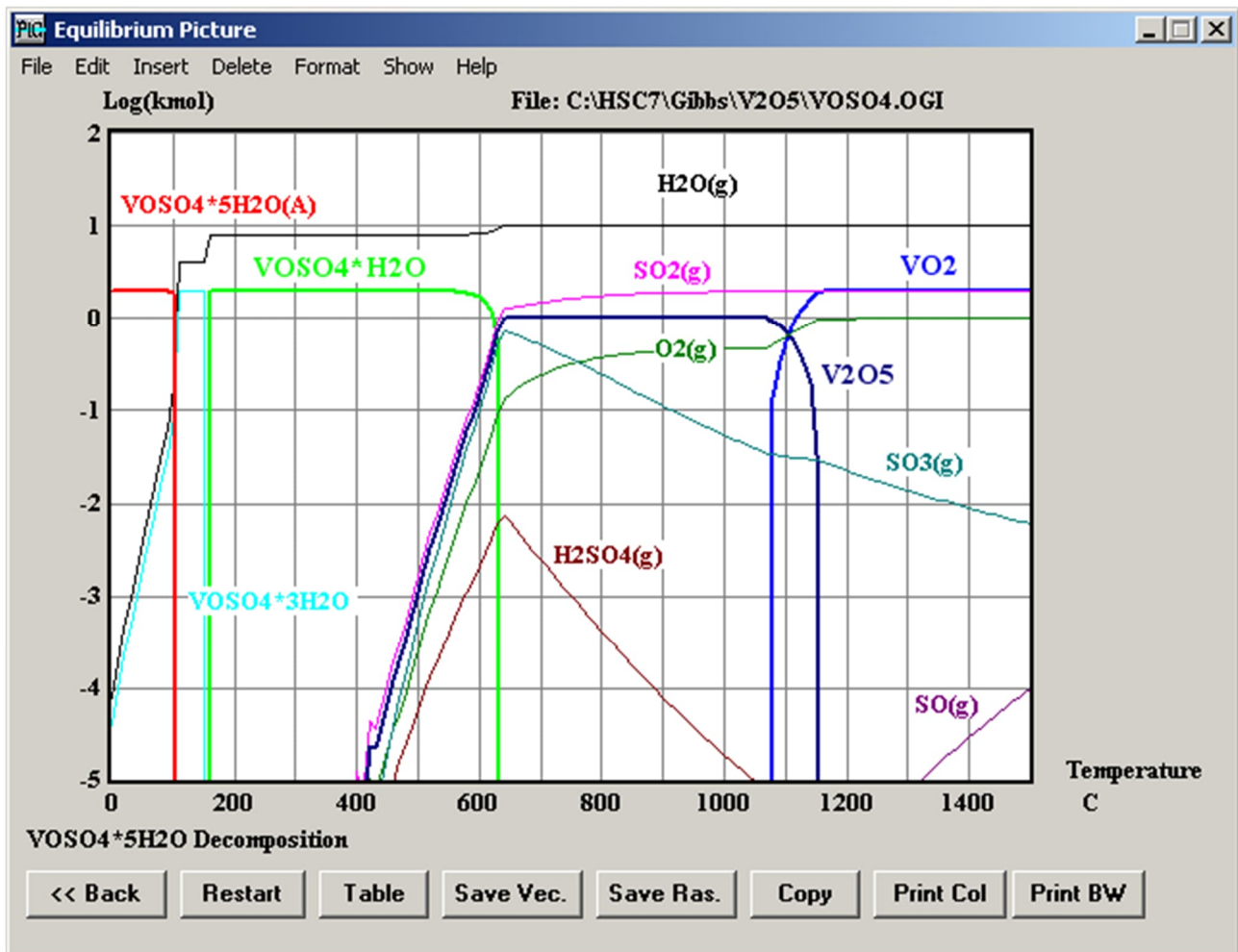
The HSC Equilibrium module calculates unit process output at the equilibrium state when the user specifies the chemical system and the raw materials. This module uses the Gibbs Energy Minimization method, which takes all the possible chemical reactions into account automatically.

In general, the old Gibbs 6.1 minimization routine calculated equilibrium compositions quickly and reliably. However, in some cases it did not calculate all the points in the equilibrium diagram. Sometimes there were even some zigzag errors in the equilibrium diagrams. Usually these problems could be solved by fine-tuning the raw material amounts, however, this is quite inconvenient.

The new Gibbs 7.0 routine is more robust and less fine-tuning is needed to obtain the correct results. This new version was completed just before the HSC 7.0 release, therefore the HSC 7.0 user still has the option to use either Gibbs 6.1 or the new Gibbs 7.0.

Updated MW Module with new H, S and Cp Estimates

The HSC 7.0 database contains more than 25000 species with enthalpy H, entropy S, and heat capacity Cp data; this data is usually based on experimental measurements. The data has been collected from more than 3000 different sources, which may contain typos and misprints. The new HSC Estimates module may be used to identify and filter these errors, because it gives a rough estimate of the H, S, and Cp values based purely on chemical formula.

