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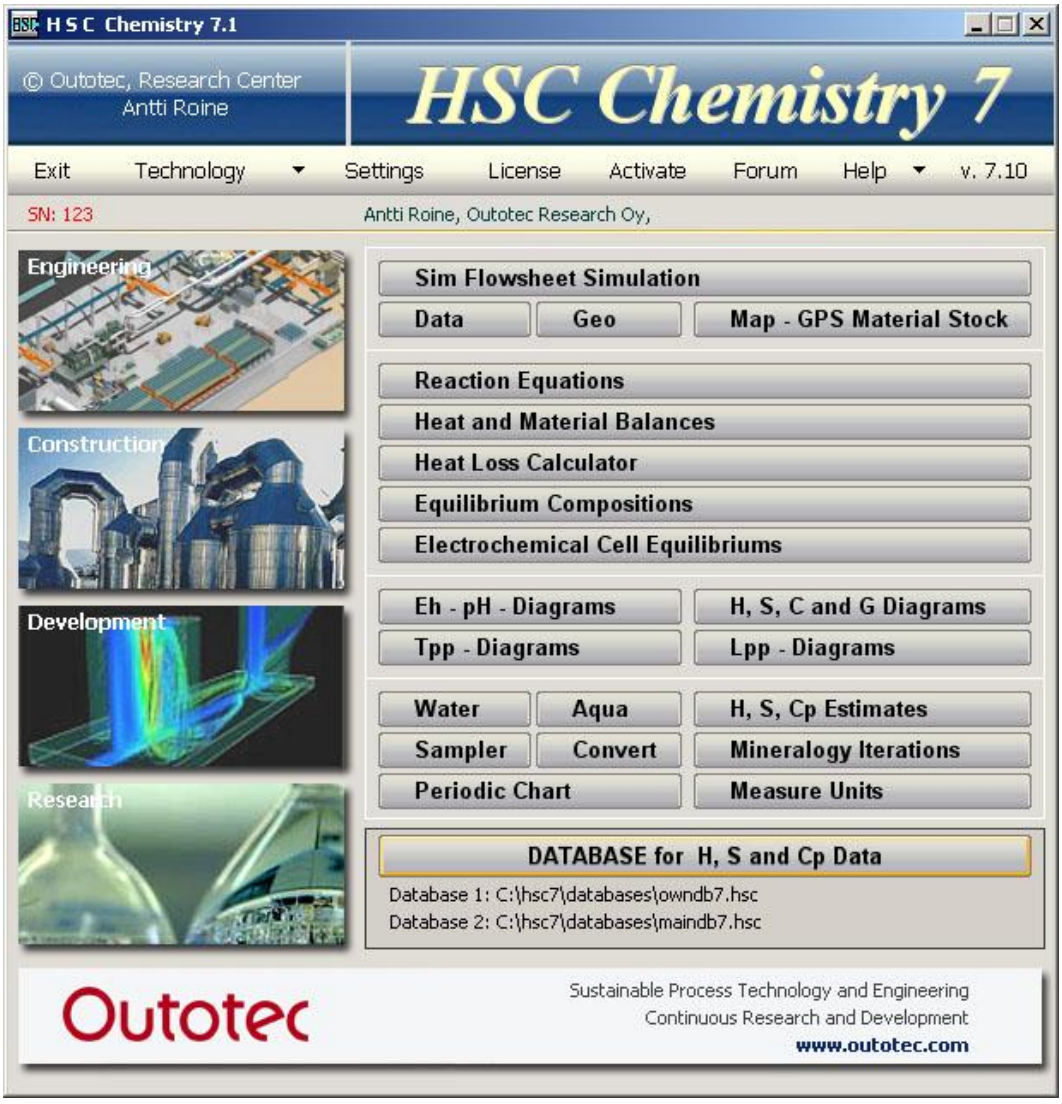
What's New in HSC 7.1?



Not only is HSC Chemistry 7.1 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 in the same package.

HSC 7.1 mainly contains small fixes to the HSC 7.0 version, but some new features have also been added. The most important improvements are the more robust Sim flowsheet and Equilibrium modules. HSC 7.1 is a free upgrade for registered HSC 7.0 customers.

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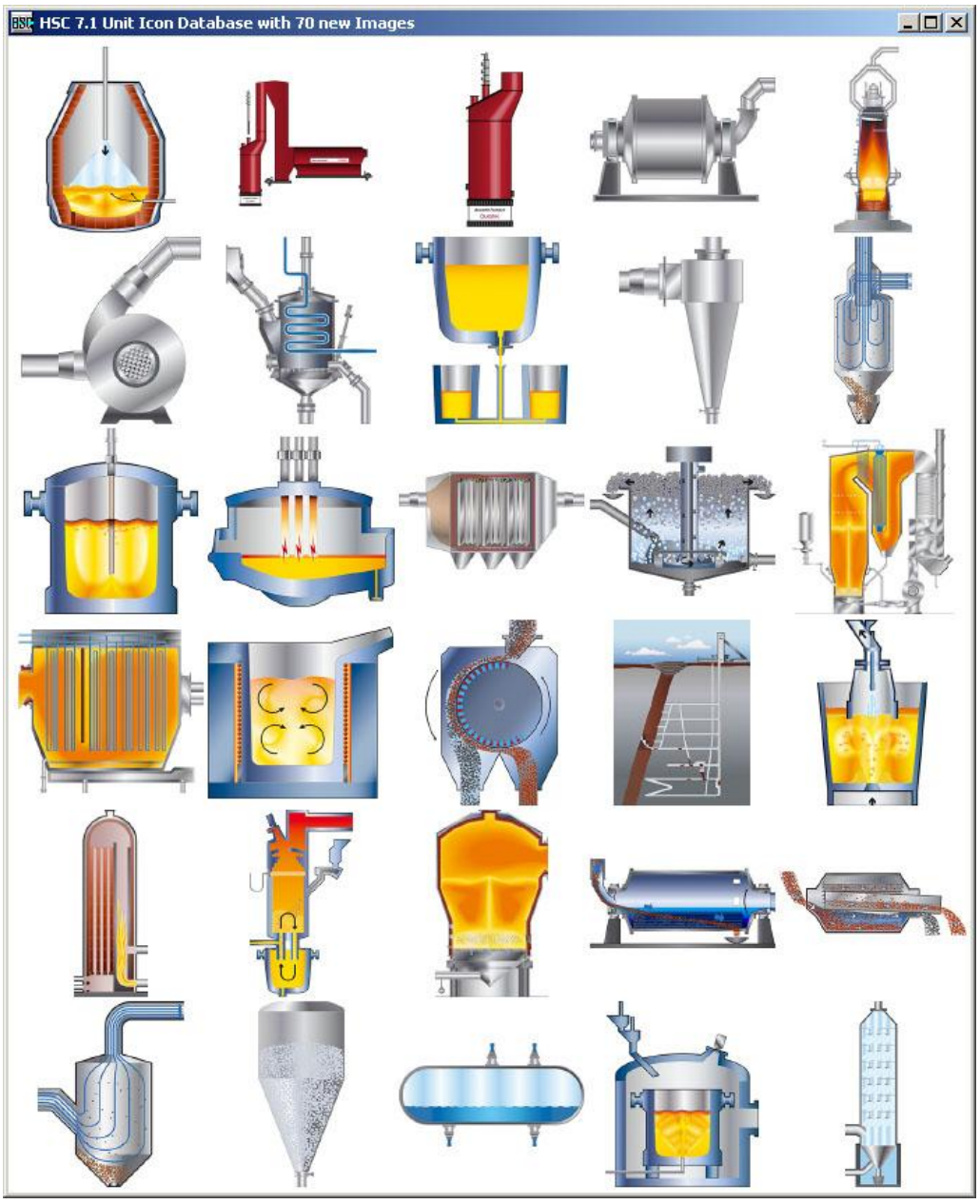
Summary of the new Features

