HSC Chemistry 7.0

HSC Chemistry is a versatile tool for thermodynamical and process calculation. HSC has a wide range of application possibilities in industry, research, and education. The software is continuously being developed to meet the high expectations of our customers. This is a brief description of the calculation modules found in the program. For more information, please visit our website: www.outotec.com/hsc

1.   Introduction

HSC Chemistry 7.0 is a software program for process flowsheet simulation, which also contains 22 other calculation modules displayed as options in the main HSC menu, and 12 databases together with extensive thermochemical, heat transfer and mineralogical data. HSC Chemistry 7.0 is compatible with Windows Vista, Vista 64, and Windows 7.

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2. Sim Flowsheet Simulation

HSC Sim includes four different modes (Particles, Reactions, Distributions and Experimental). The program calculates the steady state of the process. Each mode has its own area of application:

Minerals Processing Models:
    Grinding, flotation → Particle based models, Particles mode
Hydrometallurgical Models:
    Leaching → Chemical reaction based models, Reactions mode
Pyrometallurgical Models:
    Smelting → Element distribution based models, Distributions mode
Experimental data analysis:
   Data measured from the process → Mass balancing models, Experimental mode

HSC Sim offers an easy to use interface for process modeling. Its many automated functions speed up process calculation. The drawing procedures of the flowsheet are similar in all calculation modes.

2.1. Flowsheet module – Particles mode

HSC Sim has a special set-up and approach for processes where minerals are treated. This approach should be used for processes including crushing, grinding, flotation, gravity separation, or screening. Mineral-based models treat **particles**, which have at least the following properties:
- size (diameter)
- mineral composition as wt.%

In addition, they may have additional 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.
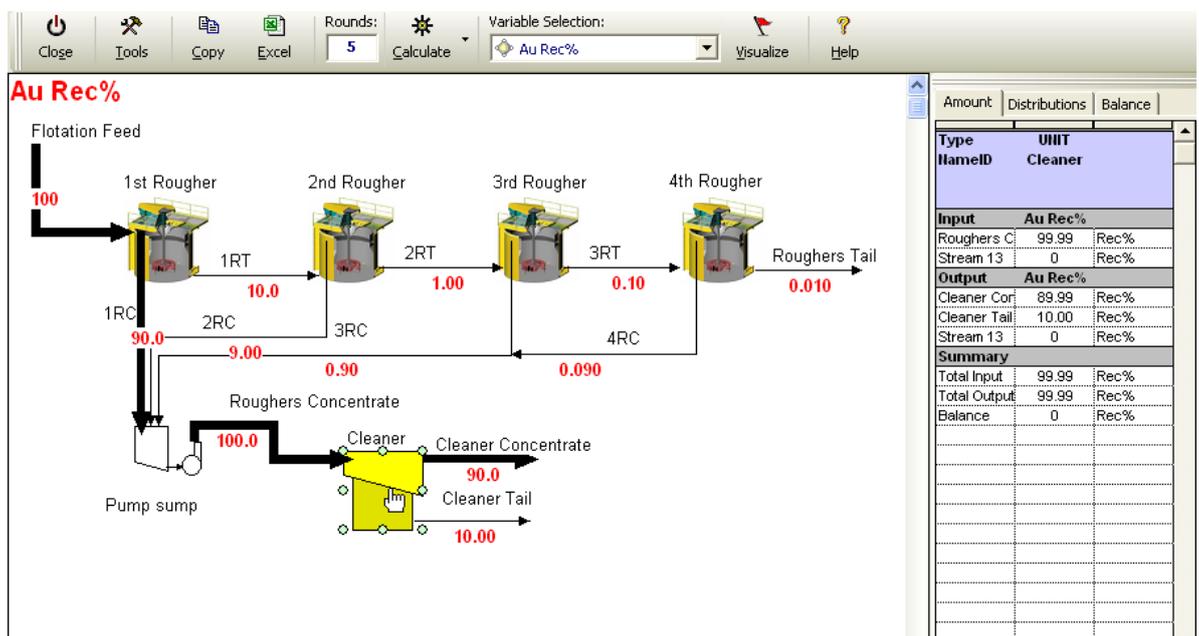
2.2.   Flowsheet module – Reactions mode

The Reactions mode is designed for processes that can be described with chemical reactions. Processes can be either small single-unit processes or complete plants with all recycle streams. The program contains ready-made Wizards to ease the making of the process.

