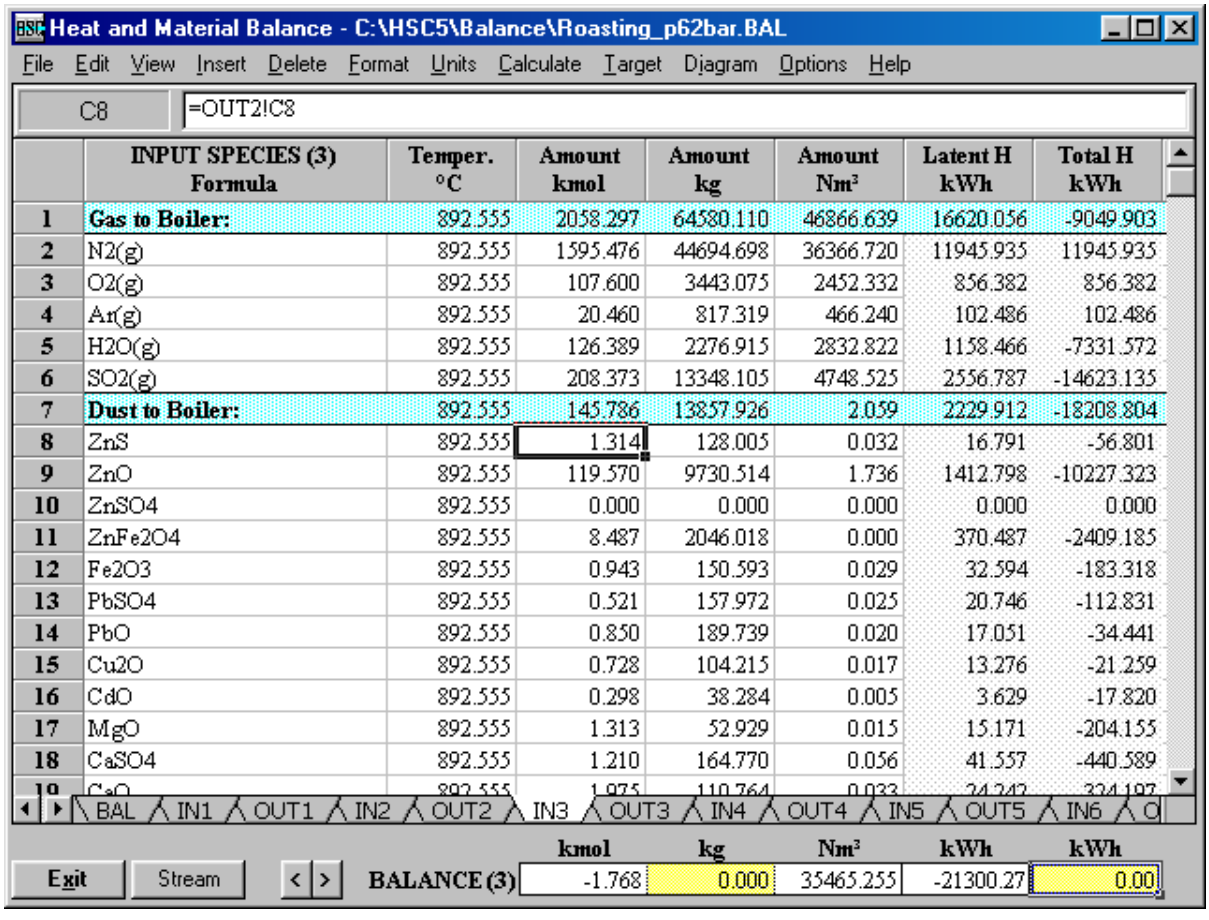
6. What's new in HSC Chemistry 5.0

The new HSC version 5 contains several new calculation routines, new properties and a larger database with updated data. The familiar HSC style user interface and file formats have been maintained in order to minimize the training requirements for current HSC users. The new features can be summarized as follows:

6.1. Updated Heat and Mass Balance Module

- HSC version 4 calculated only one balance area at a time. With the new HSC 5 up to 127 balances may be calculated simultaneously.
- Balance areas may be connected with each other using cell references or built-in element amount functions.
- Temperatures may be used as variables.
- Target routine is also available in Diagram option.
- New stream elemental composition calculator.
- Graphical objects may be added to sheets.
- Link to the new Steam enthalpy calculator (0.01 - 1000 bar).
- Link to the new Heat Loss routine.
- Many small improvements such as iteration routine fixes.



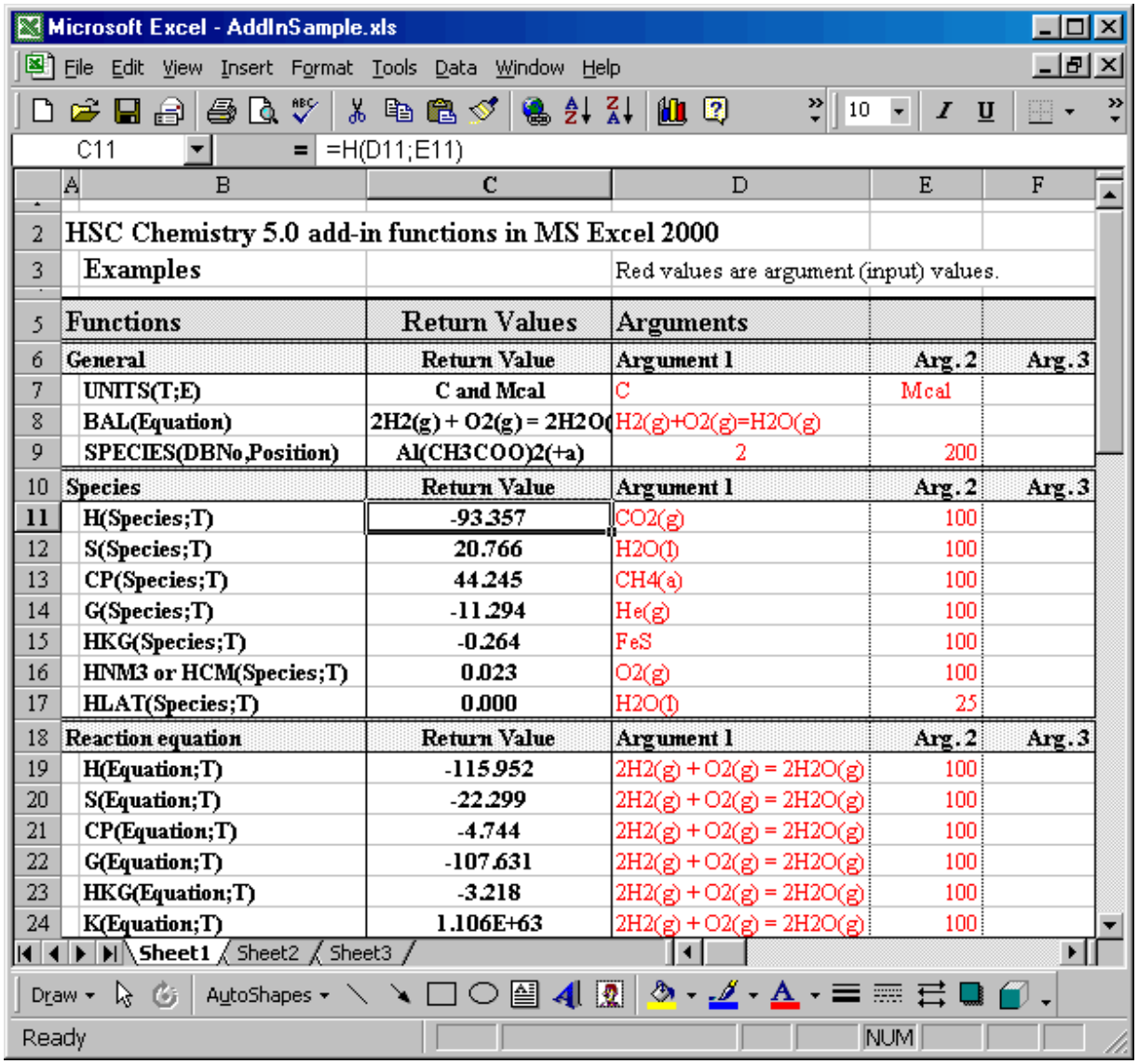
	INPUT SPECIES (3) Formula	Temper. °C	Amount kmol	Amount kg	Amount Nm³	Latent H kWh	Total H kWh
1	**Gas to Boiler:**	892.555	2058.297	64580.110	46866.639	16620.056	-9049.903
2	N2(g)	892.555	1595.476	44694.698	36366.720	11945.935	11945.935
3	O2(g)	892.555	107.600	3443.075	2452.332	856.382	856.382
4	Ar(g)	892.555	20.460	817.319	466.240	102.486	102.486
5	H2O(g)	892.555	126.389	2276.915	2832.822	1158.466	-7331.572
6	SO2(g)	892.555	208.373	13348.105	4748.525	2556.787	-14623.135
7	**Dust to Boiler:**	892.555	145.786	13857.926	2.059	2229.912	-18208.804
8	ZnS	892.555	1.314	128.005	0.032	16.791	-56.801
9	ZnO	892.555	119.570	9730.514	1.736	1412.798	-10227.323
10	ZnSO4	892.555	0.000	0.000	0.000	0.000	0.000
11	ZnFe2O4	892.555	8.487	2046.018	0.000	370.487	-2409.185
12	Fe2O3	892.555	0.943	150.593	0.029	32.594	-183.318
13	PbSO4	892.555	0.521	157.972	0.025	20.746	-112.831
14	PbO	892.555	0.850	189.739	0.020	17.051	-34.441
15	Cu2O	892.555	0.728	104.215	0.017	13.276	-21.259
16	CdO	892.555	0.298	38.284	0.005	3.629	-17.820
17	MgO	892.555	1.313	52.929	0.015	15.171	-204.155
18	CaSO4	892.555	1.210	164.770	0.056	41.557	-440.589
19	CaO	892.555	1.975	110.764	0.033	24.242	-324.197
			kmol	kg	Nm³	kWh	kWh
	BALANCE (3)		-1.768	0.000	35465.255	-21300.27	0.00

6.2. New HSC AddIn Functions for Excel 2000

HSC Excel AddIn makes native HSC functions and databases available directly within a normal Excel spreadsheet. Highly specialized applications may be created with these new Excel AddIn functions.

