

What's new in HSC Chemistry 6.0

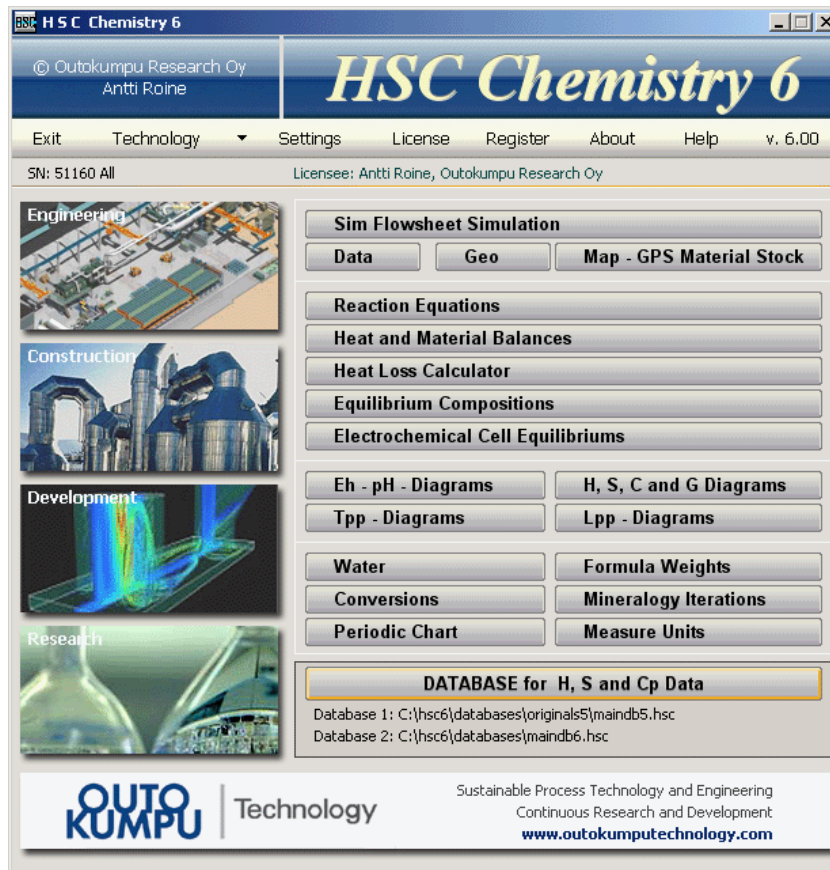


Fig. 1. HSC Chemistry® 6.0 Main Menu.

The old HSC Chemistry® 5.1 software is made for the simulation and modeling of single chemical reactions and unit processes. The new HSC Chemistry® 6.0 will expand the scope of the old HSC 5.1 software to include the simulation and modeling of the whole process, made up of several unit processes. HSC 6.0 also has many other new features:

- The new Sim module with versatile auxiliary Data, Data-Fit and Geo modules.
- Larger H, S and Cp database with more than 20000 species (HSC 5.1 has 17000 species). Several other fixes has also been made to the database.
- New Excel AddIn interface with better compatibility with different Excel versions and different computers.
- New Excel AddIn functions like StreamEQ for equilibrium calculations.
- The printing and copy-paste options of the HSC modules has been improved.
- The compability with Windows XP has been improved with several code changes and a new installation routine.
- Working demo of the new GPS based Material Map module.
- Many other small bug fixes and new properties.
- The familiar the HSC style, user interface and file formats have been maintained in order to minimize the training requirements for current HSC users.