The Reactions mode can be used to model processes like the leaching of minerals, manufacturing of bulk chemicals, liquid – liquid extraction processes, and liquid purification processes - just to mention a few examples.
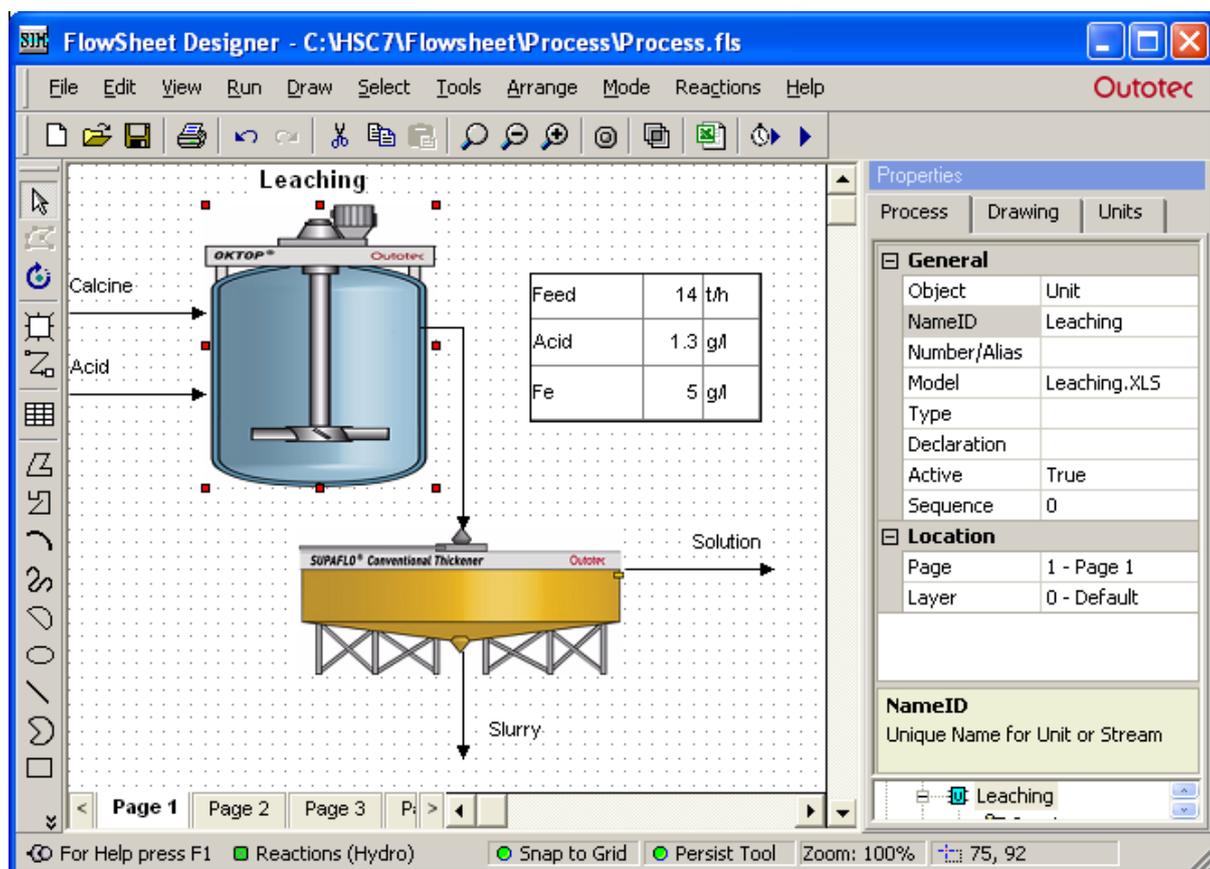
2.3. **Flowsheet module – Distributions mode**

The flowsheet principles for drawing and running the model in Sim Distribution mode are quite similar to the Sim Reactions and Particle modes. However, the unit process models are not based on a fixed variable list. Instead, the model editor looks more like the traditional HSC Balance module. The basic ideas of the model are also quite similar to the old Balance module.

The Distributions mode is meant for applications where you want to split elements into different streams with distributions. This is a common practice in pyrometallurgical calculations for which this mode was originally designed.

Sim Unit Editor: ESP_fsf

File　Edit　View　Insert　Delete　Format　Tools　Units　Run

| C12 | SO2(g) |

	A	B	C	D	E	F	G	H	I	J	R
1			OUTPUT								
2											
3											
4	Flags		Output Streams	Value	Units	Amounts			Latent H	Total H	S
5						kg	Nm3	kmol	kWh	kWh	
6			Total Gas	132221.62	Nm3/h						
7			Total Condenced	7.72	t/h	205165.22	132223.63	5954.47	17345.47	-110201.69	
8	SRC	ESP_	ESP Gas	132221.62	Nm3/h	Amounts			Latent H	Total H	
9	DST	?	Temperature	341.01	°C	kg	Nm3	kmol	kWh	kWh	
10			Pressure	1.00	bar						
11	Fix		Total	100.00	vol-%	197727.94	132221.62	5899.17	16889.87	-96908.37	22606
12			SO2(g)	13.70		51774.08	18115.29	808.23	3217.29	-63419.55	3868
13			SO3(g)	0.07		325.15	91.03	4.06	21.59	-424.90	20
14			H2O(g)	4.54		4823.69	6001.39	267.76	819.78	-17166.48	977
15			CO2(g)	4.46		11566.88	5890.86	262.83	991.86	-27736.79	1095
16			O2(g)	6.81		12852.21	9002.35	401.65	1082.25	1082.25	1556
17			N2(g)	70.43		116385.92	93120.71	4154.65	10757.11	10757.11	15087
18											
19	O		Dust	52.59							
20	O		SO3/SOX	0.50							
21	SRC	ESP_	ESP Fume	0.00	t/h	Amounts			Latent H	Total H	
22	DST	?	Temperature	341.76	°C	kg	Nm3	kmol	kWh	kWh	
23	Inert	21	Pressure	1.00	bar						
24	Fix		Total	100.00	wt-%	2.59	0.30	0.01	0.08	-0.53	
25			SeO2(g)	7.49		0.19	0.04	0.00	0.01	-0.05	

Input　**Output**　Dist　Controls　Model　Tank

| Close | Sync is ON | Open Str | Save Str | Del Str | ▲ ▼ | Ins Row | Del Row | Show/Hide | Run |

**2.4.** **Flowsheet module – Experimental mode**

The Experimental mode is for managing and processing experimental data from laboratory or pilot scale test work or from full process. Usually experimental data incomplete and contains measuring errors, which leads to problems in model fitting where balanced values are required. This mode can be used to calculate the best fit for the balance.