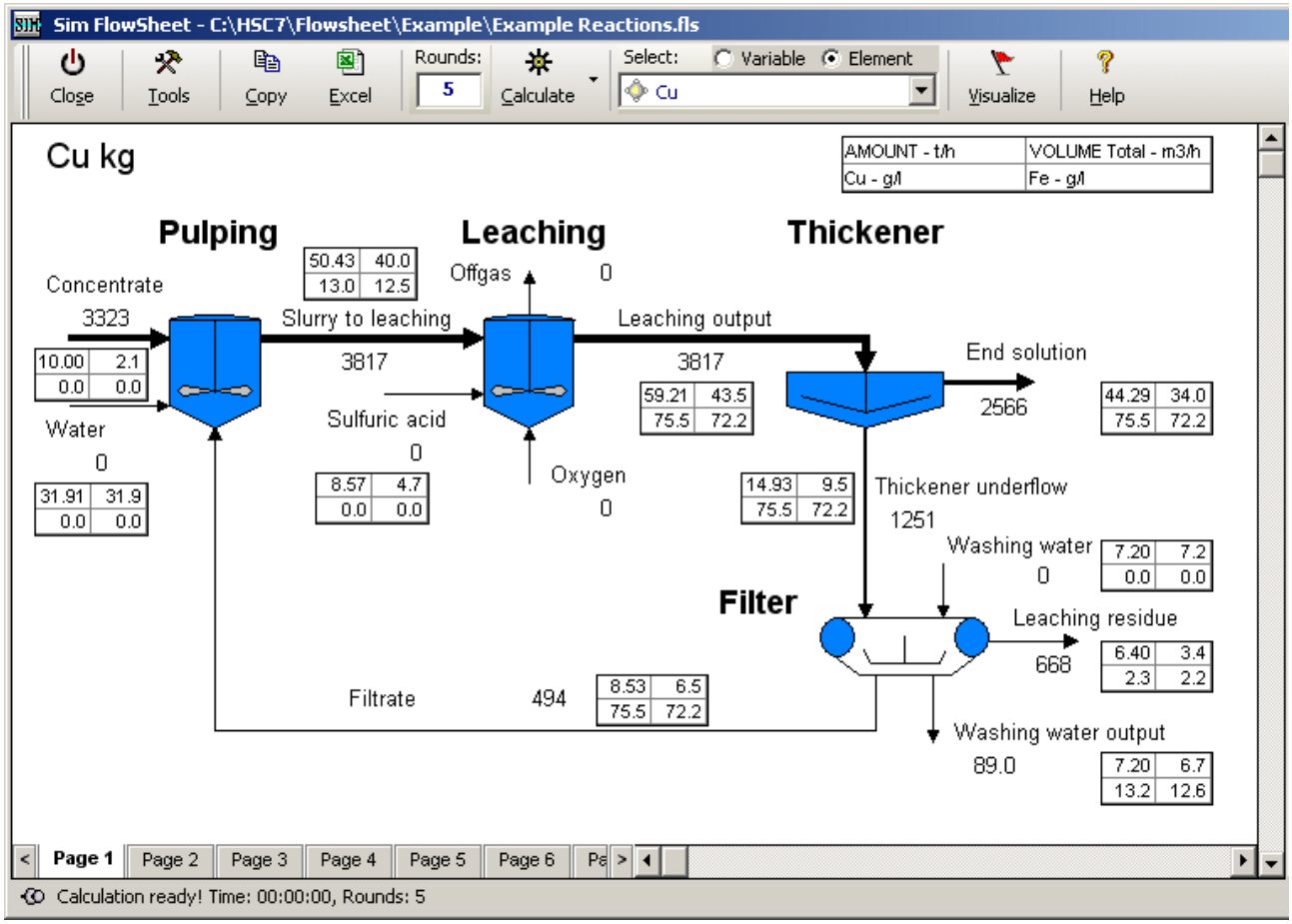
1. Installation

- HSC 7.1 compatibility with Windows 7 has been improved. The new InstallShield 2011 tool is used for the installation of HSC 7.1 instead of the old InstallShield 2009.
- Issues with some of the Unicode characters have been fixed within the HSC activation.
- Data, Geo, and Map module operation problems with the old HSC 6.1 versions have been fixed. Now all the HSC 6.1 and 7.1 modules may coexist on the same computer.