New Sim Module

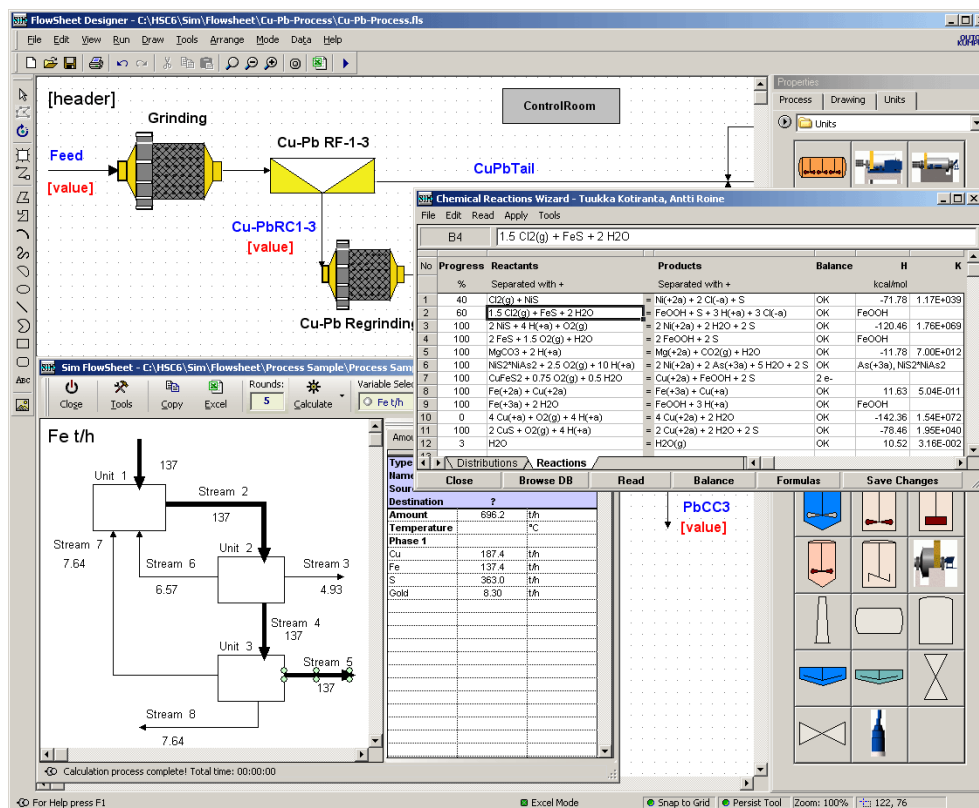


Fig. 2. HSC-Sim Module user interface with drawing and run mode.

The target has been to develop an easy-to-use simulation tool for many types of basic applications from chemical processes to economic optimization. HSC-Sim 6.0 has especially been tested with process metallurgical and mineralogical applications, but it may also be used in a wide range of other applications.

The HSC-Sim user may start from a single chemical reaction and end up with the final process model. HSC-Sim is a simple but still powerful simulation tool for the ordinary process engineer. For the old HSC users with Excel spreadsheet skills it should be easy to learn to use the new Sim module. HSC-Sim flowsheet process is made of single process units which are connected with each others with streams. Behind each process unit there is "a small HSC engine" for thermochemical simulation models.

The Sim module uses two main user interfaces: a graphical flowsheet interface and behind each process unit a spreadsheet type Model Editor interface. The basic ideas of the Sim module are quite simple:

1. The process consists of the process units which have been connected to each other with streams. The flowsheet is saved in one FLS file.
2. Behind each process unit there is a "small HSC engine" made of an Excel emulator with HSC AddIn functions or other DLL-based tools. Each unit has its own XLS file.
3. The process unit calculation models are independent of each other.
4. The streams on the graphical flowsheet specify the material and data transfer between the process units (FLS file).
5. There are two modes in the HSC-Sim module: the Designer Mode and Run Mode. The user draws and edits the flowsheet in the Designer mode. In the Run (calculation) mode the graphical flowsheet is locked.