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.

There is no need 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, then HSC will increase the mass balance node size accordingly.
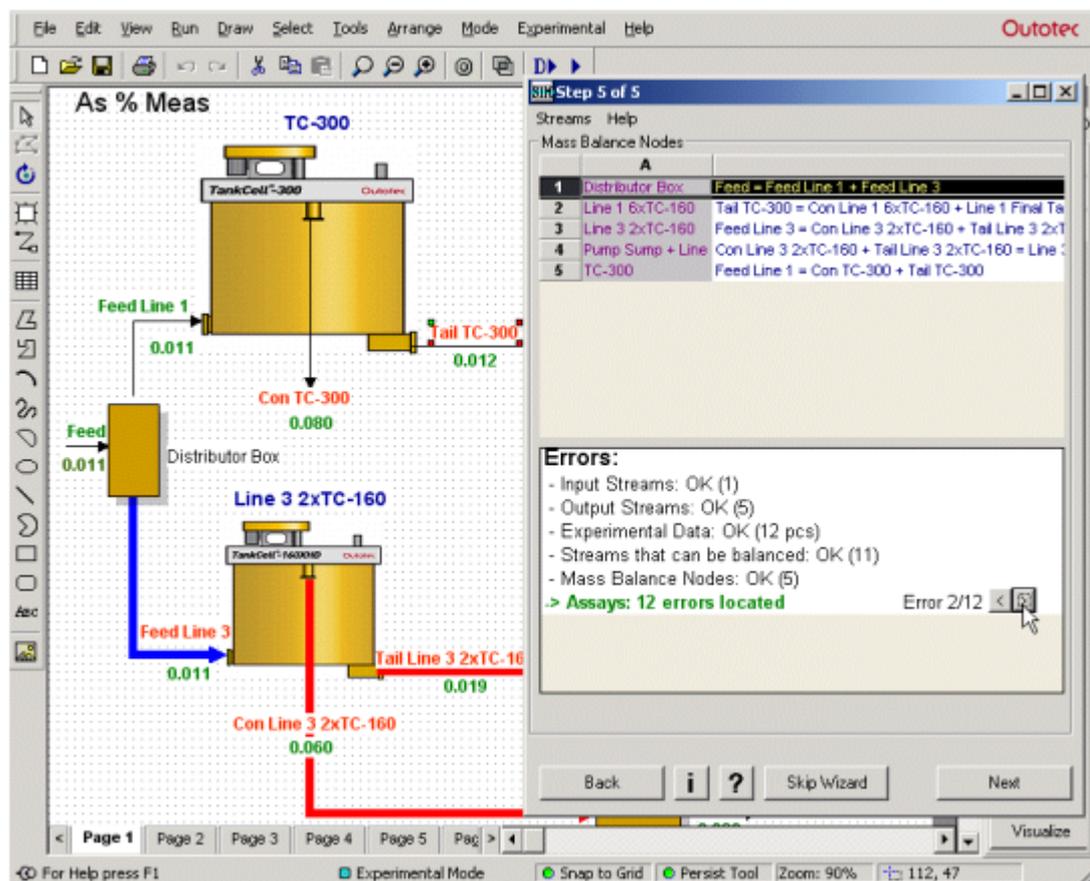
3.   Data

HSC Data is a data processing application of the HSC Chemistry program family. HSC Data has been designed to process data in Microsoft Access (*.mdb) databases, but some other database types can be opened and Microsoft Excel files and TAB-separated ASCII files can also be opened with the program.

4.   Geo

HSC Geo is a collection of tools developed originally for geologists and mineralogists. However, this mineral database is also useful for other professionals. HSC Geo tools are listed below with some of the tasks they have been designed for:

1. Mineral Database tools
    a. Search minerals and their properties in the Mineral Database
    b. Study chemical composition of minerals and how it varies within a mineral species
    c. Search minerals by elements, name
    d. Identify unknown mineral by its chemical composition
    e. Add new analyses to the database

2. Mineral Liberation tools
    a. Open MLA (Mineral Liberation Analysis of FEI) files for study of modal composition, elemental composition, mineral mode of occurrence, etc.
    b. Process MLA files for reporting (e.g. adjusting modal composition of MLA to match chemical assays)
    c. Process MLA analysis to be used in Process Simulator HSC Sim

3. Modal Analysis tools
    a. Calculate modal composition (mineral composition by weight) of samples based on chemical assays and chemical composition of minerals (element to mineral conversion). HSC Geo creates mass balance equations and solves them.
    b. Study and report the Modal Analysis result: mineral grades, the distribution of elements between minerals, calculation residual, back calculated chemical composition.