HSC estimates are based on statistical data mining methods, which utilize stoichiometric element amounts, oxidation states, interactions, etc., which may be calculated automatically from the chemical formula. This module is quite easy to use: the user types in the formula and the program gives the formula weight, oxidation states and H, S and Cp estimates.

Antti Roine, Pertti Lamberg, Tuukka Kotiranta, Justin Salminen
September 8, 2023

H Enthalpy of Aqueous Species
- kcal / mol
- 3572 Species
- Mean error = 10.28 kcal/mol
- Median error = 5.89 kcal/mol

S Entropy of Gas Species
- kcal / (mol*K)
- 7720 Species
- Mean error = 5.50 kcal/(mol*K)
- Median error = 4.16 kcal/(mol*K)
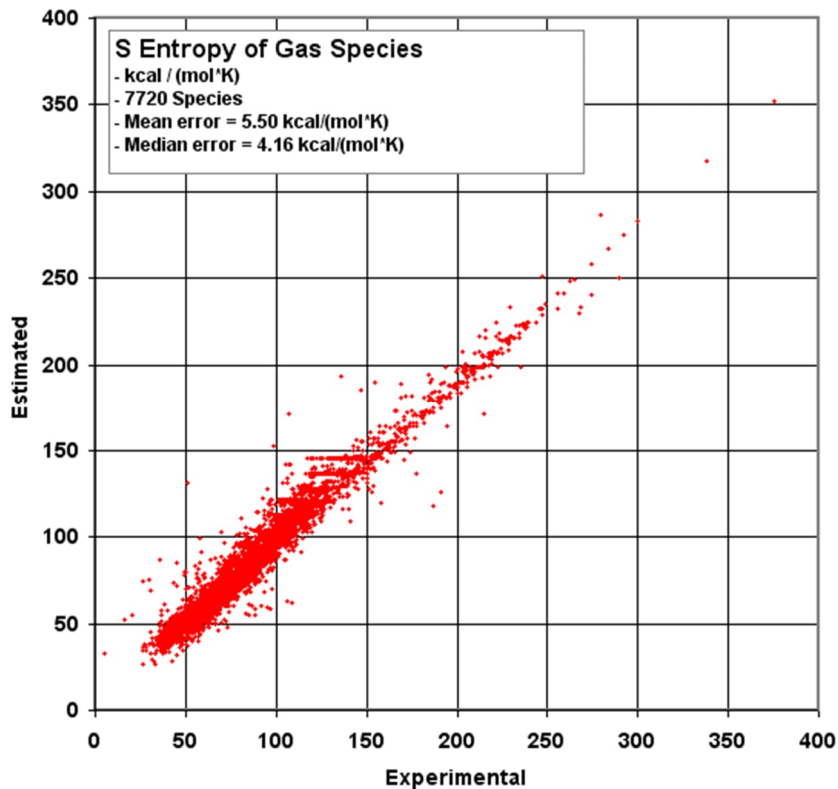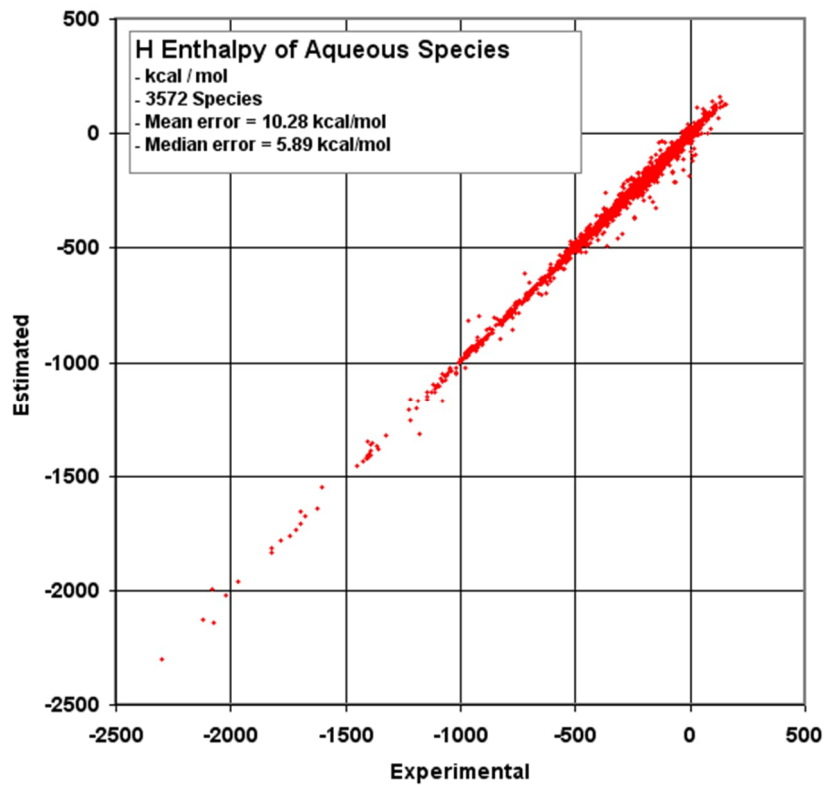
The new HSC Estimates module gives rough estimates of H, S and Cp values for the chemical species that exist in the HSC database, and also for those that do not exist in this database.