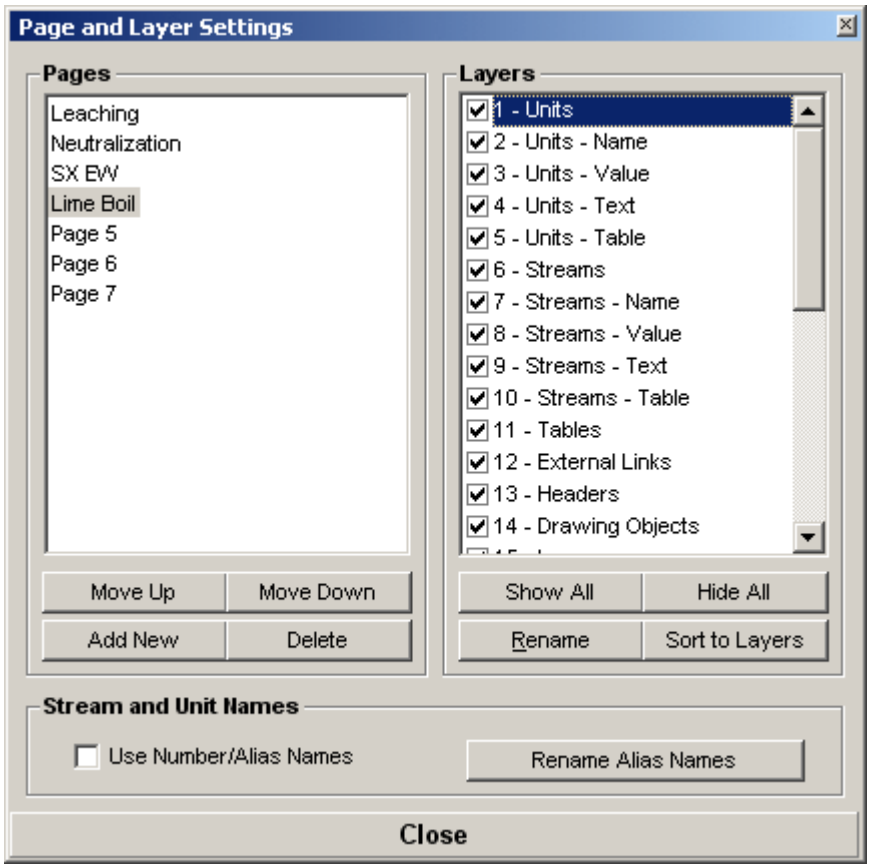


- More than 70 new unit icons have been added to the Iron-Steel, Roasting, Filter, Pyro_Ausmelt, and Energy folders of the Sim Flowsheet module unit icon database.

2. Sim Flowsheet Module



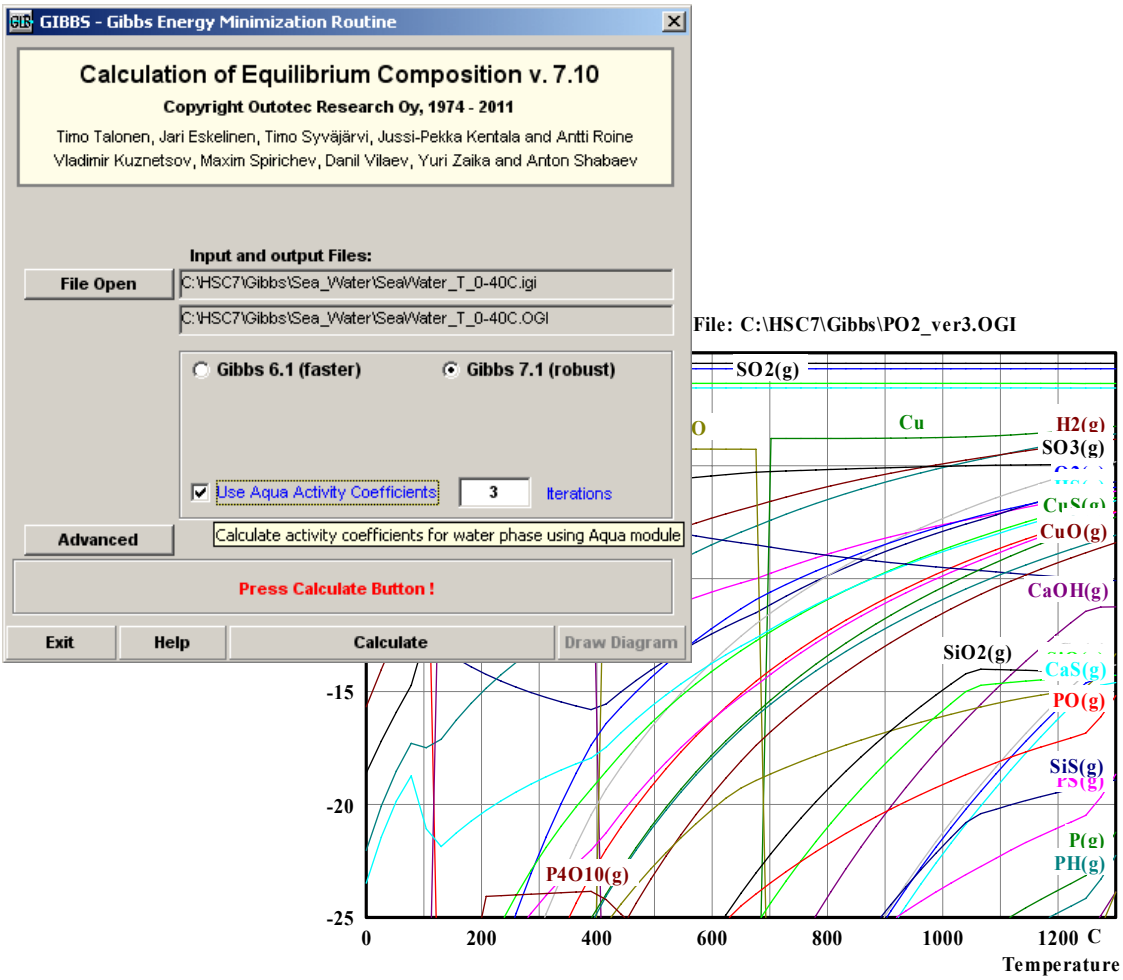
- Improved process calculation speed.
- Sim user interface remembers the size and location of the forms.
- Find Errors: Circular reference test added to "Find Errors" dialog and some other problems have also been fixed.
- Find Errors: Also warns of external controls and Sync area errors.
- Find Errors: Total error test added and error limit tests improved.
- Find Errors: Problem with missing units fixed.
- Find errors: Dialog has been updated. External controls have also been checked, mass balances are shown for the whole process, and the mass balance error calculation for one unit has been corrected.
- Circular References: Ten recalculations will be carried out if circular references are detected which improves accuracy, but slows down the calculation speed.
- Controls: Possible user errors in the controls (#REF) will not crash the calculation.
- Controls: Simple reverse/direct control operation has been improved.
- Reaction Wizard: new distribution 100% test has been added.
- Reaction Wizard: improved balance routine messages.
- List Streams: small bug in the listing has been fixed.