4. Tools for processing chemical assays of rocks and minerals
    a. Read chemical analysis of rock samples and calculate atomic%, cation%, sulfide fraction%, CIPW-normative composition, volatile free composition (VF), volatile and sulfide-free composition (VSF)
    b. Reorganize chemical assays from different sources to a standard structure ("Database Model")
    c. Save original, organized and saved data in Microsoft Access database to be further used by HSC Data
    d. Calculate mineral formula for mineral assays

5.   **Map**

HSC Map is location-based (GPS) stock control software. HSC Map is designed for feed mixture calculation and raw material stock control. The basic idea is that the user may easily collect the raw materials from the stock and calculate a single or multi mixture composition, in order, for example, to obtain the proper copper and silica content and calorific value in a feed mixture. The user may also test the calculated feed mixtures using the HSC Sim process calculator before starting to use the new mixture.

6.   **Reaction Equations**

Traditionally researchers have tested their ideas by writing out reaction equations and then calculating equilibrium constants and heats of reaction from standard thermochemical data. However, this required a time-consuming search for the data with standard state conversions.

HSC does all of the above instantly – you simply type the reaction equations in the input field and HSC gives you the heat of the reactions, equilibrium constants at any temperature, and the amount of species. HSC even checks the elemental balance and gives the potential vs. standard hydrogen electrode for electrochemical reactions.

7.   **Heat and Material Balances**

Heat balance calculations are usually carried out when developing new chemical processes and improving old ones, because no process can work if too much heat is released or if there is a lack of thermal energy to maintain the reaction temperature. 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.

8.   **Heat Loss Calculator**

The main use 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 as simple reference tables for material properties.

Heat Transfer Calculations C:\HSC7\HeatLoss\Smelting1.HTR

File Edit View Insert Delete Format Calculate Target Diagram Help

C9   1200.0003800375

Properties	Units	1	2	3	4	
Column Type:		Surface	Layer	Surface		
Material:		Molten metal	REXAL 2S EXTRA	Water, Copper elements cooling		
Surface Material:						
Thickness x	m		1.000			
Surface Area A	m²	1.000	1.000	1.000		
Conduction k (mean)	W/(mK)		3.942			
Surface Convection hc	W/(m²K)	144.000		2400.000		
Surface Radiation hr	W/(m²K)	0.000		0.000		
Left (inner) T	°C	1200	1170	22		
Right (outer) T	°C	1170	22	20		
Thermal Resistance	°C/kW	6.944	270.232	0.417		
Heat Flux	kW/m²	4.251	4.251	4.251		
Calculation Grid			10			
Distance	m	0.000	1.000	1.000		
Angle of Object	°	0		0		
Speed of Fluid/Gas	m/s	0.02		0		
Min Temperature	K	N/A	N/A	N/A		

◄ | ► \ Smelting 1200°C ∕ Smelting 1400° ∕ Smelting 1600° ◄ | ►

Get Data for Column:

Conduction

Convection

Radiation (surface)

Radiation (gas)

Radiation (particles)

TOTAL HEAT FLOW: 5.502 kW ▼

Shape and Dimensions:

◉ Wall   Draw   Width 1.00 m
○ Cube   Length 1.00 m
○ Cylinder
○ Sphere

Calculate:

Temperature profile

Heat flow

HOT => COLD

Exit   Fix Value   Diagram Table   Draw Diagram

9. Equilibrium Compositions

Equilibrium calculations offer a practical way to observe the effect on product composition of process variables such as temperature and quantity of raw materials.

With this program option you can calculate the equilibrium composition and amounts of prevailing phases in any reactor. You only need to specify the quantity of raw materials, temperatures, and the species of the system. These species can be specified by selecting the elements of the system, or typing the formulas, or by editing an old file. Activity coefficients can be given, if necessary, as constants or as a function of temperature and composition.