New Aqueous Solution Property Estimator

	SPECIES Formula	Temp. °C	Amount kmol	Amount mol-%	AC Experim.	AC Estimate	H Ideal kcal/mol	H Estimate kcal/mol	Cp Ideal cal/(mol'K)	Cp Estimate cal/(mol'K)
1	Water Phase	25	73.821	100.000			-68.071	-68.069	17.361	17.421
2	H2O	25	72.313	97.957	1.000	1.002	-68.315	-68.315	17.980	17.941
3	CO2(a)	25			1.000	1.000	-98.900	-98.900	46.940	46.940
4	CO3(-2a)	25			0.039	1.000	-161.385	-161.385	-68.914	-68.914
5	Ca(+2a)	25	0.013	0.018	0.203	0.185	-129.800	-129.282	-7.402	5.922
6	CaCl(+a)	25			1.000	1.000	-168.607	-168.607	17.476	17.476
7	CaHCO3(+a)	25			1.000	1.000	-294.350	-294.350	55.619	55.619
8	CaOH(+a)	25			1.000	1.000	-179.600	-179.600	1.490	1.490
9	Cl(-a)	25	0.737	0.998	0.666	0.693	-39.933	-39.930	-29.217	-24.138
10	ClO(-a)	25			1.000	1.000	-25.600	-25.600	-27.513	-27.513
11	ClO2(-a)	25			1.000	1.000	-15.900	-15.900	-19.067	-19.067
12	H(+a)	25			0.590	1.000				
13	OH(-a)	25			0.255	1.000	-54.977	-54.977	-32.423	-32.423
14	HCO3(-a)	25	0.003	0.004	0.570	0.589	-165.392	-165.219	-8.284	-4.949
15	HS(-a)	25			1.000	1.000	-3.850	-3.850	-22.375	-22.375
16	HSO3(-a)	25			1.000	1.000	-149.670	-149.670	-1.268	-1.268
17	HSO4(-a)	25			1.000	1.000	-211.974	-211.974	5.399	5.399
18	K(+a)	25	0.013	0.018	1.000	0.605	-60.270	-60.298	2.040	7.824
19	KSO4(-a)	25			1.000	1.000	-276.980	-276.980	-10.718	-10.718
20	Mg(+2a)	25	0.072	0.098	0.240	0.248	-111.616	-110.840	-5.119	-3.048
21	MgCl(+a)	25			1.000	1.000	-150.933	-150.933	24.980	24.980
22	Mg(HCO3)(+a)	25			1.000	1.000	-275.750	-275.750	60.526	60.526
23	MgOH(+a)	25			1.000	1.000	-152.955	-152.955	30.750	30.750
24	Na(+a)	25	0.632	0.856	0.668	0.651	-57.433	-57.441	9.168	14.698
25	NaCO3(-a)	25			1.000	1.000	-223.720	-223.720	-126.237	-126.237
26	NaSO4(-a)	25			1.000	1.000	-273.620	-273.620	-60.058	-60.058
27	O2(-a)	25			1.000	1.000	12.718	12.718	-88.120	-88.120
28	S2(-2a)	25			1.000	1.000	7.200	7.200	-64.548	-64.548
29	SO3(-2a)	25			1.000	1.000	-151.900	-151.900	-66.927	-66.927
30	SO4(-2a)	25	0.038	0.051	0.104	0.126	-217.400	-217.119	-63.323	-72.568

Aqueous solutions are widely used in the process industry in a huge number of applications. Process models may be created using pure substance data and assuming ideal behavior for the aqueous solutions. However, the accuracy of the models may be improved by taking into account the naturally existing non-ideal behavior of ions in the solution.

Well-known non-ideal models for aqueous electrolytes properties have been included in the new **Aqua module**. The activity coefficient models include the extended Debye-Hückel model here called Davies model, Pitzer model, and Harvie's modification. An extensive database including about 1000 Pitzer parameters for different systems have been collected to date. The Pitzer parameter database currently has 407 cation-anion pairs, 102 cation-cation and anion-anion pairs, 114 ternary coefficients, and 289 ion-neutral pairs. Many of these parameters are tabulated as temperature-dependent functions.

The user is given the option to choose between simpler and more rigorous models and to select the number of parameters used.

In the HSC Aqua module, the **Water Phase** sheet is used for calculating the activity coefficients, enthalpies and heat capacities for homogeneous (single phase) aqueous systems. The user specifies the system by inserting the ionic or molecular formulas of the solute species in the **SPECIES Formula** column, the temperature in the **Temp °C** column, and the amounts in the **Amount kmol** column.