- Improved dialog has been added for maintaining Alias Names.
- Convenient new method has been added to the "Tree View" of the process - just keep the left mouse button down and you will see the different streams of the selected unit.
- Sim Menu selection "Arrange, Make Same Size,..." has been improved.
- Duplicate stream synchronization within File Links and Info Toolbars has been improved.
- Save dialog opens when Sim is closed from the top-right cross if changes have been made. Sim also remembers the last folder when closed from the top-right cross.
- Remote Control: Ergonomy of the Remote Control dialog has been improved. The occasional remote control bug has been fixed.
- New DLL unit interface and option have been added to the menu. This makes it possible to replace the visible unit calculation model with the DLL file. These DLL models read data from the Input sheet and return results to the Output sheet. The user may create these DLL files using C++, VB6, Delphi, etc.
- Sim registers the unit DLL files automatically in the folder: C:\HSC7\Sim\Wizards\Unit-DLL
- Table object: The Copy-Paste and cell formula bugs have been fixed with the cell reference links.
- Table object: The Save and Open bug has been fixed with cell comments.
- Table object: The visual problems with zoom have been fixed.
- Table object: The editing problems in the Run window have been fixed.
- Table object and Reaction Wizard: the Ctrl-C and Ctrl-V keys enabled.

- Select Stream: Tables problem fixed.
- Duplicate Stream: Table bug fixed.
- Stream Stick ends bug with the unit selection fixed.
- Occasional bug with the Sim mode changes fixed.
- Bug with "File, Import Model,…" dialog fixed in case of invalid file formats.
- New "Edit, Copy and paste to all streams,…" option has been added to the Reaction and Particle modes.
- New "File, Import Variable List" option has been added to file menu in the Reaction and Particle modes.
- Distribution mode (Pyro): The user may complete and end the stream drawing with the "Enter" key. In the old Sim 7.0 only a mouse double click completed the stream drawing.
- Distribution mode (Pyro): External control problem fixed.
- Distribution mode: Link label problem fixed.
- Distribution mode: Element amount = 0 -> division by zero bug fixed.
- Distribution mode: New option "Fixed Input" in the Dist sheet.
- Distribution mode: New option "Refresh Cell Formats" in the Format sheet.
- Distribution mode: Sync problem with row delete operation fixed.
- Distribution mode: Limitation of 20 streams has been removed. “View all” now shows all the rows.
- Distribution mode: Problem with "Find Streams" in Run window has been fixed.
- Distribution mode: New drop down list for the measure units.
- Two Sim system memory leaks have been fixed.
- Cell Defined Name problems in the spreadsheet have been fixed.
- Spreadsheet: cosmetic cell number format problem fixed: 0.00E-01 -> 0.00E+00
- Spreadsheet: Cell comments problem with save method fixed.
- Element balances: Red color highlights negative amounts.
- "Refresh All Formulas" tool does not change the background color of the values. This way links will show up better in the streams.
- Improvements in the mass balancing and data reconciliation module to speed up the solution in complex cases.
- New model fitting module enabling to give additional constraints and use data organized in the experimental mode directly to derive model parameters for flotation, classification, and general polynomial, exponential and log functions.
- Wizards: Small improvements have been made to the Excel wizards. StreamEQ and StreamEQA wizards updated.
- Old, unnecessary menu options removed: "Save snapshot,” "Manage Snapshots,” etc.
- Report form/Particle mode: % Solids balance calculation fixed.