Calculations can be repeated at stepwise intervals over a range of raw material quantities or reaction temperatures in order to visualize the effect of these process variables. For example, you can observe the effect of temperature on arsenic evaporation from copper-iron sulfides, or the effect of chlorine feed on titanium chlorination.
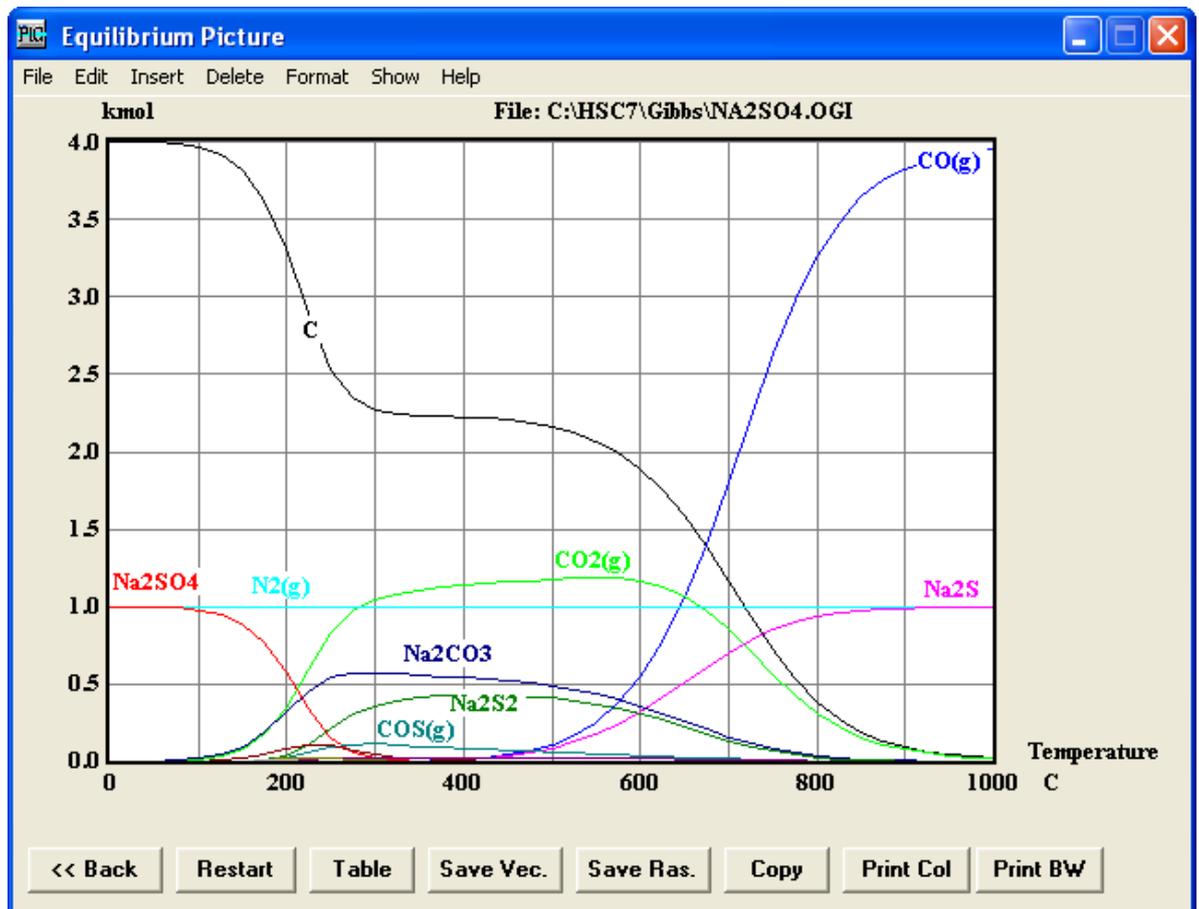
10. Electrochemical Cell Equilibriums

The Cell Equilibriums module calculates the equilibrium composition of an electrochemical cell using the same calculation method as the Gibbs solver in the Equilibrium Compositions module. However, this module is especially designed for electrochemical cell calculations, such as batteries. In addition to the phase compositions, it also gives the electrochemical potentials of the electrodes.

11. Eh – pH – Diagrams

Eh-pH-diagrams, also known as **Pourbaix Diagrams**, show the thermodynamic stability areas of different species in an **aqueous 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 with 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.
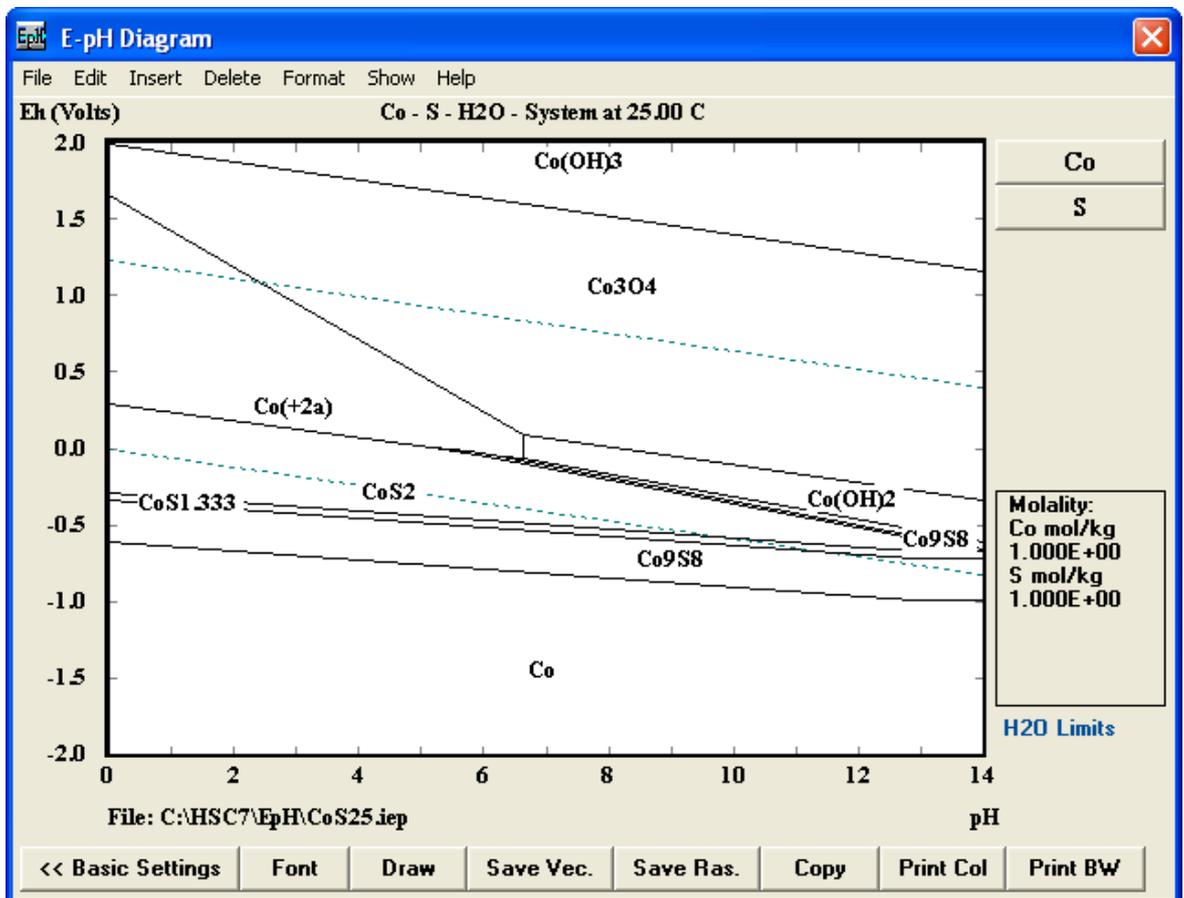
12. H, S, C and G Diagrams