At this point the user can also define the model that he wishes to use in the calculations. This is done with the help of the **Davies**, **Pitzer**, and **Harvey** checkboxes. The Water Density Calculator can now also be accessed through HSC Aqua by pressing the **Densities** tab.

The HSC Aqua **Binary System Sheet** can be used for calculation of activity coefficients, osmotic coefficients, enthalpies of solution, and heat capacities of binary electrolyte systems. These include for example NaOH, KOH, NaCl, KCl, HCl, LiCl, $CaCl_2$, $ZnCl_2$, Na_2SO_2, $CaSO_4$ $CuSO_4$, $CoSO_4$, $NiSO_4$, $MgSO_4$, $MnSO_4$, $ZnSO_4$, $AgNO_3$, and many others.

The cobalt sulfate binary system, shown above, tabulated into the **Water Phase** and calculation example in the **Binary System Sheet**.

The mean activity coefficient, $\gamma_\pm$ (Mean AC) of $CoSO_4$ as a function of the square root of molality at 25°C. The HSC Aqua **Binary System Sheet** was used with Davies and Pitzer models.

a. $CoSO_4$
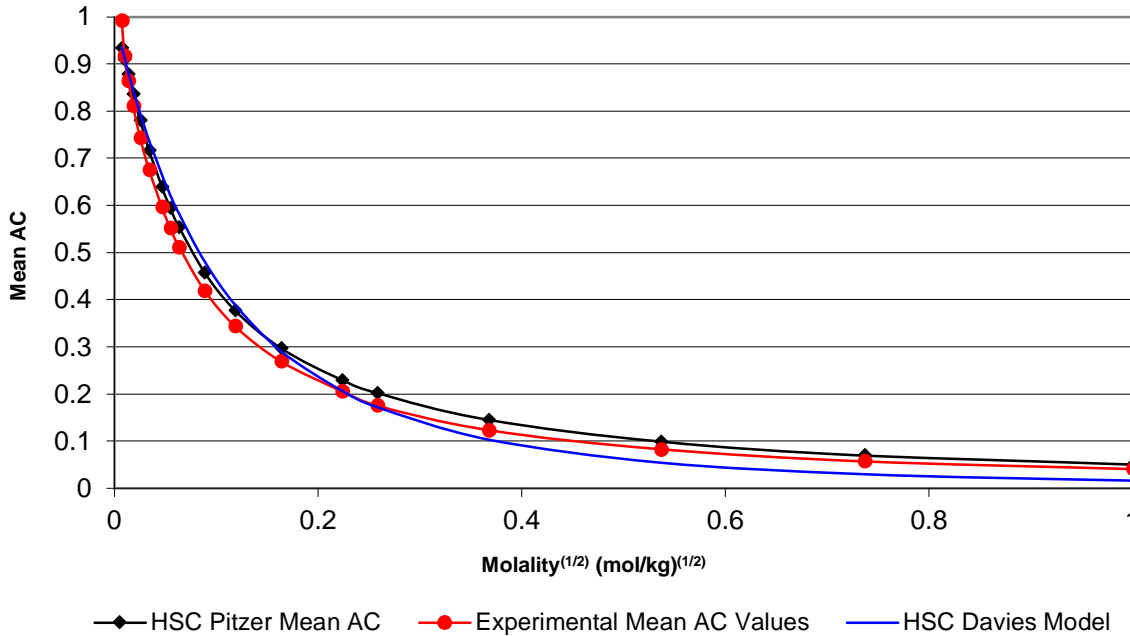
The mean activity coefficient, $\gamma_\pm$ (Mean AC) of NaCl as a function of the square root of solute molality at 25°C is shown below. The ideal behavior is shown as a straight line named "**Ideal**". The HSC Aqua **Binary System Sheet** was used with the Davies and Pitzer options. Reference data was also used for comparison.
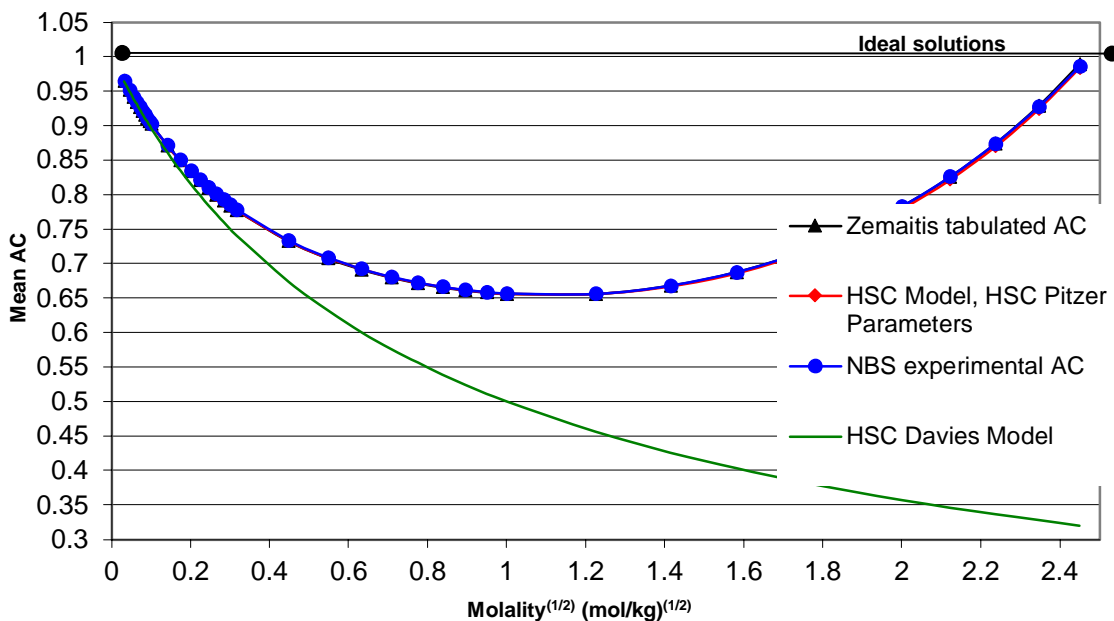
The temperature dependency of the mean activity and osmotic coefficients of KCl at different temperatures and solute molalities. The HSC Aqua **Binary System Sheet** was used with Harvey's model.