These functions work like normal Excel functions such as the **SUM** function. For example, **H("FeO";500)** function returns the enthalpy of FeO at 500 Kelvin. Another example is **WTP("Na";"Na2SO4")** function which returns the weight percent of sodium in sodium sulfate.

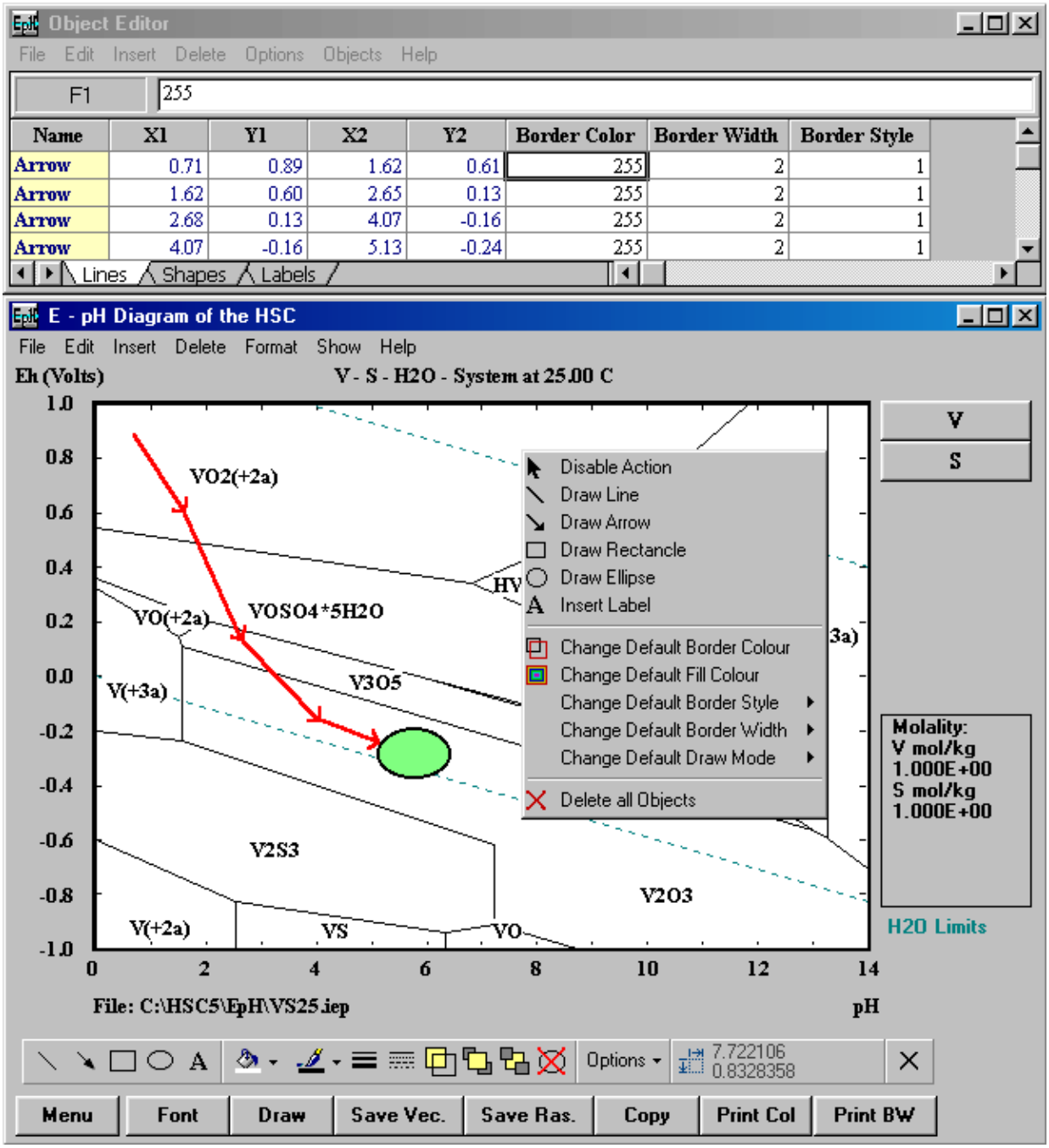
Up to 45 different HSC functions are available in Excel which automatically reads the HSC database.



6.3. New Drawing Toolbar

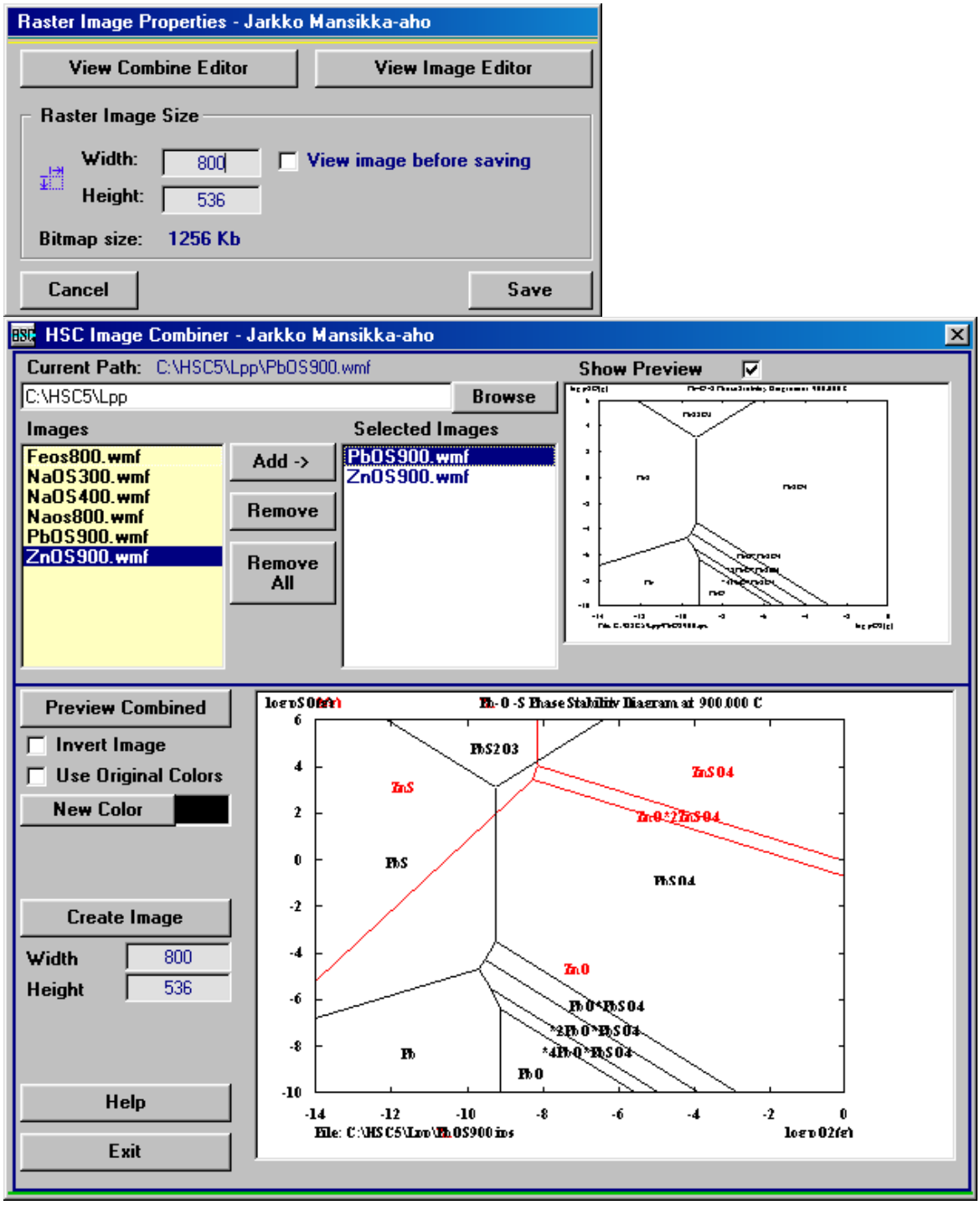
The new Drawing Toolbar may be used to draw basic graphical objects (lines, arrows, rectangles, ellipses) in HSC diagrams. These shapes may be used, for example, to illustrate experimental conditions. Versatile formatting options may be used to edit lines or add fill colour, line widths and styles.

Drawing Objects may be created and edited with the mouse or using the Object Editor, which enables very exact editing with numerical values. Drawing Objects may be fixed so that they can be used in all diagrams or they may be saved for later use in files.