The diagram 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.
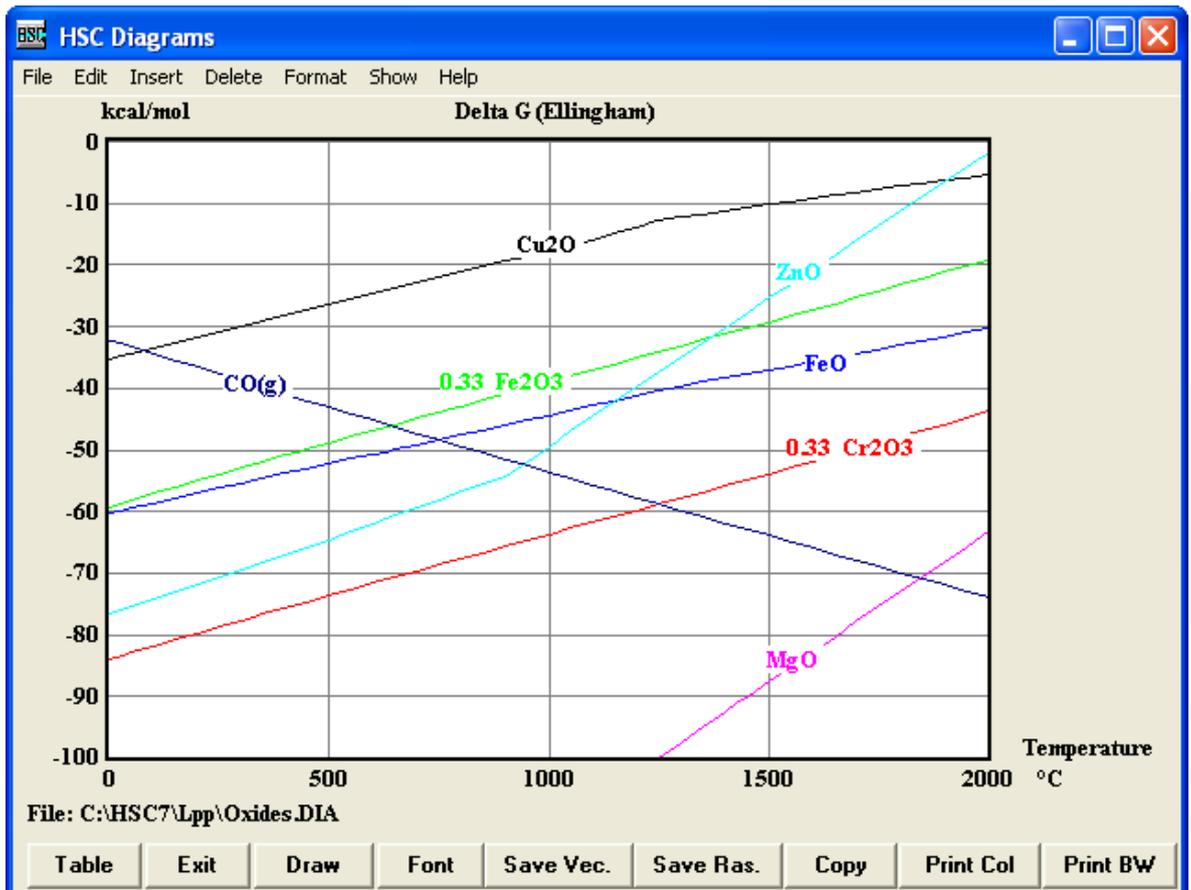
13.   Phase stability diagrams

The phase stability diagrams show the stability (*predominance*) areas of condensed phases in a ternary system as a function of temperature or in isothermal conditions, with the remaining constraints as the other axis. These diagrams are very useful when a quick estimation of the prevailing phases is needed. It is assumed that all phases are pure substances. Mixture phases are not taken into account in basic phase stability diagrams.