KCl, temp. dependence

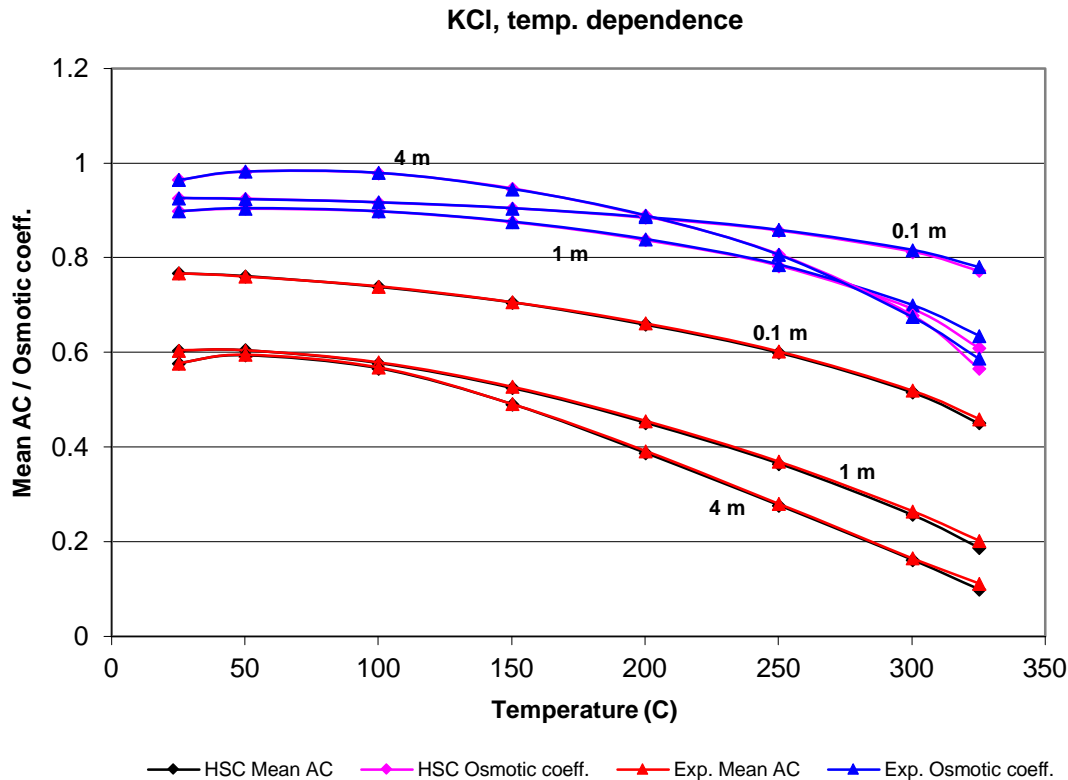The enthalpy aqueous solutions and especially the activity coefficients depend on the concentrations of the species. The new Aqueous Estimator module provides you with an easy way to estimate activity coefficients, enthalpies and heat capacities of dilute, moderate, and concentrated electrolyte solutions as a first guess for process design purposes.

These estimated values may be utilized in process models and other HSC calculation modules. At this point, only homogeneous liquid phases can be calculated, i.e. precipitated phases are not yet included.

The user has to specify the temperature, species, compositions, and temperature of the water solution and the module estimates activity coefficients, enthalpies, and heat capacities.

Updated H, S and Cp Database

The HSC database has traditionally been an extensive and easy to use source of thermochemical data of pure substances. This data has been collected from more than 3500 different scientific articles and publications.

HSC database development work was started some 30 years ago and work is still ongoing. The new HSC 7.0 database contains several improvements:

1) More than 4000 new species and data.
2) Updated and fixed data for some 4700 species.
3) Less duplicate species.
4) More density and CAS data.