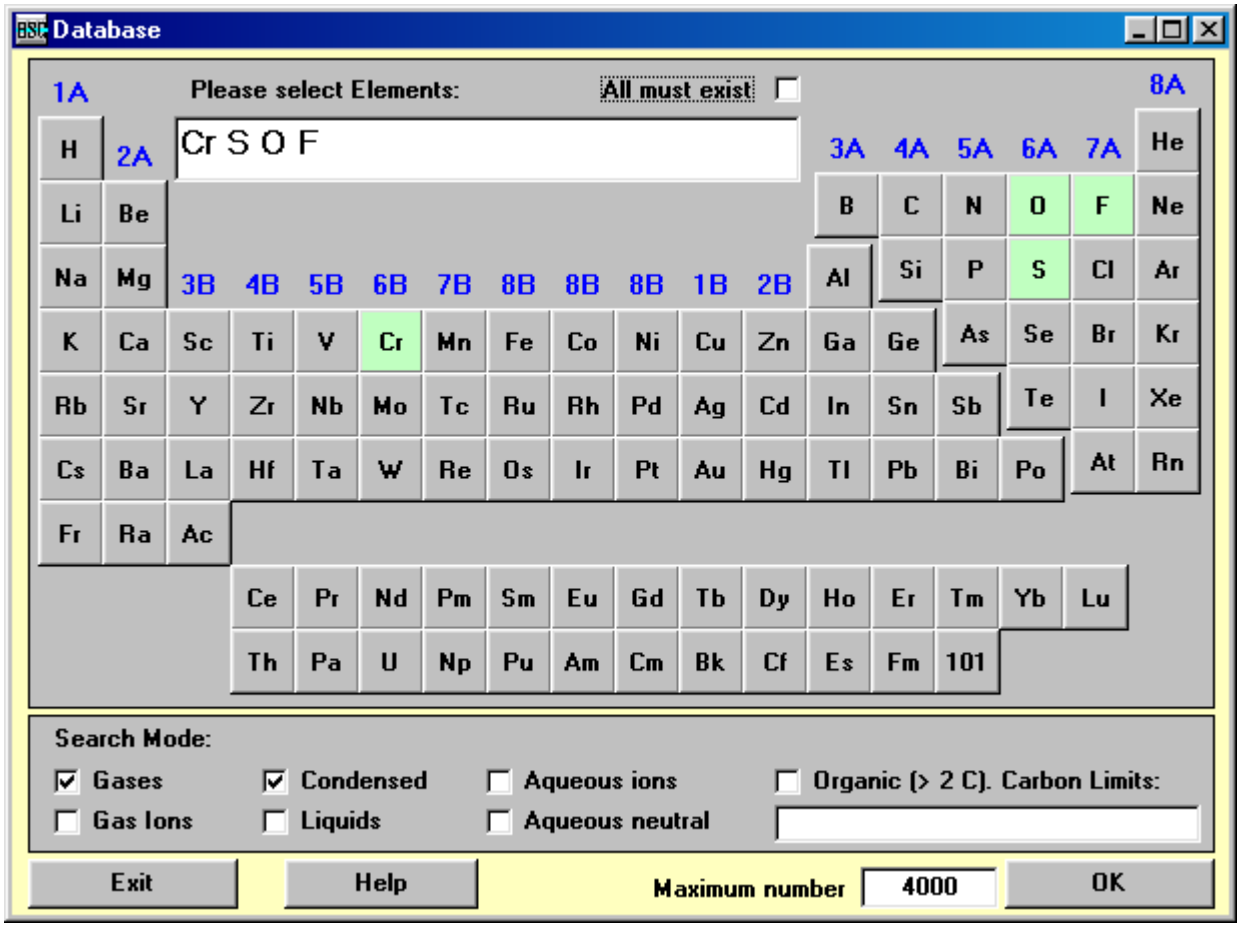
6.4. New Diagram Options

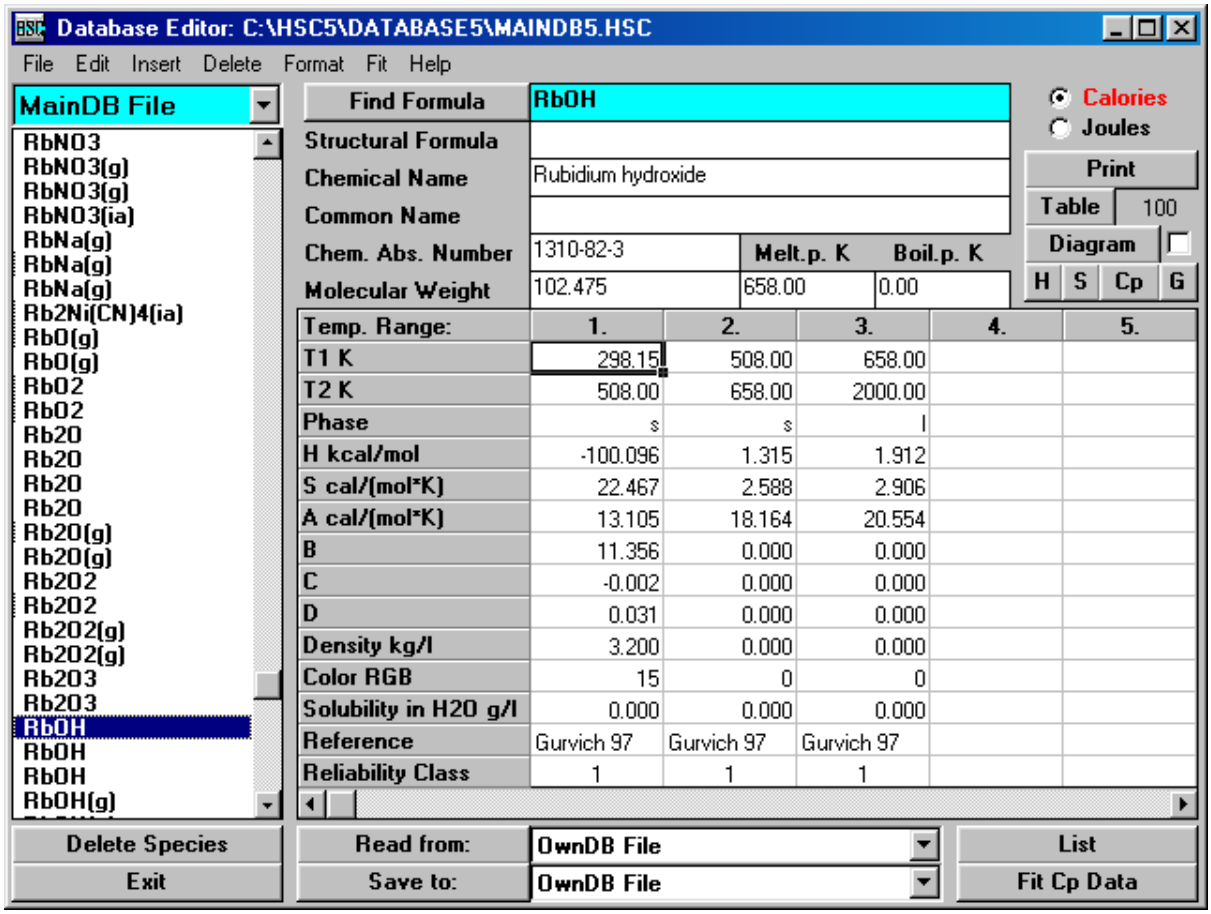
- HSC 4 was able to save diagrams using only one WMF format. Now more than 30 file formats are available, such as JPG, BMP, etc.
- Diagrams may also be edited using the new HSC Image Editor.
- Several diagrams may be combined with the new HSC Image Combiner if the same X- and Y-scales have been used.
- There is a new Diagram Grid format option as well as some new formatting options for diagram curves.