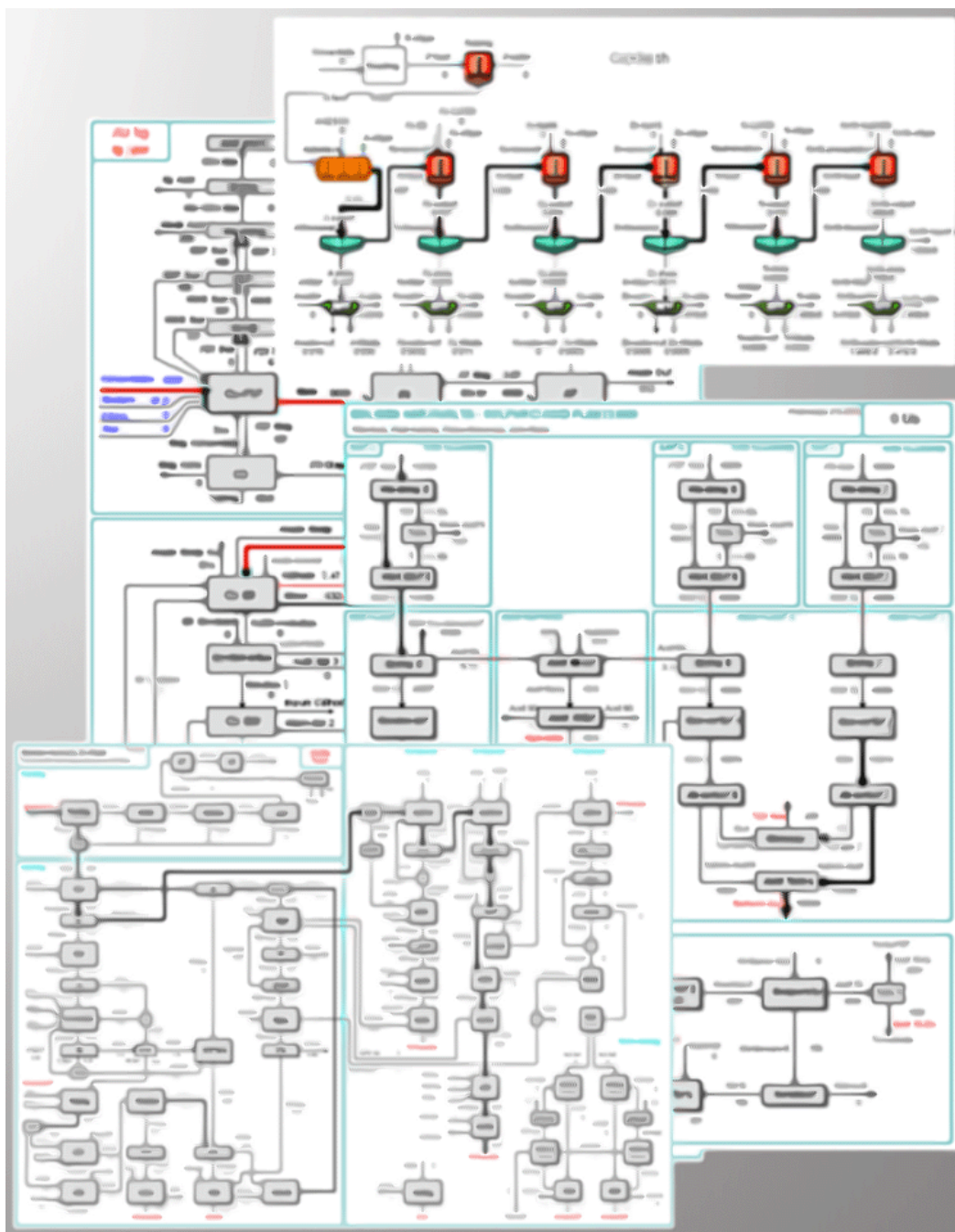


Fig. 3. Some process examples. The Sim module development started some 4.5 years ago and it has been tested with numerous new and old real process flowsheets. It has been used internally in Outotec Oyj for more than 2 years already. The flowsheet samples have been blurred due to confidentiality in this figure.