The HSC 7.0 H, S and Cp database now contains more than 25000 species.

Updated Mineral Database
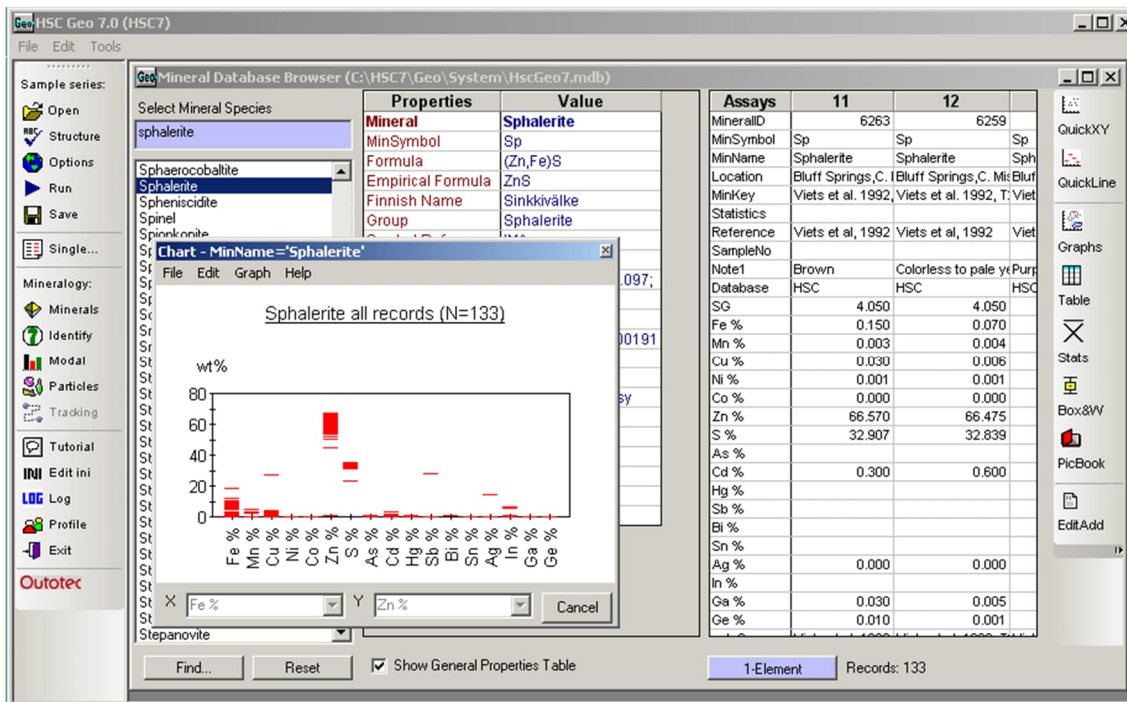
The number of minerals has been increased from 3581 to 13346 minerals. In the database the chemical composition of minerals is stored as elemental weight percentages but in the database viewer, the composition can be viewed as oxide% or as the number of atoms per formula unit.

The chemical composition of selected mineral species can be compared in different graphs including XY-, Line- and Box & Whisker charts.

The new Edit/Add window provides a quick and easy way for the user to add new mineral analyses.

You can search the database for minerals by the elements included / not included in the formula, by name or by typing the chemical composition and finding the best matching species in the database.

All HSC modules use the same mineral database and database browser.
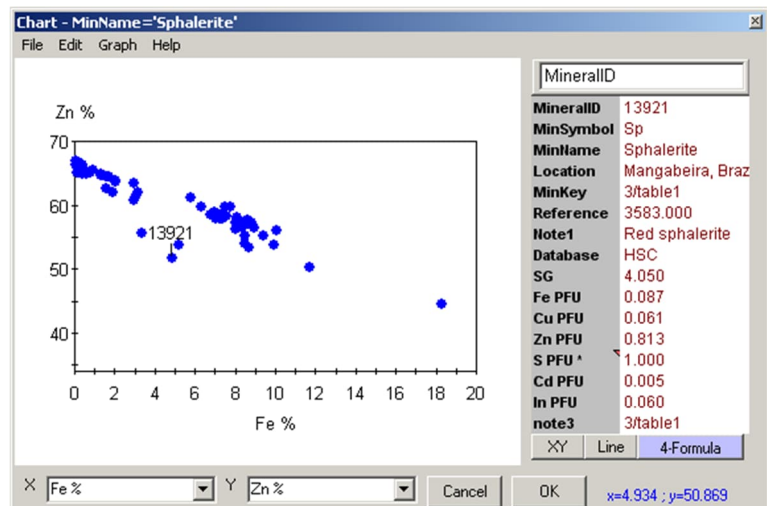
Also, the Excel add-in function "=MineralProperty(MineralName, Property) " queries the properties from the HSCGeo7.mdb database.