6.5. Larger Database with new Options

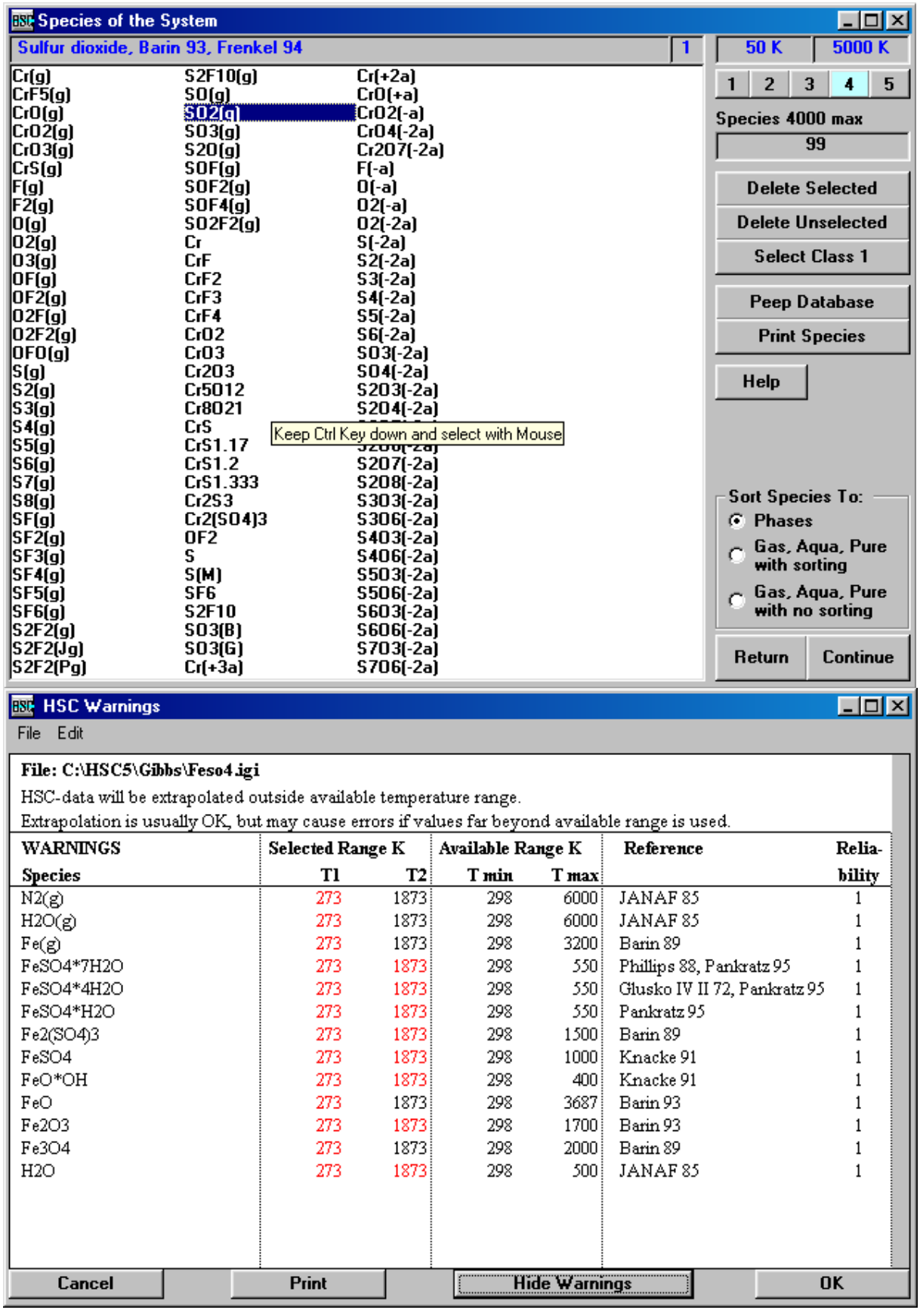
- The number of species in the database has been increased from 15000 to more than 17000. The quality of the database has been improved and the temperature ranges of the available data have also been expanded; more than 5000 changes have been made.
- New water data at pressures from 0.01 - 1000 bar are now available.
- Limitation of 2000 species has been removed from the Search routine.
- New Search mode has been added (All elements must exist).
- New fast Table and Diagram routines have been added to Database Editor.
- Several other small improvements have also been made.





6.6. Improved Equilibrium Module

- Calculation reliability has been improved in many of the test cases.
- New database search options without the limit of 2000 species.
- New Species Name display added to the database search routine.
- New Warnings routine for temperature range extrapolation.
- Small fixes e.g. species name length increased from 20 to 24 characters.


Species of the System
Sulfur dioxide, Barin 93, Frenkel 94
1
50 K
5000 K
1 2 3 4 5
Species 4000 max
99
Delete Selected
Delete Unselected
Select Class 1
Peep Database
Print Species
Help
Cr(g) CrF5(g) CrO(g) CrO2(g) CrO3(g) CrS(g) F(g) F2(g) O(g) O2(g) O3(g) OF(g) OF2(g) O2F(g) O2F2(g) OFO(g) S(g) S2(g) S3(g) S4(g) S5(g) S6(g) S7(g) S8(g) SF(g) SF2(g) SF3(g) SF4(g) SF5(g) SF6(g) S2F2(g) S2F2(Jg) S2F2(Pg)
S2F10(g) SO(g) SO2(g) SO3(g) S2O(g) SOF(g) SOF2(g) SOF4(g) SO2F2(g) Cr CrF CrF2 CrF3 CrF4 CrO2 CrO3 Cr2O3 Cr5O12 Cr8O21 CrS CrS1.17 CrS1.2 CrS1.333 Cr2S3 Cr2(SO4)3 OF2 S S(M) SF6 S2F10 SO3(B) SO3(G) Cr(+3a)
Cr(+2a) CrO(+a) CrO2(-a) CrO4(-2a) Cr2O7(-2a) F(-a) O(-a) O2(-a) O2(-2a) S(-2a) S2(-2a) S3(-2a) S4(-2a) S5(-2a) S6(-2a) SO3(-2a) SO4(-2a) S2O3(-2a) S2O4(-2a)
Keep Ctrl Key down and select with Mouse
S2O6(-2a) S2O7(-2a) S2O8(-2a) S3O3(-2a) S3O6(-2a) S4O3(-2a) S4O6(-2a) S5O3(-2a) S5O6(-2a) S6O3(-2a) S6O6(-2a) S7O3(-2a) S7O6(-2a)
Sort Species To:
Phases
Gas, Aqua, Pure with sorting
Gas, Aqua, Pure with no sorting
Return
Continue
HSC Warnings
File Edit
File: C:\HSC5\Gibbs\Feso4.igi
HSC-data will be extrapolated outside available temperature range.
Extrapolation is usually OK, but may cause errors if values far beyond available range is used.
WARNINGS
Species
Selected Range K
T1
T2
Available Range K
T min
T max
Reference
Relia-bility
N2(g) 273 1873 298 6000 JANAF 85 1
H2O(g) 273 1873 298 6000 JANAF 85 1
Fe(g) 273 1873 298 3200 Barin 89 1
FeSO4*7H2O 273 1873 298 550 Phillips 88, Pankratz 95 1
FeSO4*4H2O 273 1873 298 550 Glusko IV II 72, Pankratz 95 1
FeSO4*H2O 273 1873 298 550 Pankratz 95 1
Fe2(SO4)3 273 1873 298 1500 Barin 89 1
FeSO4 273 1873 298 1000 Knacke 91 1
FeO*OH 273 1873 298 400 Knacke 91 1
FeO 273 1873 298 3687 Barin 93 1
Fe2O3 273 1873 298 1700 Barin 93 1
Fe3O4 273 1873 298 2000 Barin 89 1
H2O 273 1873 298 500 JANAF 85 1
Cancel
Print
Hide Warnings
OK

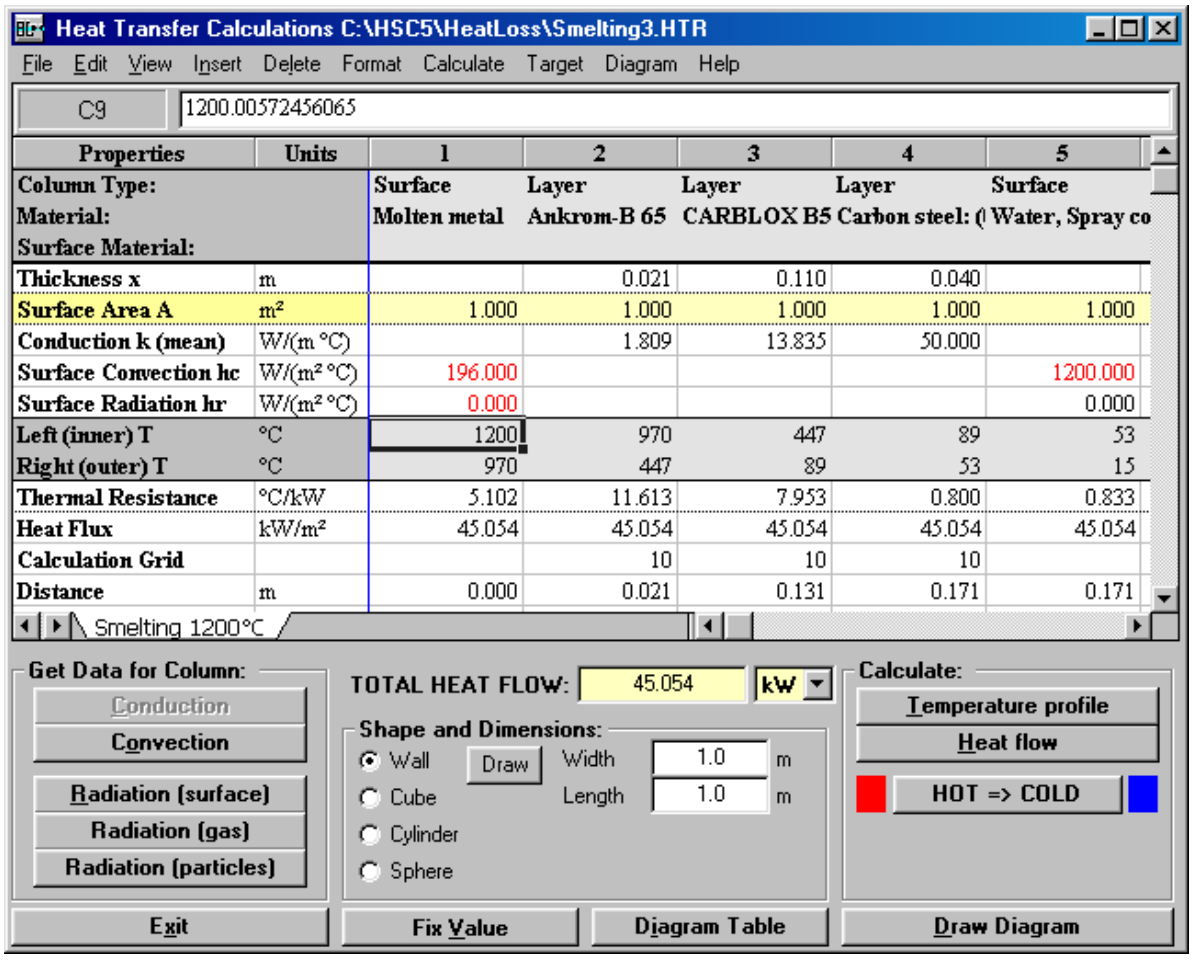
6.7. New Heat Loss Module

The new Heat Loss module may be used, for example, to estimate heat loss values needed in the Balance module. The user must first specify the wall layers, layer materials and thickness of these layers. Two basic types of calculations may be carried out:

1 **Temperature profile** with fixed heat loss and one temperature point.
2 **Heat Loss** with two fixed temperature points will return the heat loss but also the temperature profile.