3. Equilibrium Module



- A more robust equilibrium calculation routine Gibbs 7.1 has been added to the HSC Equilibrium module. This routine is also faster and more accurate, especially for very small element amounts.
- An aqua option has been added to Gibbs 7.1. This makes it possible to calculate the activity coefficients of the water mixture phases automatically.
- Activity coefficient formulas have been enabled on Gibbs 7.1.
- Limitation of 20 elements in IGI files has been removed.
- New View, Element Matrix, option added. This makes it possible to check the element amounts given in the raw materials, etc.
- Element search dialog no longer adds duplicate N2(g) species.
- Ergonomics of the Pic.exe diagram drawing routine has been improved.
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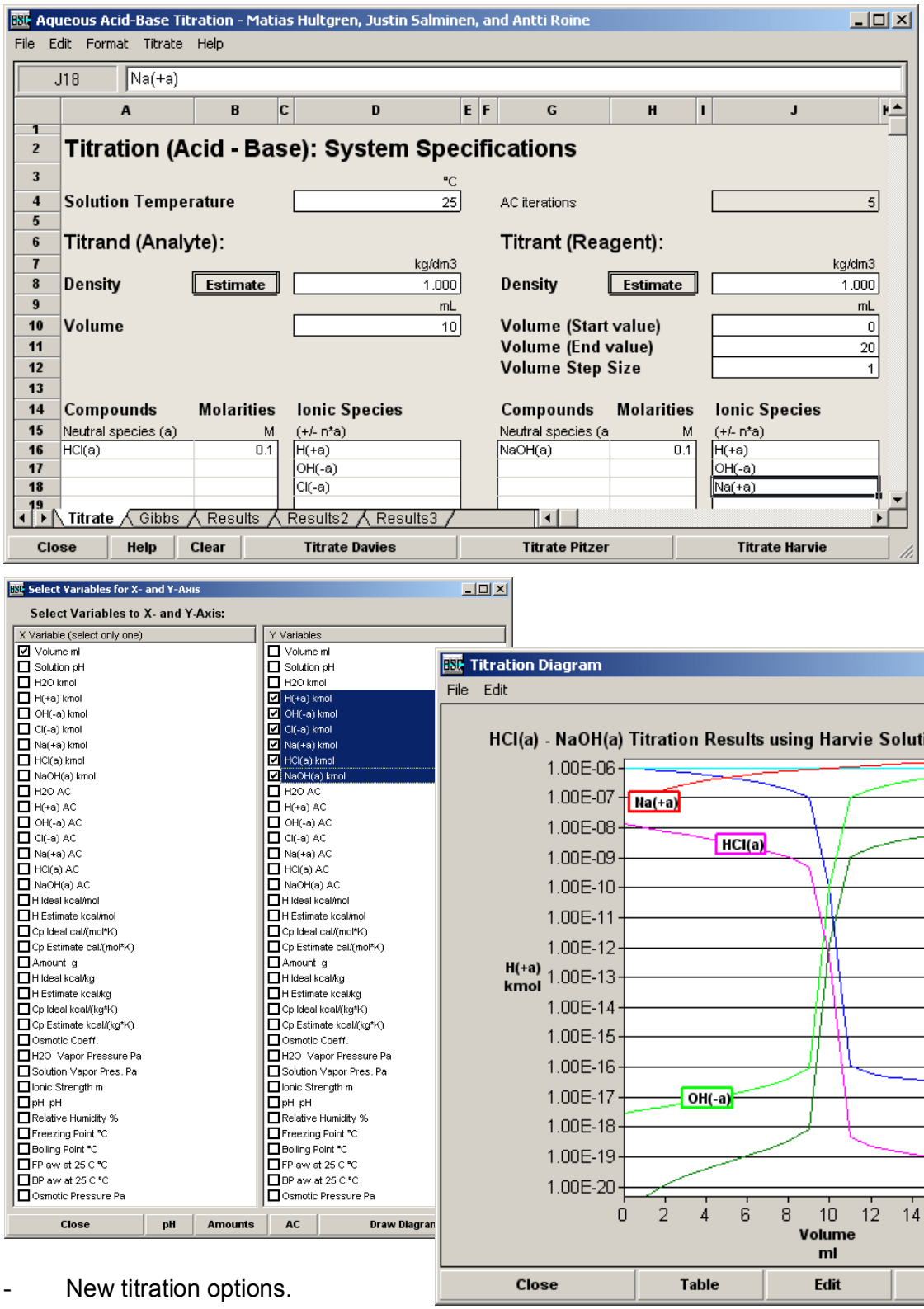
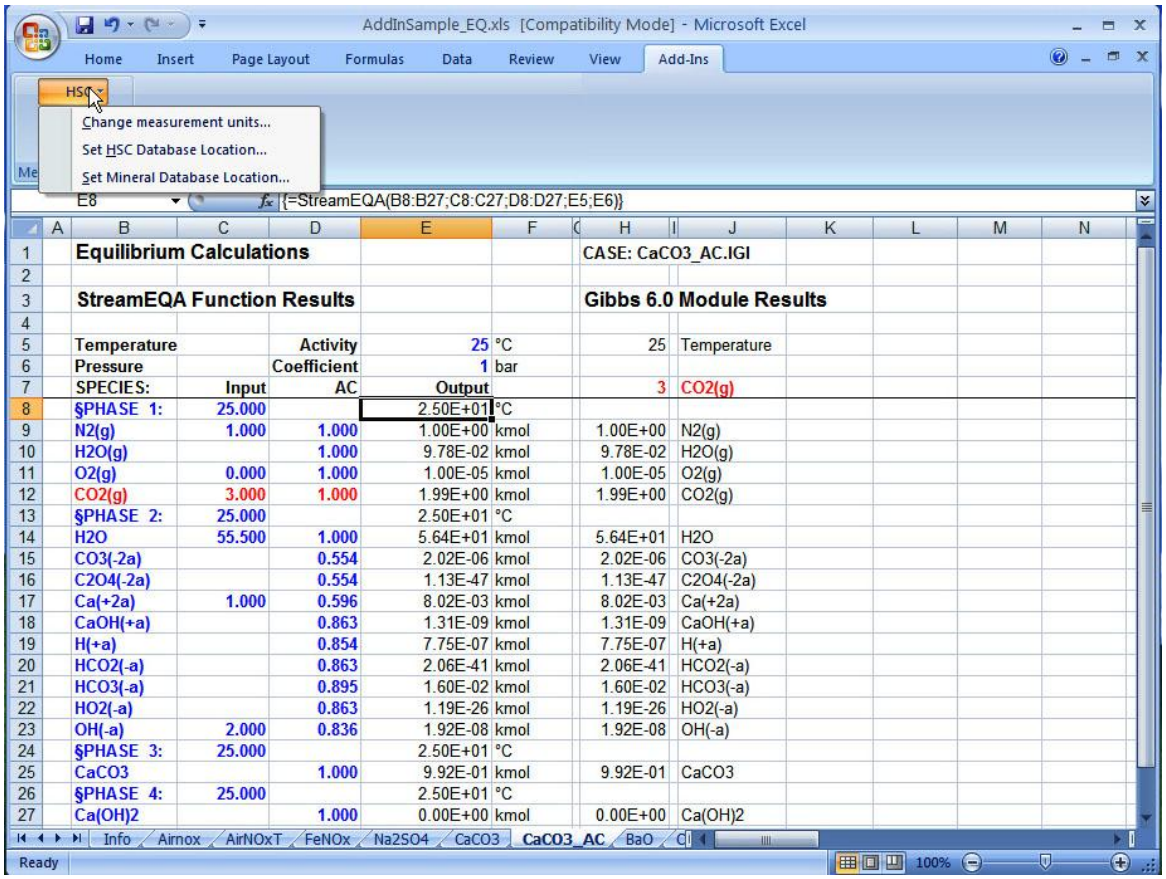
4. Aqua Module



- New titration options.
- Improved calculation speed.
- New properties: Boiling point elevation, freezing point depression, osmotic pressure estimation, water vapor pressure estimations, relative humidity estimations.