Updated Help Module
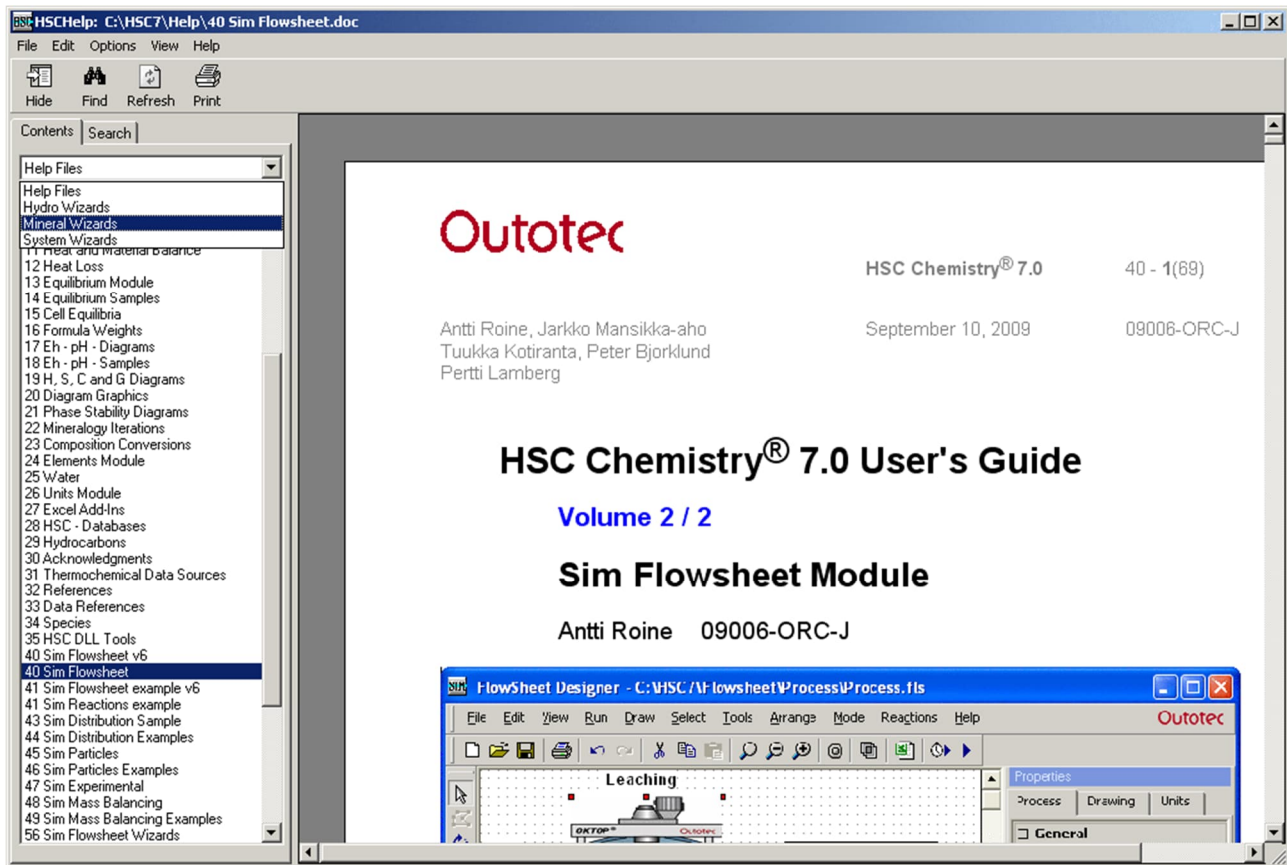
The HSC help files contain the same information as the manuals. The new Help module has been updated, and is now faster and more robust. Many unit models (applied as wizards) have been documented and can be found as help files both in HSC Sim and in the Help module.

Operating System Requirements

HSC 7.0 was developed under Windows 2000 and XP systems. HSC 7.0 has also been tested under Vista, Vista 64 and Windows 7 (beta). The old Windows versions 98, NT and Me are no longer supported.

Other improvements

- The updated liquid H, S and Cp data estimation routine also works if Cp data starts at a temperature lower than 298 Kelvin.
- Program hang problems with some printer drivers have been fixed.
- Thumbnail unit icons loading speed has been improved.
- Improved navigation window for the units and streams.
- Streamlines are automatically cut off when streams cross each other.
- More object types have been added to the select menu.