The calculation routine handles conduction, convection and radiation properties as functions of temperature, but fixed values may also be used by selecting the value and pressing the Fix Value button. These fixed values are shown in red on the calculation sheet.

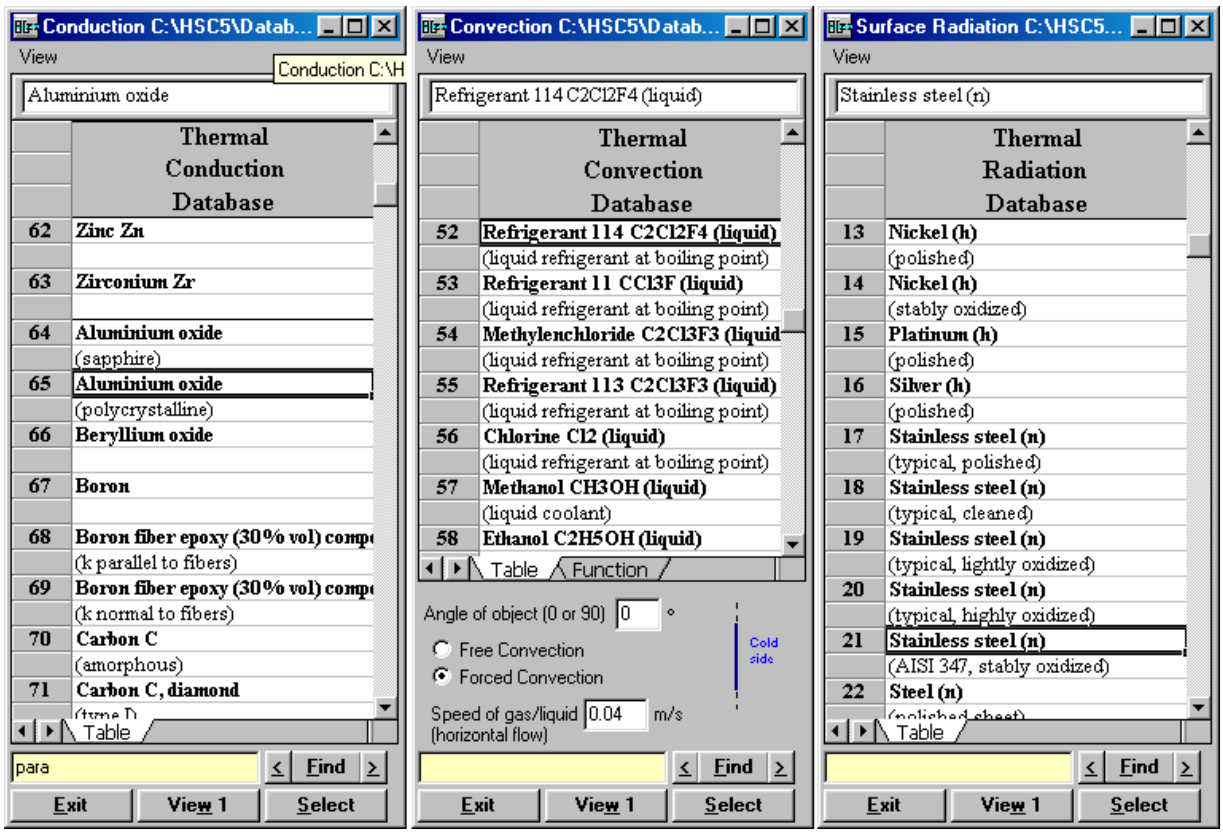
Temperature profile as well as some other user specified values may also be presented in graphical form. The Target Dialog may be used to find, for example, minimum layer thickness. The calculation specifications may be saved to files for later use.

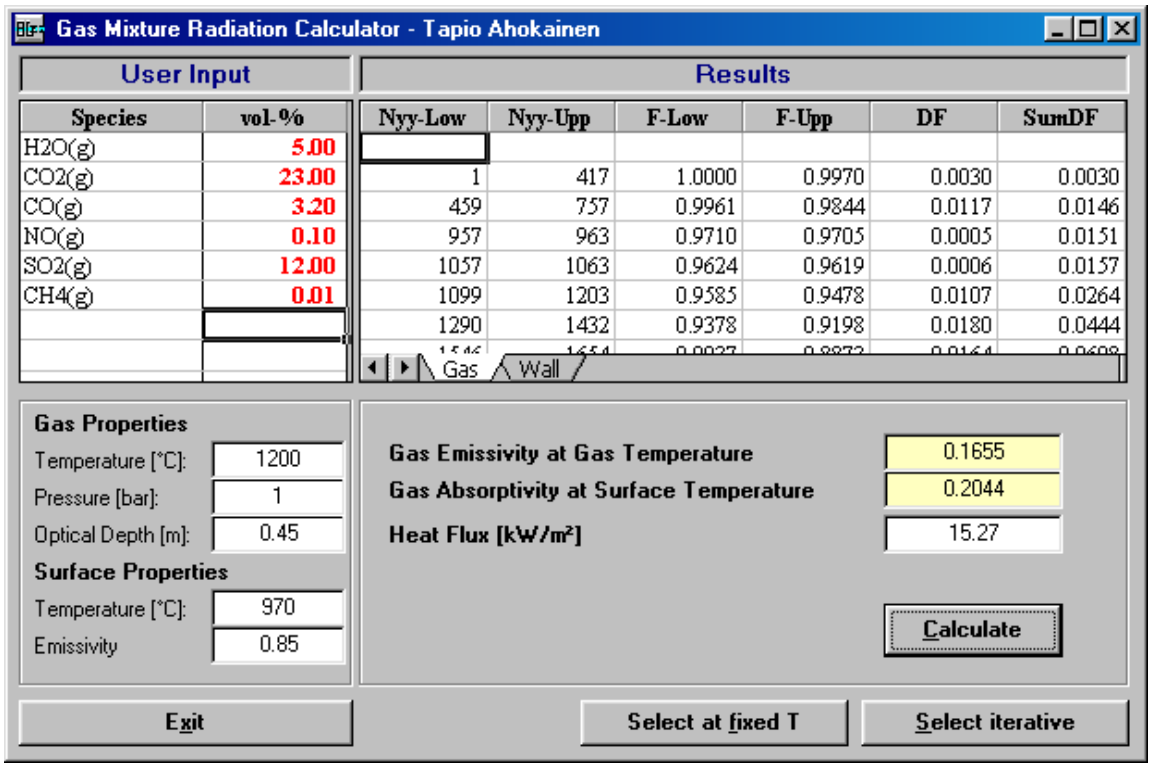


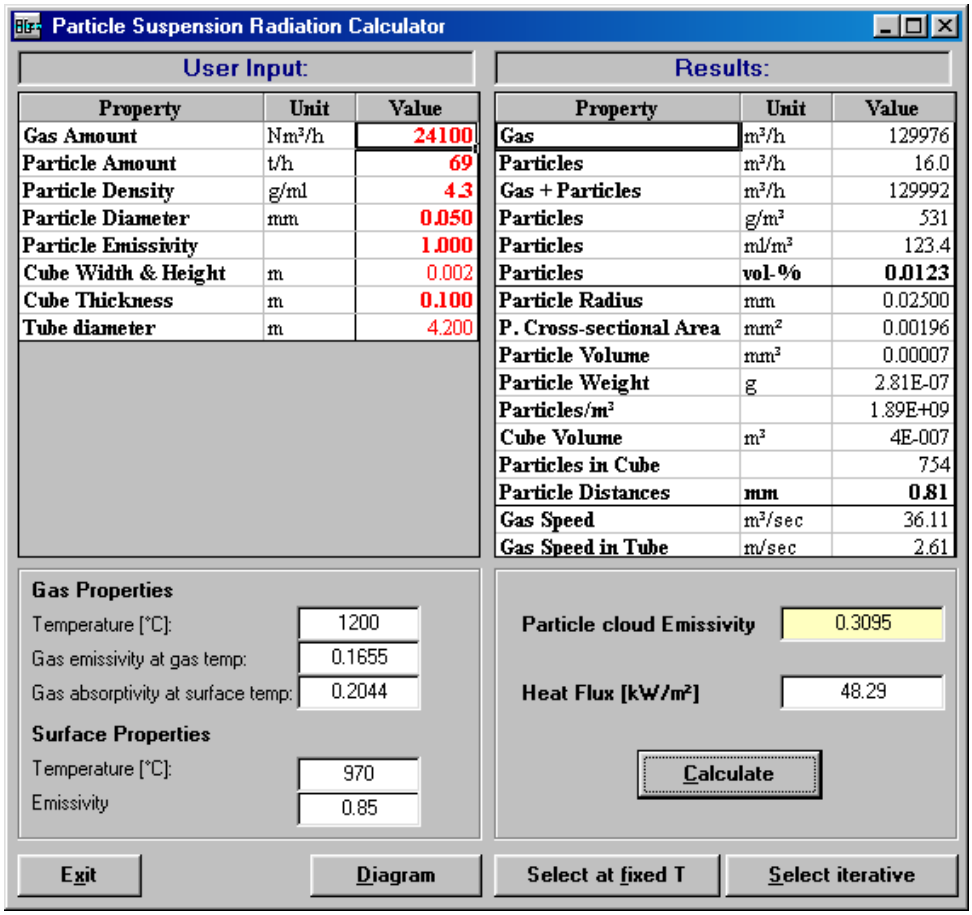
The Heat Loss module is integrated with three databases and two calculators:

- Conduction database with 718 substances
- Convection database with 111 substances and 4 functions
- Radiation database with 61 surface materials
- Gas Radiation Calculator with H2O, CO2, CO, NO, SO2 and CH4 data
- Particle Radiation Calculator.