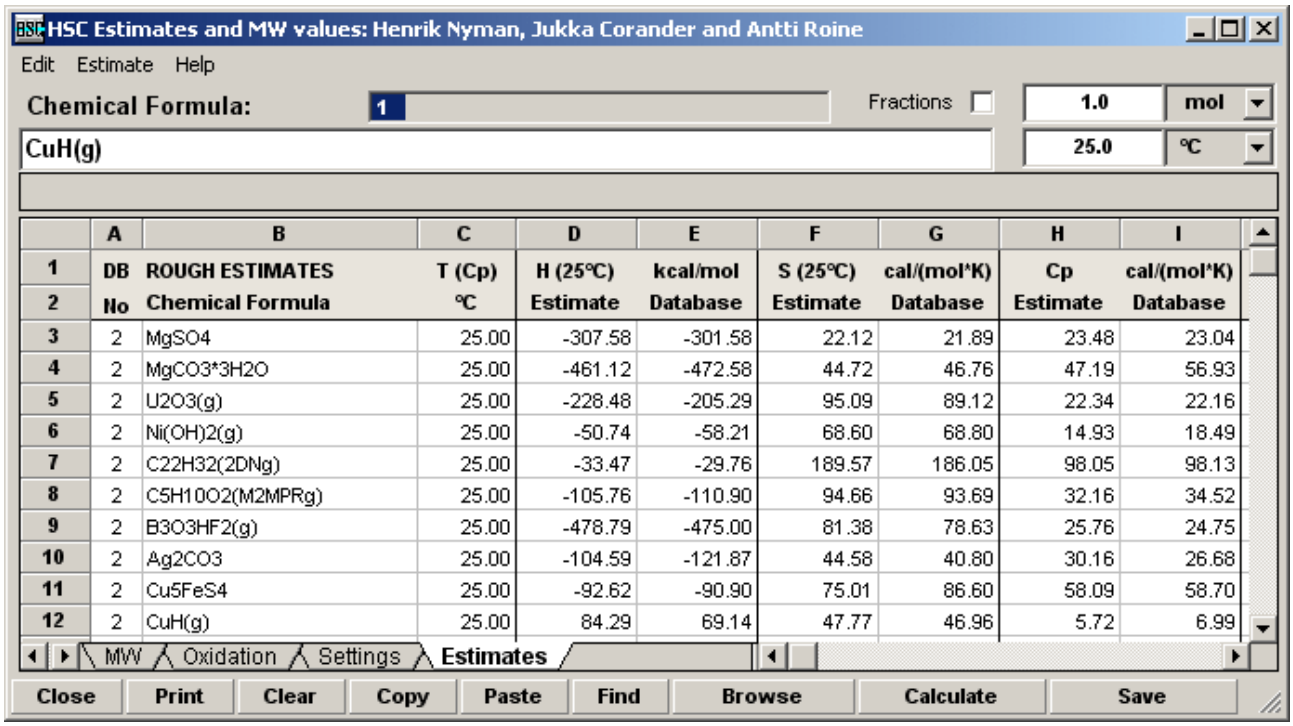
5. Add-In Functions



1	**Equilibrium Calculations**					**CASE: CaCO3_AC.IGI**		
3	**StreamEQA Function Results**					**Gibbs 6.0 Module Results**		
5	Temperature		Activity	25	°C	25	Temperature	
6	Pressure		Coefficient	1	bar			
7	SPECIES:	Input	AC	Output		3	CO2(g)	
8	§PHASE 1:	25.000		2.50E+01	°C			
9	N2(g)	1.000	1.000	1.00E+00	kmol	1.00E+00	N2(g)	
10	H2O(g)		1.000	9.78E-02	kmol	9.78E-02	H2O(g)	
11	O2(g)	0.000	1.000	1.00E-05	kmol	1.00E-05	O2(g)	
12	CO2(g)	3.000	1.000	1.99E+00	kmol	1.99E+00	CO2(g)	
13	§PHASE 2:	25.000		2.50E+01	°C			
14	H2O	55.500	1.000	5.64E+01	kmol	5.64E+01	H2O	
15	CO3(-2a)		0.554	2.02E-06	kmol	2.02E-06	CO3(-2a)	
16	C2O4(-2a)		0.554	1.13E-47	kmol	1.13E-47	C2O4(-2a)	
17	Ca(+2a)	1.000	0.596	8.02E-03	kmol	8.02E-03	Ca(+2a)	
18	CaOH(+a)		0.863	1.31E-09	kmol	1.31E-09	CaOH(+a)	
19	H(+a)		0.854	7.75E-07	kmol	7.75E-07	H(+a)	
20	HCO2(-a)		0.863	2.06E-41	kmol	2.06E-41	HCO2(-a)	
21	HCO3(-a)		0.895	1.60E-02	kmol	1.60E-02	HCO3(-a)	
22	HO2(-a)		0.863	1.19E-26	kmol	1.19E-26	HO2(-a)	
23	OH(-a)	2.000	0.836	1.92E-08	kmol	1.92E-08	OH(-a)	
24	§PHASE 3:	25.000		2.50E+01	°C			
25	CaCO3		1.000	9.92E-01	kmol	9.92E-01	CaCO3	
26	§PHASE 4:	25.000		2.50E+01	°C			
27	Ca(OH)2		1.000	0.00E+00	kmol	0.00E+00	Ca(OH)2	