Mineral Based Models

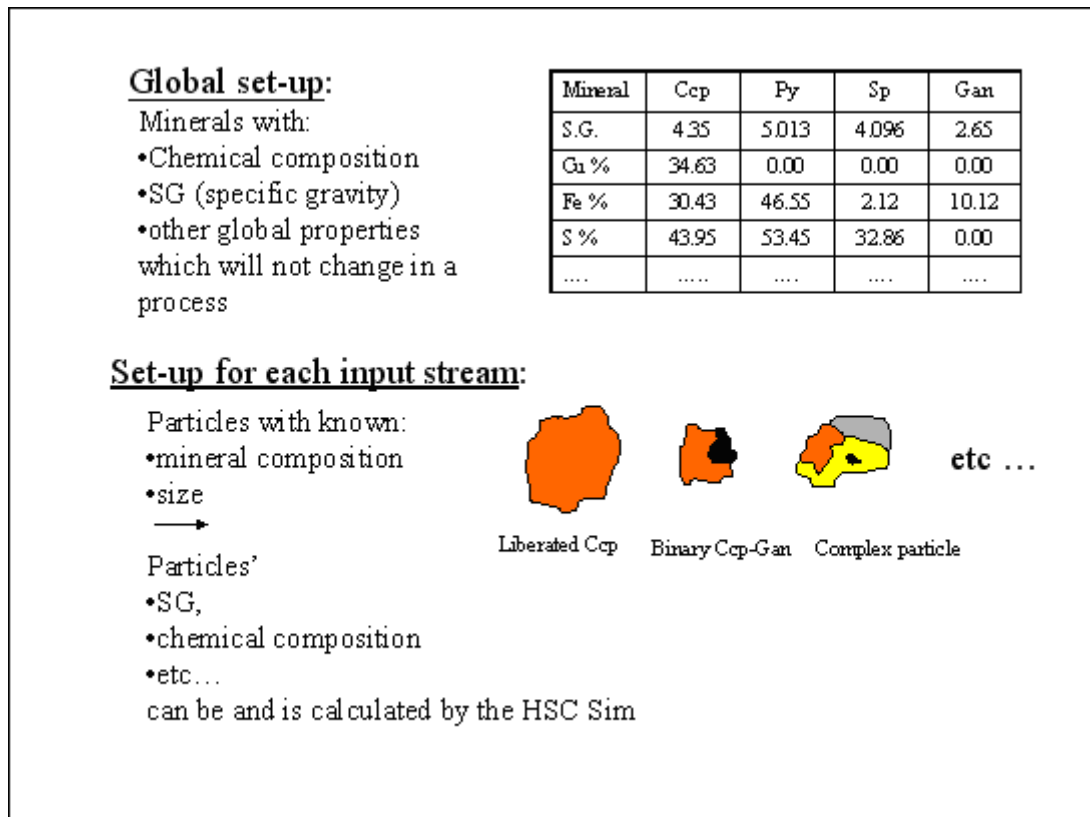


Fig. 4. Global and set-up for each input stream in Mineral Based models.

HSC-Sim has a special set-up and approach for processes where minerals are treated. In the processes including crushing, grinding, flotation, gravity separation or screening this approach should be used. Particles with at least A) size (diameter) and B) mineral composition (wt-%) data can be handled in mineral-based models.

In addition, they may have additional parameters like mineral volume-%, mineral area-% (on the surface of a particle), 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. Particles can be generated through mineralogical information. There are two levels of information required, **Fig. 4.**

The HSC Geo module makes possible to calculate, for example, composition of the sulfide fraction and volatile-and-sulfide-free composition from chemical analysis of a rock certain petrochemical indices like CIPW norm. It includes mineralogical database of ca. 5500 minerals and their chemical compositions.

HSC Geo also contains a versatile tool for modal calculations, i.e. to convert chemical analysis to mineralogical composition.

HSC Data is a general data processing tool with which you may use for statistical analysis, xy/ternary/spider diagram drawing, linear modeling and population analysis based on numerical data in normal Access database.