The user may edit or add new data to these databases.

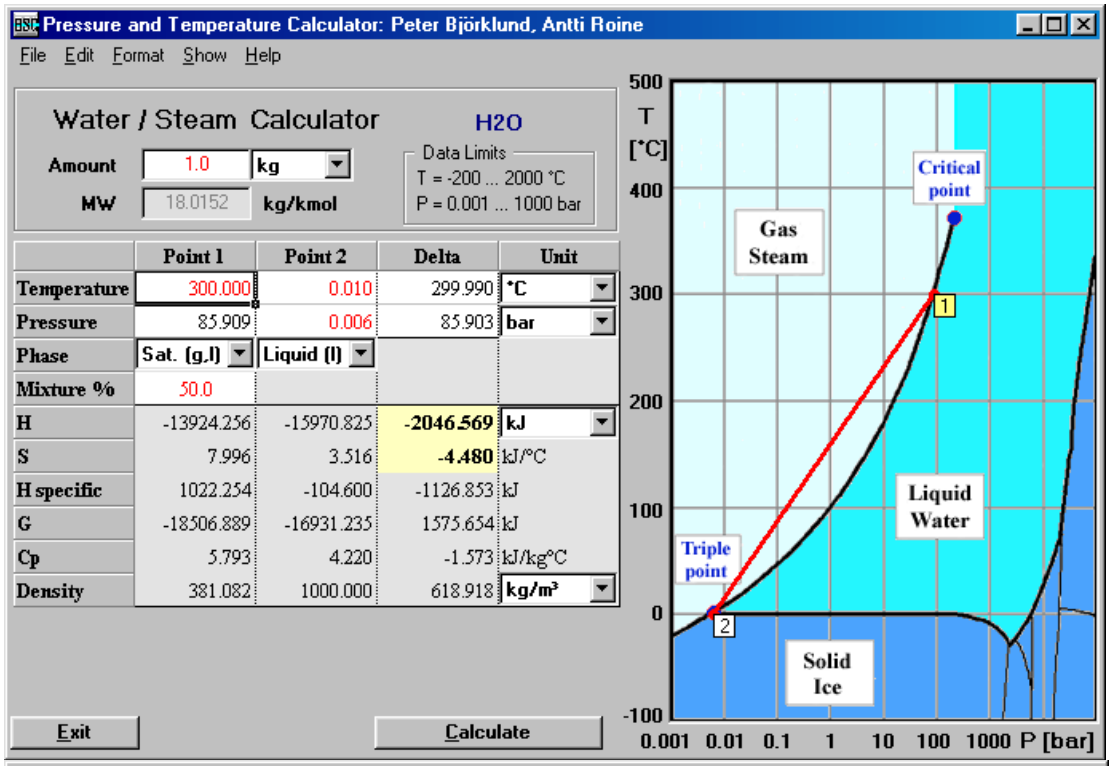

Conduction C:\HSC5\Datab...
View
Conduction C:\H
Aluminium oxide
Thermal Conduction Database
62 Zinc Zn
63 Zirconium Zr
64 Aluminium oxide
(sapphire)
65 Aluminium oxide
(polycrystalline)
66 Beryllium oxide
67 Boron
68 Boron fiber epoxy (30% vol) compo
(k parallel to fibers)
69 Boron fiber epoxy (30% vol) compo
(k normal to fibers)
70 Carbon C
(amorphous)
71 Carbon C, diamond
Table
para
Find
Exit
View 1
Select
Convection C:\HSC5\Datab...
View
Refrigerant 114 C2Cl2F4 (liquid)
Thermal Convection Database
52 Refrigerant 114 C2Cl2F4 (liquid)
(liquid refrigerant at boiling point)
53 Refrigerant 11 CCl3F (liquid)
(liquid refrigerant at boiling point)
54 Methylenchloride C2Cl3F3 (liquid
(liquid refrigerant at boiling point)
55 Refrigerant 113 C2Cl3F3 (liquid)
(liquid refrigerant at boiling point)
56 Chlorine Cl2 (liquid)
(liquid refrigerant at boiling point)
57 Methanol CH3OH (liquid)
(liquid coolant)
58 Ethanol C2H5OH (liquid)
Table
Function
Angle of object (0 or 90)
0
°
Free Convection
Forced Convection
Speed of gas/liquid (horizontal flow)
0.04
m/s
Cold side
Find
Exit
View 1
Select
Surface Radiation C:\HSC5...
View
Stainless steel (n)
Thermal Radiation Database
13 Nickel (h)
(polished)
14 Nickel (h)
(stably oxidized)
15 Platinum (h)
(polished)
16 Silver (h)
(polished)
17 Stainless steel (n)
(typical, polished)
18 Stainless steel (n)
(typical, cleaned)
19 Stainless steel (n)
(typical, lightly oxidized)
20 Stainless steel (n)
(typical, highly oxidized)
21 Stainless steel (n)
(AISI 347, stably oxidized)
22 Steel (n)
Table
Find
Exit
View 1
Select

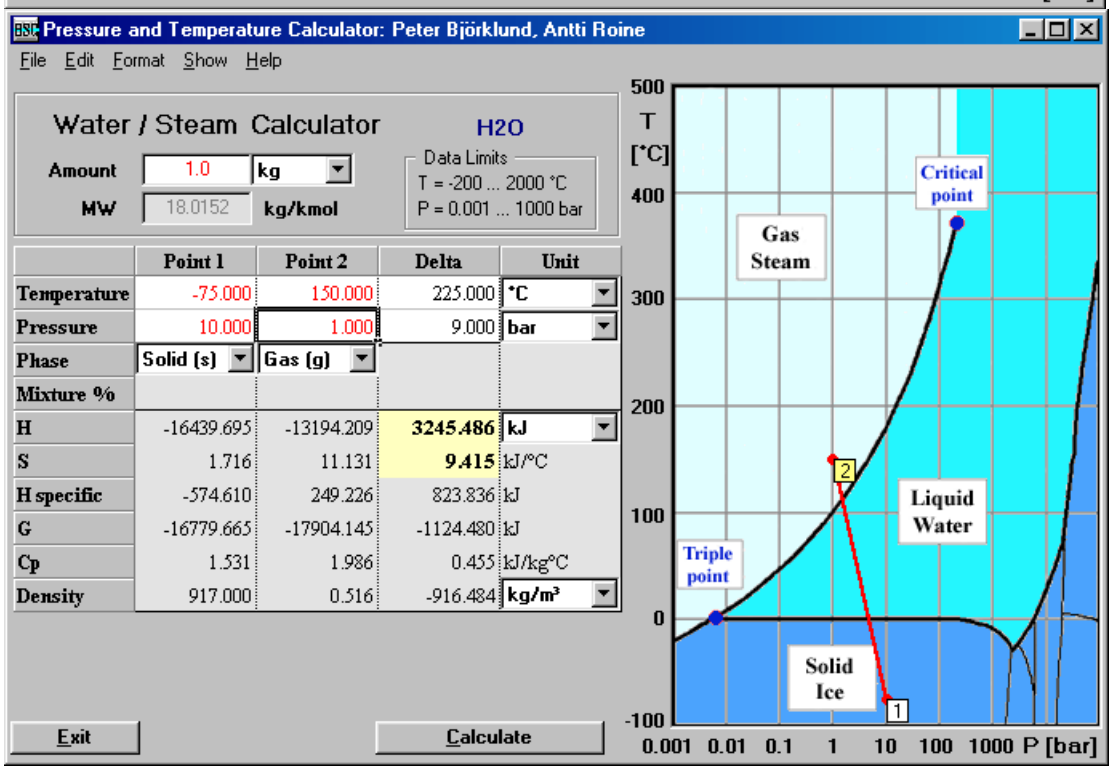

Gas Mixture Radiation Calculator - Tapio Ahokainen
User Input
Species vol-%
H2O(g) 5.00
CO2(g) 23.00
CO(g) 3.20
NO(g) 0.10
SO2(g) 12.00
CH4(g) 0.01
Results
Nyy-Low Nyy-Upp F-Low F-Upp DF SumDF
1 417 1.0000 0.9970 0.0030 0.0030
459 757 0.9961 0.9844 0.0117 0.0146
957 963 0.9710 0.9705 0.0005 0.0151
1057 1063 0.9624 0.9619 0.0006 0.0157
1099 1203 0.9585 0.9478 0.0107 0.0264
1290 1432 0.9378 0.9198 0.0180 0.0444
Gas
Wall
Gas Properties
Temperature [°C]: 1200
Pressure [bar]: 1
Optical Depth [m]: 0.45
Surface Properties
Temperature [°C]: 970
Emissivity 0.85
Gas Emissivity at Gas Temperature 0.1655
Gas Absorptivity at Surface Temperature 0.2044
Heat Flux [kW/m²] 15.27
Calculate
Exit
Select at fixed T
Select iterative