- New functions: StreamEQAqua, StreamEQ6, StreamEQA6, StreamEQAqua6, StreamExTkg, StreamExTNm3, ExPh, StreamExPkg, StreamExPNm3, ExCh, StreamExCkg, StreamExCNm3, AquaAC, AquaH, AquaCp, StreamEQA, StreamEQEle, StreamEQAEle
- Several StreamEQ and StreamEQA issues have been fixed:
  - StreamEQ recalculation problem fixed.
  - The negative input amounts to StreamEQ are automatically converted to zero. If the §! flag is used then the negative input amounts create an error.
  - Element amount may also be zero in the StreamEQ and StreamEQA functions.
  - Limit of 20 elements has been removed, the limit is now 100 elements.
  - In Excel the new "HSC, Set HSC Database Location..." dialog makes it possible to see and change the H, S, and Cp database paths.
  - StreamEQ and StreamEQA error message boxes no longer show up (fire) too often.
  - The section mark § stands for the ordinary phase in StreamEQ and StreamEQA functions; however the "§!" flag string puts the error messages ON.
  - The double section mark §§ in the last phase converts this to the invariant phase, which means that the species are regarded as pure substances.
- New database option in the HSC menu of Excel.
- New document "27 Creating HSC Add-Ins.doc" has been added to the manual. This gives instructions to create custom-made Add-In functions for Sim.

6. H, S, and Cp Estimation Module



	A	B	C	D	E	F	G	H	I
1	DB	ROUGH ESTIMATES	T (Cp)	H (25°C)	kcal/mol	S (25°C)	cal/(mol*K)	Cp	cal/(mol*K)
2	No	Chemical Formula	°C	Estimate	Database	Estimate	Database	Estimate	Database
3	2	MgSO4	25.00	-307.58	-301.58	22.12	21.89	23.48	23.04
4	2	MgCO3*3H2O	25.00	-461.12	-472.58	44.72	46.76	47.19	56.93
5	2	U2O3(g)	25.00	-228.48	-205.29	95.09	89.12	22.34	22.16
6	2	Ni(OH)2(g)	25.00	-50.74	-58.21	68.60	68.80	14.93	18.49
7	2	C22H32(2DNg)	25.00	-33.47	-29.76	189.57	186.05	98.05	98.13
8	2	C5H10O2(M2MPRg)	25.00	-105.76	-110.90	94.66	93.69	32.16	34.52
9	2	B3O3HF2(g)	25.00	-478.79	-475.00	81.38	78.63	25.76	24.75
10	2	Ag2CO3	25.00	-104.59	-121.87	44.58	40.80	30.16	26.68
11	2	Cu5FeS4	25.00	-92.62	-90.90	75.01	86.60	58.09	58.70
12	2	CuH(g)	25.00	84.29	69.14	47.77	46.96	5.72	6.99

- HSC 7.0 estimation methodology makes it possible to estimate the enthalpy, entropy, and heat capacity values of any chemical substance, and no information of the geometrical bond structure is needed. The given species do not need to exist in the HSC database.
- HSC 7.1 improves estimates with updated estimation parameters.
- HSC 7.1 improves Cp temperature function estimates in particular.

7. H, S, and Cp Database

- Some 200 bug fixes have been made to the HSC 7 database based on the Estimation module results.

8. Heat and Material Balance Module

- Spreadsheet: Duplicate cell Defined Name "PrintArea" problem has been fixed.

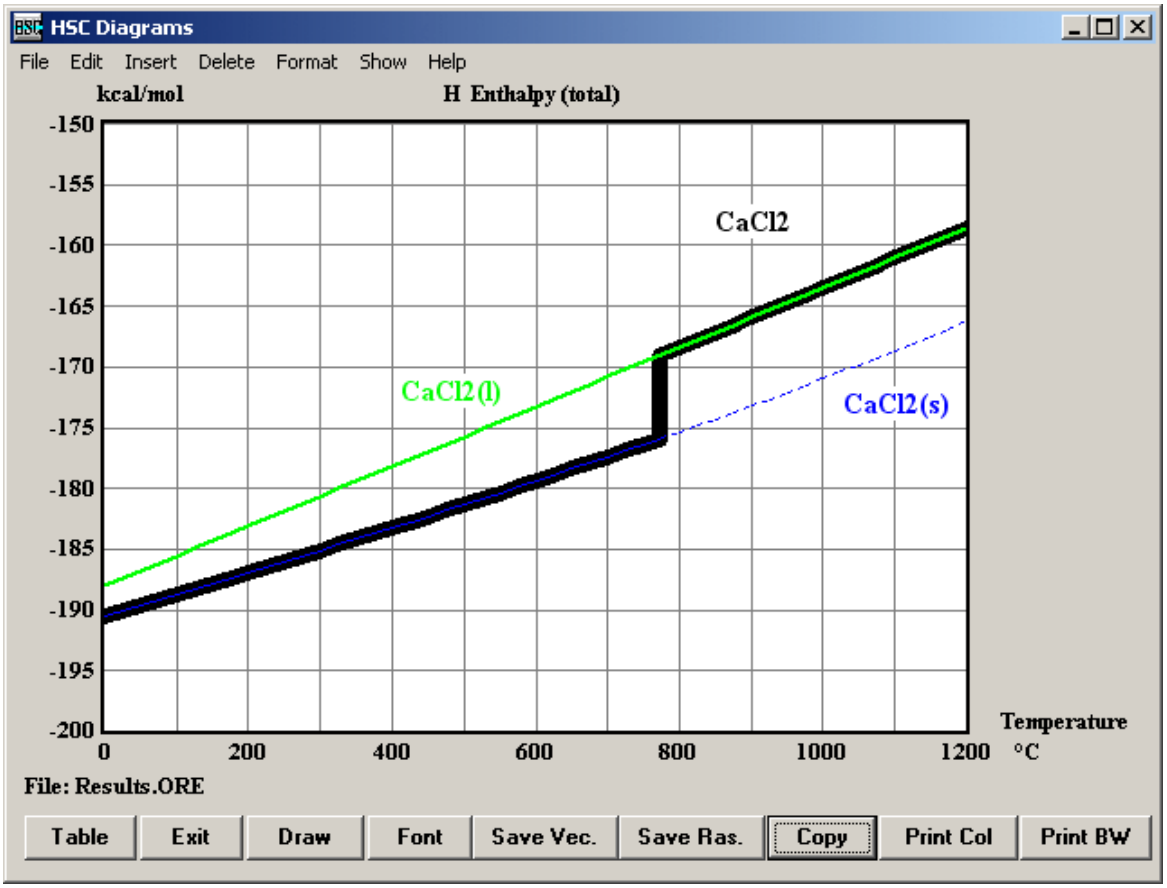
9. Sampler Module

- Semi-empirical process models are based on the theoretical and experimental data. Sampler module may be used to estimate sample sizes and sampling errors in the experimental work.