- A new Set to Default option was added to Sim to make selection of default stream and unit formatting options easier.
- New Frame, Drawing Title table and Meter objects have been added to Sim.
- A new Go To property was added to Sim drawing objects.
- The shape and visualization of stream arrows was improved.
- New mouse right button menu in Sim module.
- Copy-Paste properties from Sim to the other Windows applications was improved.
- New 0/0 = 0 option was added to Sim, this relieve #DIV/0! error problem.
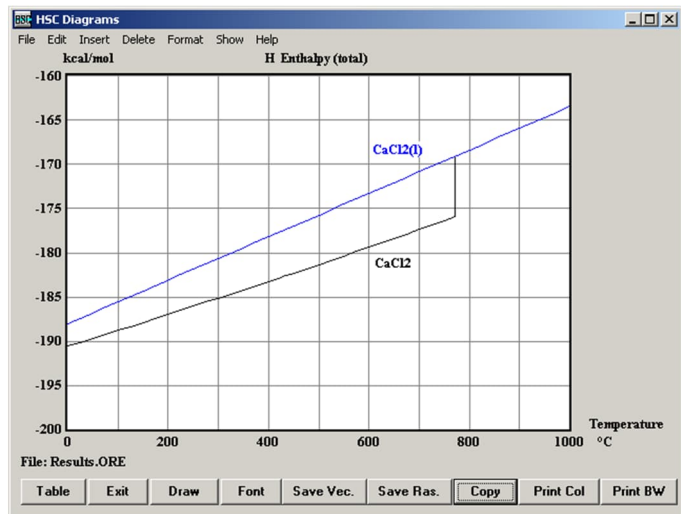
Preliminary News of HSC 8.0

1. Will be released at the end of 2013.
2. Simulation of dynamic processes will be possible. HSC 7.0 and older versions are based on steady-state simulation.
3. Excel Wizards will be added for dynamic simulation.
4. Making a simulation will be kept as easy to use as previously.
5. Version 8.0 will include an Experimental Database and tools to compare different tests graphically and process the data in a versatile way.
6. Improvements in Data Fitting. HSC 8.0 will have a standard and smooth way from 1) experimental data through 2) mass balance and data reconciliation to 3) model fitting and model building, and finally to 4) simulations.
7. There will be an even larger H, S and Cp database.
8. New elegant diagram tool.
9. … and many other new properties and fixes…

This all depends of course on user feedback, so please send us your feedback ☺

HSC Chemistry 7.0 Training

A two-day HSC training course is available. This may be a public one for all HSC users or it can be arranged internally for one company. The first day focuses on general issues, HSC databases and traditional calculation modules and the second day focuses on flowsheet simulation. Course content can be adjusted according to audience interest. For example, the focus may be on mineral processing, hydro or pyrometallurgy, flowsheet simulation, etc. Typical topics may include:

A) General Introduction of the HSC Package (First Day)
- History of HSC Chemistry, its internal structure, etc.
- Some basic principles of thermochemistry related to HSC
- HSC user interface
- Internal structure of the HSC databases
- Some important general aspects to be taken into account
(specification of phases and species, syntax of formulas, etc.)

B) Demonstration of the HSC Calculation Modules (First Day)
- All the calculation modules will be presented with the basic principles and selected hands-on calculation examples. Participants will have the opportunity to ask questions.

C) Calculation Workshop (Second Day)
- Sample cases will be solved with the most important calculation modules.

D) Introduction of Flowsheet Simulation module (Second Day)
- Basic principles and features
- Some sample cases will be demonstrated

E) Simulation Applications in Minerals Processing (Second Day)
- Grinding and Flotation Circuits
- Gravity separation
- Full mineral processing circuits (crushing, grinding, classification, gravity separation, flotation, dewatering)

The target of the HSC Introductory Course is to teach the participants what can be done with the HSC package and what cannot be done. After the course, the participants will understand the basic HSC operation principles and the major procedures needed to solve more complicated problems with the HSC package. The course will also illustrate thermochemistry application possibilities in practical problems.

The majority of HSC users utilize perhaps only 1-3 of the HSC calculation modules. This course will help to understand the capabilities of all 22 calculation modules and 12 databases. The course will focus on the most common questions and problems raised by HSC users over the last few years.

The HSC Introductory Course is intended for beginner and intermediate users. However, more advanced users may also find it useful because they will have the opportunity to raise questions concerning more difficult issues.

Tailor-Made HSC 7.0 Process Models

HSC provides easy tools for creating process models. However, some expertise and professional skill is needed to create models of large processes. Robust models are easier and faster to create if you have long experience of this work. However, less experience is needed to run and use process model applications.

Consequently, the easiest way to start the simulation of your plant is to order a tailor-made process model application from Metso. These models may help to identify bottlenecks and run the process in a more efficient way. This work is always done on a confidential basis.

Antti Roine, Pertti Lamberg, Tuukka Kotiranta, Justin Salminen

September 8, 2023

New HSC Chemistry 7.0

Metso's innovative process calculation software contains a updated flowsheet simulation module and a thermochemical database expanded to over 25,000 species. With 22 calculation modules and 12 databases at your fingertips, HSC 7 is an invaluable tool for any process engineer or scientist because one laboratory experiment may cost much more than a single HSC license.

Great step forward for green chemistry

Everything works in cycles in the natural ecosystem, water, carbon, energy, etc. Industrial ecosystems have the same target. The HSC flowsheet simulation tool may be used to optimize chemical and energy cycles in industrial processes. These process models makes it possible to maximize process output and efficiency, and to convert waste materials into valuable raw materials using recycling within industrial ecosystems.

HSC may also be used to focus expensive experimental research rapidly towards ideal process conditions, for example, in chemistry, metallurgy, minerals processing, energy production, and many other areas of industry.