New Excel Add-In Functions

Stream/Flow	Return Value	Argument 1	Arg. 2	Arg. 3	Arg. 4	Arg. 5
34 STREAMH(Species;Amount;T)	5.723	Fe	1	100		
35 FLOWH(Species;Amount;T)		Cu	1			
36		Zn	1			
37 STREAMHKG(Species;Amount;T)	6.364	Cu(+2a)	21.85	100		
38 FLOWHKG(Species;Amount;T)		Fe(+2a)	6.72			
39		Zn(+2a)	2			
40 STREAMHNM3(Species;Amount;T)	2.187	N2(g)	17.78	100		
41 FLOWHNM3(Species;Amount;T)		O2(g)	4.79			
42		Ar(g)	0.23			
43 STREAMHLAT(Species;Amount;T)	14.060	Cu2S	1	100		
44 FLOWHLAT(Species;Amount;T)		FeS	1			
45		ZnS	1			
46 STREAMS(Species;Amount;T)	200.629	N2(g)	0.78	100		
47 FLOWS(Species;Amount;T)		O2(g)	0.21			
48		Ar(g)	0.01			
49 STREAMCP(Species;Amount;T)	29.252	N2(g)	0.78	100		
50 FLOWCP(Species;Amount;T)		O2(g)	0.21			
51		Ar(g)	0.01			
52 STREAMG(Species;Amount;T)	-72.677	N2(g)	0.78	100		
53 FLOWG(Species;Amount;T)		O2(g)	0.21			
54		Ar(g)	0.01			
55 DensityA(Species;Amount;T)	1260.348	NaCl	0.2	50		
56		FeSO4	0.1			
57						
58 Stream/Flow iteration (reverse)	Return Value	Argument 1	Arg. 2	Arg. 3	Arg. 4	Arg. 5
59 STREAMTH(Species;Amount;H;Tmin;TMax)	100.00	Fe	1	5.72	0	1000
60 FLOWTH(Species;Amount;H;Tmin;TMax)		Cu	1			
61		Zn	1			
62 STREAMTHKG(Species;Amount;H;Tmin;TMax)	100.00	Cu(+2a)	21.85	6.36	0	1000
63 FLOWTHKG(Species;Amount;H;Tmin;TMax)		Fe(+2a)	6.72			
64		Zn(+2a)	2			
65 STREAMTHNM3(Species;Amount;H;Tmin;TMax)	100.00	N2(g)	17.77905	2.19	0	1000
66 FLOWTHNM3(Species;Amount;H;Tmin;TMax)		O2(g)	4.786145			
67		Ar(g)	0.227884			
68 STREAMTHLAT(Species;Amount;H;Tmin;TMax)	100.00	Cu2S	1	14.06	0	1000
69 FLOWTHLAT(Species;Amount;H;Tmin;TMax)		FeS	1			
70		ZnS	1			
71 STREAMTS(Species;Amount;S;Tmin;TMax)	100.00	N2(g)	0.78	200.63	0	1000
72 FLOWTS(Species;Amount;S;Tmin;TMax)		O2(g)	0.21			
73		Ar(g)	0.01			
74 STREAMTCP(Species;Amount;CP;Tmin;TMax)	100.00	N2(g)	0.78	29.25	0	1000
75 FLOWTH(Species;Amount;H;Tmin;TMax)		O2(g)	0.21			
76		Ar(g)	0.01			
77 STREAMTG(Species;Amount;G;Tmin;TMax)	100.00	N2(g)	0.78	-72.68	0	1000
78 FLOWTG(Species;Amount;G;Tmin;TMax)		O2(g)	0.21			
79		Ar(g)	0.01			

Fig. 5. New Stream Functions in AddInSample.xls.

The HSC 6 Excel AddIn functions use the new HSC6.XLL interface instead of the old HSC5.XLA. This improves the compatibility with different Excel versions and makes possible easier file exchange within different computers. Several new AddIn functions have also been added which makes it possible to calculate stream properties, for example, in simulation models, Fig. 5.

The new **StreamEQ** function enables the user to carry out equilibrium calculations in MS Excel, Fig. 6. The new **DensityA** function makes it possible to calculate the density of several aqueous solutions, etc.