10. Help Module

- Rendering of images improved, not only the quality of the images but also the scrolling speed of the Help files.

11. General Fixes



- New force to solid (s) method. This makes it possible to force the HSC calculation modules to use solid data for a species at any temperature.

  In earlier HSC versions, the user had to force HSC to use liquid data at all temperatures with a (l) suffix in the formula. For example, **CaCl2(l)** will force HSC to use liquid calcium chloride data at all temperatures. HSC saves (l) data in the active Own database.

  Now with the (s) suffix, the user may force HSC 7.1 to use solid data at all temperatures. For example, **CaCl2(s)** forces HSC to use solid calcium chloride data at all temperatures. HSC does not save (s) data in Own database but uses only the s-records in the Main database and skips the l-records.

  This new feature may be used, for example, in the equilibrium module to illustrate melting points.

- The bug with table printing for some PDF printers has been fixed.
- In some computers the default font of the HSC modules caused cosmetic problems. Now Windows standard "Arial" font is used as default HSC font in most of the modules.
- "Outotec Research Oy" was integrated with "Outotec (Finland) Oy" at the beginning of 2011. The name "Outotec Research Oy" was changed to ""Outotec, Research Center"
- + Large number of small cosmetic fixes and improvements have been made.

11. HSC 7.14 Fixes and New Properties

- Sim: Slightly more robust control routine (tries harder to find the solution)
- Sim: "Paste formulas" bug was fixed
- Sim Reactions mode: wt-% formula bug has been fixed
- Sim Reactions mode: StreamEq wizard asks also distributions of the products
- Sim Reactions mode: Reaction wizard, Distributions sheet rows Hide/Show option
- Sim Distributions mode: Table row 65536 overflow bug was fixed
- Sim Distributions mode: Dist sheet opens now at left columns
- Sim Distributions mode: “Move Stream Down" bug fixed
- Sim: Particles mode: Redirecting feed stream bug has been fixed
- Sim: Particles mode: Mineral setup protection error corrected
- Sim: Possible to reorganize the order of the output streams in the units
- Aqua: Mg-SO4 Pitzer parameters updated.
- Occasionally file open took lot of time, because network printer linked to this file was not found. HSC 7.14 does not anymore look for network printers, when opening unit, ini, table and Excel files.
- Several small fixes

12. HSC 7.17 Fixes and New Properties

- Sim: Unit and Stream names may start with number. In HSC 7.14 there were occasional problems.
- Sim: “Tools, Insert Stream Header Table” inserts table into visible top-left corner.
- Sim: Incomplete Copy-Paste of flowsheet tables to Word was fixed.
- Sim Particles: Occasional bug when applying wizards in mineral mode (incomplete mineral by size tables) has been fixed.
- Sim Particles: In mass balacing the recovery by size calculation bug has been fixed.
- Sim Particles: In 2D mass balancing the composition for intermediate streams is calculated.
- Sim Particles: Occasional incomplete wizard run and mineral setup problems was fixed.
- Sim Hydro and Distribution: Elemental Balances calculates also total process balances.
- Sim Pyro: Occasional stream measure unit problem when rerouting streams was fixed.
- Geo: new window (database table) for viewing mineral database has been added.
- Geo: Occasional concentration calculation bug in Geo was fixed.
- Equilibrium Module: Works if the HSC has not been installed into default folder C:\HSC7\
- PIC: Table option opens sheet 1. Improper X-axis selection do not crash program.
- HSC tables: Mouse wheel stuck into hidden table rows was fixed. Support of CSV-file format was added.
- HSC occasional memory leak with some Add-In functions was fixed.
- HSC 7.16 conflict with HSC 6.1 was fixed.
- etc.

13. HSC 7.19 Fixes and New Properties

- Sim: Problem with "Fit to Window" Zoom option when closing Run mode was fixed.
- Sim: Controls iteration routine improved with difficult control functions, which reach infinite values within given min and max variable range. This new routine will be used if Max Iters is larger than 10, for example, 30.
- Sim: Controls sheet format improved
- Sim: Controls ON/OFF settings new change option
- Sim: Particle mode controls may refer to mineral setup and minera feeds.
- Sim: Control monitor stability improved. Missing unit in controls do not crash model.
- Sim: Insert Cell sync problem fixed.
- Sim: Remote control SET can change also cells with formula. Original formula will be recovered after the remote run.
- Sim: Remote control SET works also with empty cells.
- Sim: Remote control works better with Distribution mode also, like SET, Set Link, Multiply links, and Show Link methods.
- Sim: Distribution mode – Browse HSC Database dialog added.
- Sim: Edit Table dialog “Link to Unit” stablity fixed
- Sim: Page change do not cause problems to Edit Table dialog
- Sim: Distributions mode – new Mixer Wizard, which makes easy to create mixer and splitter units.
- Sim: “Recover Original Aspect Ratio” option works now with all objects.
- Sim: F2-key sets focus to unit or stream name ID.
- Equilibrium Module: H, S and Cp value viewer was added to Pic.exe. This viewer is able to remove species from the chemical system. The co-operation within HSC.exe, Gibss.exe and Pic.exe routines was improved.
- Equilibrium Module: Error 20007 fixed.
- Gibbs: The maximum number of species per phase was increased from 999 to 9999.
- Aquadll.dll: Temperature unit bug with Kelvins was fixed.
- HSC7.DLL slightly faster and “Others” species handling improved.
- Sampler: Few bugs fixed.
- etc.