13.1.   Tpp – Diagrams

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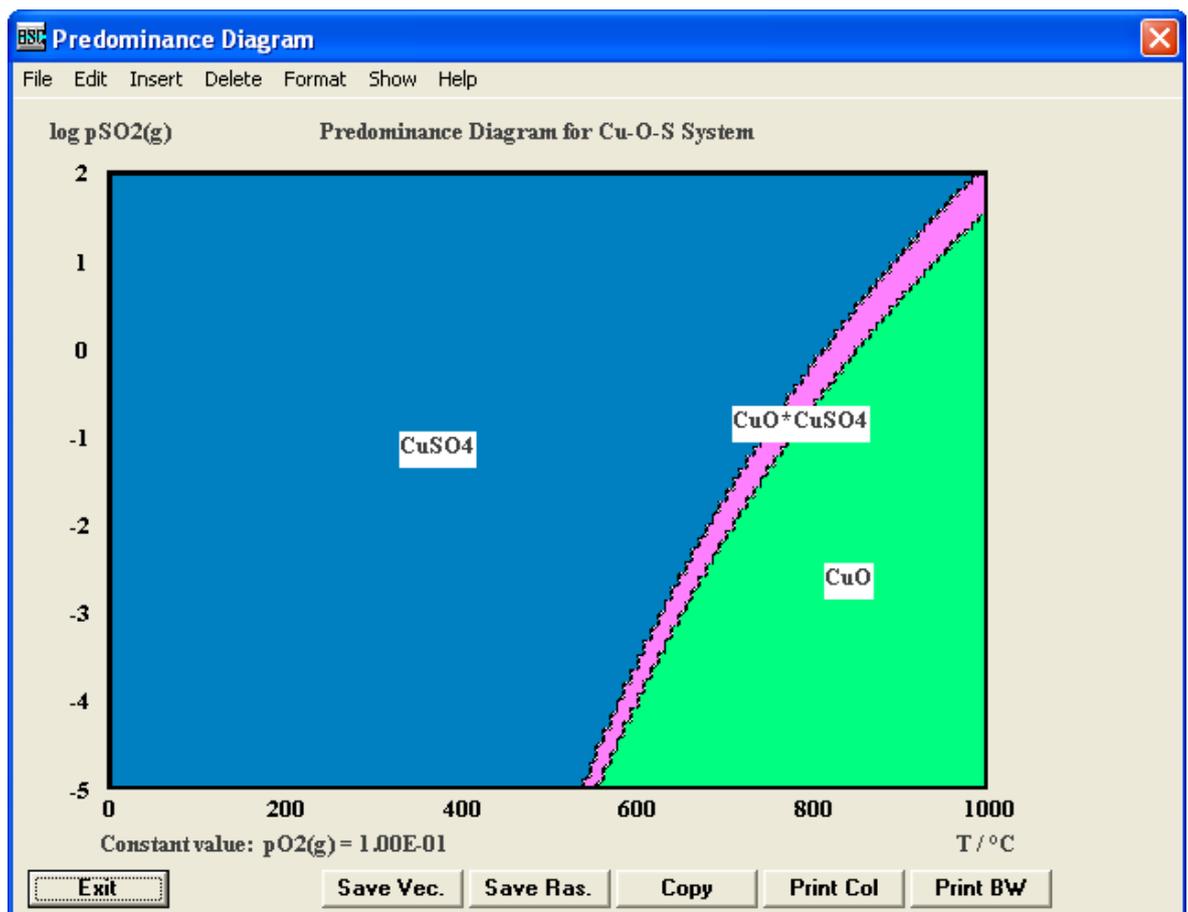
13.2. Lpp Diagrams

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.
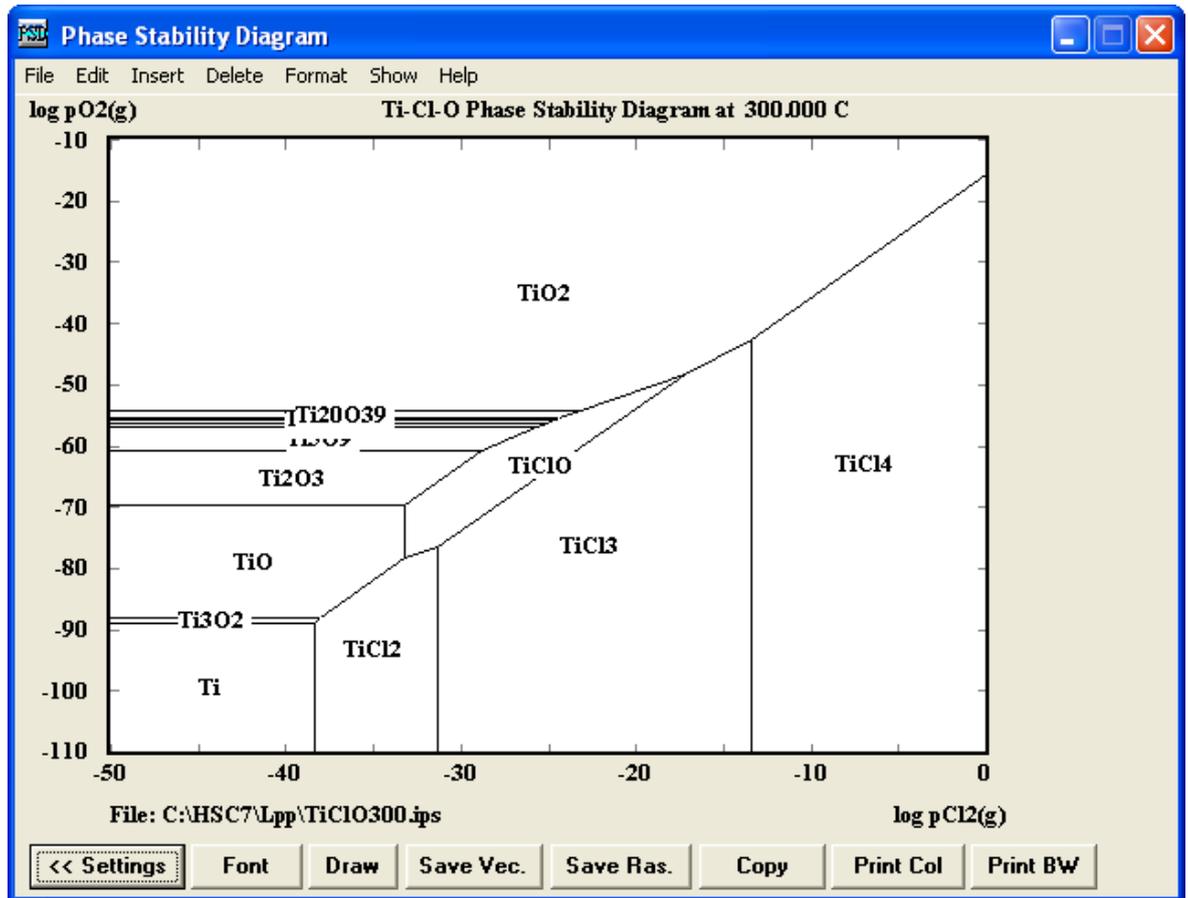
14. Water