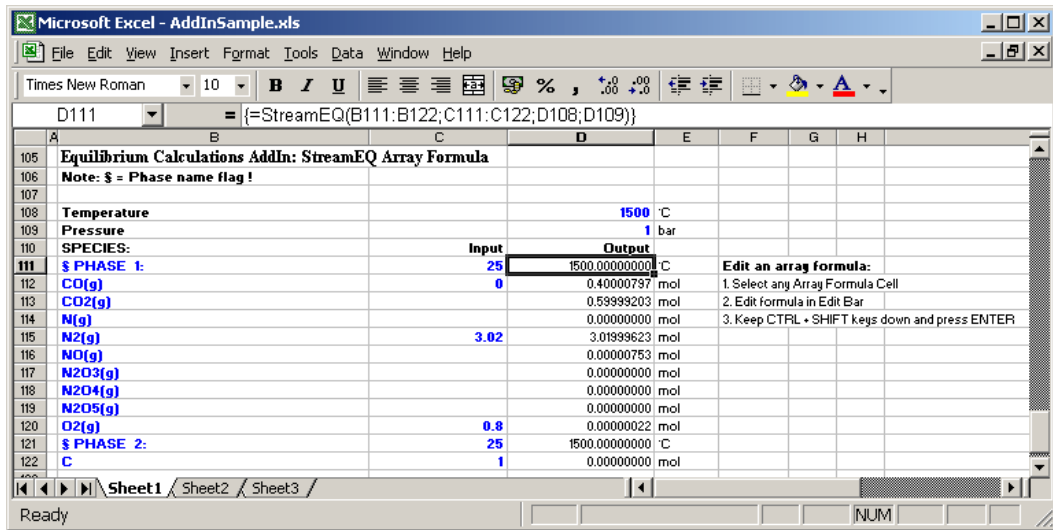


Fig. 6. New StreamEQ Function for equilibrium calculations.

Other New Features

The new Data, Data-Fit and Geo modules are useful tools when creating process models using HSC-Sim. However, these modules may also be used in many other applications. For example, the HSC-Sim Data-Fit module may be used to convert experimental data points into functions which can be used in the unit models, Fig. 7.

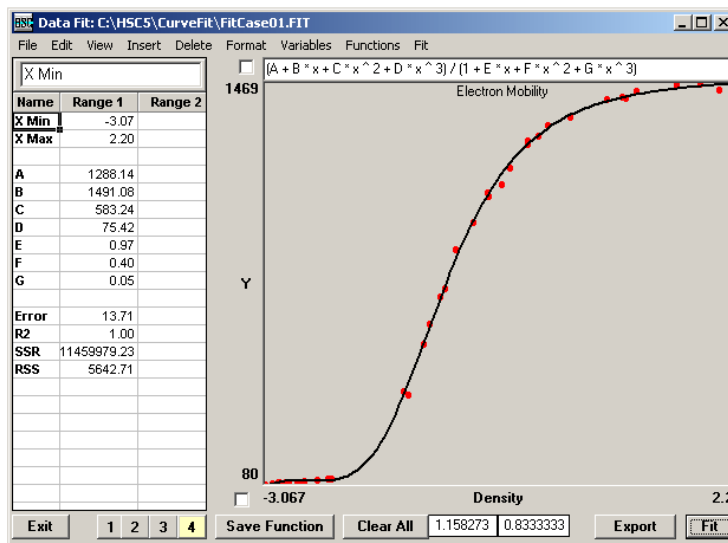


Fig. 7. New Data-Fit module.

A working demo of the new GPS based Material Map module makes it possible to create location-based material maps. However, the plants and stocks are different, therefore, some tailoring and tuning is usually needed. Please ask for a quote for this work from Outotec Research Oy.

The high quality thermochemical H, S and Cp data is needed in many process calculations. The HSC 6.0 extensive thermochemical database with more than 20000 species is unique and valuable source for this basic data. This data is automatically used in all HSC calculation modules but it may also be used in other programs and as a quick reference on the available data sources.