Particle Suspension Radiation Calculator
User Input:
Results:
Property Unit Value
Gas Amount Nm³/h 24100
Particle Amount t/h 69
Particle Density g/ml 4.3
Particle Diameter mm 0.050
Particle Emissivity 1.000
Cube Width & Height m 0.002
Cube Thickness m 0.100
Tube diameter m 4.200
Property Unit Value
Gas m³/h 129976
Particles m³/h 16.0
Gas + Particles m³/h 129992
Particles g/m³ 531
Particles ml/m³ 123.4
Particles vol-% 0.0123
Particle Radius mm 0.02500
P. Cross-sectional Area mm² 0.00196
Particle Volume mm³ 0.00007
Particle Weight g 2.81E-07
Particles/m³ 1.89E+09
Cube Volume m³ 4E-007
Particles in Cube 754
Particle Distances mm 0.81
Gas Speed m³/sec 36.11
Gas Speed in Tube m/sec 2.61
Gas Properties
Temperature [°C]: 1200
Gas emissivity at gas temp: 0.1655
Gas absorptivity at surface temp: 0.2044
Surface Properties
Temperature [°C]: 970
Emissivity 0.85
Particle cloud Emissivity 0.3095
Heat Flux [kW/m²] 48.29
Calculate
Exit
Diagram
Select at fixed T
Select iterative

6.8. New Steam Calculator Module

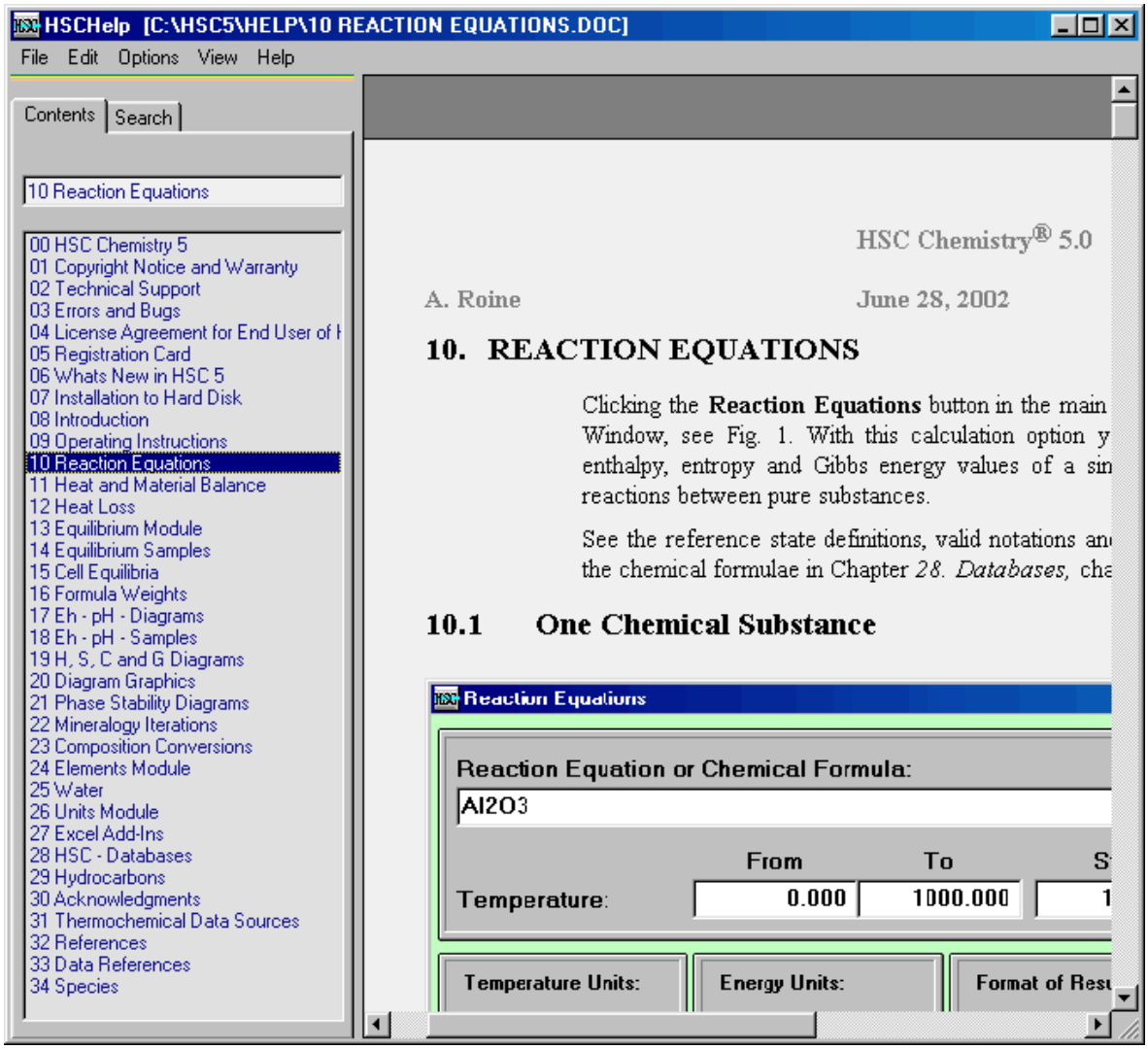
The new Steam Calculator module offers a much more convenient way to estimate enthalpies, entropies and densities of steam, water and ice than the traditional Steam Tables and Mollier Diagrams within 4 - 2273 K and 0.01 - 1000 bar. Steam enthalpies may be needed, for example, when calculating the heat and material balances of boilers or turbines.





6.9. New Help Routine

The new Help routine contains all the information, graphics and formulae of the HSC printed manual with convenient search, print, edit and save options.



6.10. Other Improvements

- The new folder structure divides HSC files into logical groups.
- HSC tables now also have Excel 97 and 2000 file support.
- The length of formulas has been increased from 20 to 24 characters in the EpH module.
- Form resize properties have been improved.
- Many small bug fixes and cosmetic adjustments etc.

6.11. New Windows Me, 2000 and XP Compatibility

- New installation routine.
- New compiler and programming tool versions used.
- HSC 5.0 is compatible with Windows 95, 98, NT, Me, 2000 and XP.

6.12. What's New in HSC 5.1 vs. 5.0

1. Database fixes:
   - HSC now finds all the F- and Zr- containing species.
   - Database Editor bug which sometimes created empty records to Own Database has been fixed.
   - Al(NO3)3(a) -> Al(NO3)3(ia)
   - AlF(+2a), AlF2(+a), AlF3(a) added
   - AmSO4(-a) -> Am(SO4)2(-a) (Typo in HSC database)
   - BF4Na S -34.728 replaced with NaBF4 S 34.728 cal/mol*K
   - (Co(NH3)5H2O)Cl3 -> Co(NH3)5*H2O*Cl3 (Duplicate)
   - CrS1.333 H 37.3 -> -37.3 kcal/mol (Typo in HSC database, Mills 74)
   - Cr2NiO4 replaced with NiO*Cr2O3 (duplicate)
   - FeCr2O4 replaced with Cr2FeO4 (duplicate)
   - HFe2O(-a) removed (Typo in Slop 98: HFe2O(-a) -> HFeO2(-a)
   - H2O Cp constant when T > 600 K
   - HO(g): typo in H and S values fixed
   - HOI(g) -> HIO: Reliability Class 1 -> 5 (Gas in Pankratz 95 ?). Compare to HIO(g)(Cor 90, Landolt 01)
   - I(-3a) -> I3(-a) (Typo in HSC database, Fabricius 94)
   - K3AlCl9 -> K3Al2Cl9 (Typo in Karapet 70)
   - K3Al2F6 -> K3AlF6 (Typo in Karapet 70)
   - MoF2 too stable: Reliability Class 2 -> 5 (Ruzinov 75)
   - MoO2(+2a), CH3COO(-a), CH3COOH added
   - Na2O melting point -1405K -> 1405 K
   - NaAlO2 replaced with Na2O*Al2O3 (duplicate)
   - Np(+4a) data NAGRA 91 -> Phillips 88
   - Np(OH)3(+a) H 313.983 -> -313.983 kcal/mol (Typo in HSC database)
   - Np(H2PO4)(+a) -> Np(H2PO4)2(+a) (Typo in HSC database)
   - PbSO4*PbO was removed (Enthalpy value typo in Bard 85)
   - (Pt(NH3)4)Cl2 -> Pt(NH3)4Cl2
   - (Pt(NH3)4)I2 -> Pt(NH3)4I2
   - Pu(+4a) data NAGRA 91 -> Phillips 88
   - PuO2(SO4)(-2a) -> PuO2(SO4)2(-2a) (Typo in HSC database)
   - SCN(-a) replaced with CNS(-a) (duplicate)
   - SrZr(Si2O7) was renamed SrZrSi2O7 (Huntelaar 95)
   - UO2(G) -> UO3(G): (Typo in HSC database, Phillips 88)
   - UO2.25 replaced with U4O9 (duplicate)
   - U3O5 deleted: (Typo in Samsonov 78, data seems to be for U3O8)
   - ZrF2 too stable: Reliability Class 1 -> 3 (Barin 77, Glushko 94, Landolt 00)
   - Some aqueous (a) species was changed to (ia).
   - Some new species
   - Small fix in "All must exist" option in Find Elements dialog.