This calculator is a very useful replacement for **steam table books** and **Mollier diagrams**. 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.

15. Aqua

Non-ideal aqueous electrolyte models have been added to the HSC software in the newly developed ''HSC AQUA module''. Up to this point the HSC Chemistry software has not included non-ideal models for aqueous electrolyte solutions. HSC includes an impressive number of standard state data for neutral components and ionic species. For the calculation of the excess Gibbs energy of individual species and the activity coefficient of mixtures, models need to be included in the HSC data bank. Electrolytes have so far been treated as ideal solutions where the activity coefficients of the individual solution species are set to one.

Predictive and semi-empirical models for ionic activities, mean activity coefficient, and osmotic coefficient have been introduced. In addition, an estimation of solution enthalpies and heat capacities is included. These working equations were derived from activity coefficient models. The activity coefficient models available are 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 990. This includes 407 cation-anion pairs, 102 cation-cation and anion-anion pairs, 114 ternary coefficients, and 289 ion-neutral pairs.

Aqueous Solution Equilibrium Property Estimator: Matias Hultgren, Justin Salminen, Risto Pajarre and Pertti Ko...

A1 | Water Phase

	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	0.057	100.000			-69.974	-69.939	16.107	16.617
2	H2O	25	0.055	96.496		1.018	-68.315	-68.325	17.980	17.828
3	Co(+2a)	25	0.001	1.752		0.051	-13.900	-12.635	-7.620	11.130
4	SO4(-2a)	25	0.001	1.752		0.051	-217.400	-216.135	-63.323	-44.573

Water Phase / Binary System Sheet

Davies Pitzer Harvie   Binary Systems   Small Amounts

| Close | View Database | Ins | Del | Read Test | Calculate |

16. H, S, Cp Estimates

The HSC Estimates module gives a rough estimate of the 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. 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.

17. Conversions

The Composition Conversion module is a simplified version of the Mineralogy Iteration module. It is included in HSC Chemistry because the Composition Conversion module can easily give the compositions and amounts of species in wt% and kg units.

18. Mineralogy Iterations

Composition conversions, between substance (mineralogy) and elemental analyses, are often needed in chemical R&D work. The Mineralogy module can easily convert mineralogical compositions into elemental ones, but is not always able to make the reverse conversion.

19. Periodic Chart

The Elements module offers an element database in spreadsheet format with some 56 different element properties. It is easy for users to add their own data to this table.

20.   Measure Units

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

21.   Excel Add-In Functions

With HSC 7.0 Add-In Functions it is possible to use the HSC 7.0 database directly under Microsoft Excel and carry out several thermochemical and other type of calculations in that way. In order to use these functions in Excel they must, however, first be activated. The Add-In also provides the MineralProperty Function. This function accesses the HSC Mineral Database and enables you to query the properties of stored minerals.

22.   Databases

HSC contains 12 databases for use by the modules. Some databases are used only in one module, but some contain more general information, like the main database for enthalpy (H), entropy (S), and heat capacity (Cp). The HSC Main Database and Mineralogical Database are the largest ones.

22.1.   DATABASE for H, S and Cp Data

All the calculation options of HSC Chemistry utilize the same databases, and therefore they are an essential part of the program. The enthalpy (H), entropy (S), and heat capacity (C) values of the elements and compounds are saved in the database together with a variety of additional information.

HSC Chemistry can handle two active databases simultaneously, denoted as the **Own** and the **Main** database. The current version of the **Main** database contains thermochemical data of more than 25000 species, including pure substances and aqueous species. The **Own** database is reserved for the data specified by the user. It is empty when the user gets the software, but up to 60000 species can be saved into one **Own** database.

22.2.   Mineralogical Database

The Mineralogical Database includes chemical composition and other information for 13346 minerals. The HSC Geo module has tools for the efficient use of the database, but it can also be read from Excel with Add-Ins.