2. Tpp- Module fixes:

- Scale and Print Dialog bug fixed.
- Diagram Area Color Dialog bug fixed.
- Print and Label dialogs with H, S and Cp diagrams.

3. Water-module:
   - Fixed: Small changes in Point 1 did not always effect the Phase option.
   - More density values at higher pressures and temperatures.

4. Equilibrium Module:
   - Species selection dialog: Sort mode bug fixed.
   - Automatic addition of N2(g).
   - Warning of SGM limitations.
   - Gibbs-routine fix: Diagram button may be pressed before the calculations are ready without crashing application.
   - Pic-routine improvement: Enter -key moves forvard after X- and Y-axis species selection.
   - Gibbs- and SGM-routines: Problem with phase transition data below 298.15 K fixed.

5. New "Key Word Find" Option in Database Menu finds, for example, all the species which contain the Key Word "benzene".

6. "Key Word Find" may also be used from Database Peep routine.

7. Clearer option captions in Database Menu.

8. More warning dialogs.
   - Peep Database dialog: Warning of high number of print pages.
   - Element Find Dialog: More Tool Tip Text.
   - Lpp module: Improved "Triple Point Outside Range" warning.

9. Several small fixes in Help- and Manual- files.

10. Maximum number of records in HSC databases was increased from 32767 to 2147483647 records.

11. "HSC DLL Tools" opens native HSC functions and database for use in Visual Basic applications and other programming environments.

12. "WNDTLS32.DLL could not be found" error message bug in HSC Help was fixed.

13. Heat and Material Balance Module:
   - Stream temperature link refresh bug was fixed.
   - "Calculate Recalc" option clears also columns 0 - S.
   - Arrow Graphical Object added.
   - New "Ideal Gas Density" option.

14. Some other small fixes. For example, HSC main menu flicker n some computers was fixed.
Many thanks for the feedback reports to all active HSC users!

6.13. What's New in HSC Chemistry 4.0

The new HSC version 4.0 contains several **new calculation modules**, **new properties** and a **larger database** with a lot of updated data. The familiar HSC style user interface has been maintained in order to minimize the training requirements of current HSC users. The new features can be summarized as follows:

1. The number of substances in the database has been increased from 11000 to more than 15000. A lot of old data has also been updated and extended.
2. Improved graphics, printing and format properties in all modules.
3. Target calculations in the Heat Balance module for automatic iterations.
4. Improved calculation reliability and speed in the Equilibrium module.
5. Eh-pH-diagrams with concentration and temperature lines.
6. A new Tpp-module for stability diagrams with partial pressure and temperature axes.
7. A new Diagram module for H-, S-, Cp-, G-, DH-, DG- T graphics.
8. A new Mineralogy module for fast conversion between mineralogical and elemental compositions.
9. A new Element module with basic data of elements and graphics.
10. A new Units module with a useful units conversion calculator.
11. A lot of small fixes and tuning of properties based on user feedback.
12. New 32-bit HSC version for Windows 95, 98 and NT.

The following sections will give a idea of these new features in more detail.

Installation

The HSC 4.0 installation routine has been updated and is now compatible with Windows® 95, 98 and NT. However, system requirements are still quite reasonable.

Heat and Material Balances

Several new features have been added to the Heat and Material Balance module:

1. The new **Target calculation** feature can be used to iterate sequential variable values in order to reach certain target values. For example, the user can set the zero heat balance as a target and find out the feed amount which satisfies the given target condition.
2. The **graphics feature** enables the user to draw diagrams of heat balance calculation sheets. The user may easily select one variable and range for the x-axis and several others whose values are drawn on the diagram as a function of x-variable change.
3. The user can easily **import additional MS Excel® sheets** to the module. These sheets can be used to calculate input data for the INPUT-sheet or process results of the OUTPUT-sheet. Files can be saved in Excel format for further treatment of results.
4. Several small improvements and new properties. For example, the user can now resize the forms without step values. The printing capabilities have been improved, for example, the final temperature calculation results can also be printed now.

Equilibrium Calculations

Equilibrium Calculations is one of the most used modules in HSC software, therefore a lot of effort has been spent on improving it. For example:

1. The calculation reliability and speed of Gibbs solver is better than in the previous version.
2. The processing of Excel type activity formulae has been improved.
3. The species table form can easily be resized.
4. The diagrams can be printed in any size. A greater number of lines can be visualized simultaneously by increasing the height of the printed diagram.
5. The enthalpy of the reaction can be drawn on the diagram.
6. The maximum number of pure substances in the diagrams has been increased from 99 to 999.
7. This module now makes input-files for ChemSage 2, 3 and 4 versions.(ChemSage is a registered trademark of GTT-Technologies)

Formula Weights

The new feature of the formula weight calculator allows the user to specify the amount of the species in kilograms or moles. This enables the module to calculate the amounts of elements in addition to the compositions and formula weights.

Tpp Phase Stability Diagrams

This new module allows you to draw phase stability diagrams with temperature as the x-axis and a selected partial pressure as the y-axis. Diagrams with partial pressures on both axes can also be drawn. Partial pressures of sulfur, oxygen, sulfur dioxide, carbon monoxide, etc. can be used depending on the selected system.

These diagrams can be used, for example, to estimate what kinds of phases prevail in the roasting furnace in different conditions or to evaluate which condensed substances may become stable when the process gas temperature decreases.

Eh - pH - Diagrams

Eh-pH-diagrams are used to estimate the prevailing species in aqueous solutions as a function of pH and chemical potential. A completely new option has been added to this module. The new features can be summarized in the following list:

1. The new routine can be used to combine several diagrams with different concentrations, temperatures or main elements into a single diagram. The traditional concentration diagrams are widely used, but more special temperature and main element diagrams may also give valuable information.
2. The possibility to change the size of printed diagrams is also very useful when there are several small stability areas in the same diagram.
3. The selection of different electrode potential scales is also a useful new feature, where Hydrogen, Calomel and Ag/AgCl-scales can be used.
4. Improved calculation reliability.
5. The calculation system specification can easily be modified with the user's own Gibbs energy data. These modifications can be saved for later use.

H, S, C and G - Diagrams

The new diagram module can be used to draw several different types of thermochemical diagrams. The same new versatile graphics and printing features are included as in the other modules. The main features can be summarized as follows:

1. Eight different diagram types can be drawn as a function of temperature:
    - H Enthalpy (total)
    - H Enthalpy (latent)
    - S Entropy
    - Cp Heat Capacity
    - G Gibbs Energy
    - DH
    - DS
    - DG (Ellingham diagrams)
2. Several species can be selected to the enthalpy diagrams simultaneously to compare total or latent enthalpies.
3. DG diagrams (Ellingham diagrams), offer a very fast way to compare the relative stabilities of substances. For example, you can find out which oxide or chloride compound is the most stable one. This information is useful when comparing the reduction and oxidation tendencies of different elements.
4. This module can also be used to compare the basic thermochemical data from different sources, in order to see the differences and select the best data for subsequent calculations.

Mineralogy Module

Composition conversions between substance (mineralogy) and elemental analyses are often needed in chemical R&D work. The new Mineralogy module easily converts mineralogical compositions into elemental compositions.

The conversion of the elemental composition of a substance into a mineralogical one is a more difficult task, for example, due to small analytical errors. This module offers three tools for converting elemental analyzes into mineralogical ones:

1. The **Solve method**, which uses matrix-algebra to solve the mineralogy. It is useful if the given amounts of elements fit the given substances exactly.
2. The **Automatic iterative method**, which fits the given elements to the given substances by changing the species contents to achieve the given elemental compositions.
3. The **Manual iterative method**, which may be needed especially if the same element exists in several species.

Elements Module

The thermochemical behavior of species is based on the properties of elements. The location of the element in the periodic system tells us a lot about its chemical nature. The new Elements Module offers a fast way to compare the basic properties of elements in tabular and graphical format.

The database contains data on 56 different properties of elements. As in other HSC modules, the user is permitted to modify and add new data to this database according to personal requirements.

Units Module

Traditionally, several types of energy, temperature, mass and volume units have been used in thermochemical calculations. Therefore, some inconvenient conversions are needed to compare the results from different sources. The new Units Conversion module is an easy tool for fast unit conversions in thermochemical as well as other engineering fields. The specifications of this module can be summarized as follows:

1. Some 90 different quantities and 444 units are available. The user can easily add his/her own units and coefficients into the conversion calculator database.
2. The Units Module also offers data sheets for chemical constants, particle mesh sizes, air humidity and water pressure tables. The user can modify these tables according to personal requirements.

Database

The thermochemical database is an essential part of HSC Chemistry, because the accuracy of the calculation results of all HSC modules depends on the quality of the basic data in the integrated database. Considerable development work has been carried out, which can be summarized as follows:

1. The number of species in the database has been increased from 11000 to more than 15000. This data is not critically evaluated, but gives fast access to data and references, which can be found from literature.
2. The quality of the database has been improved and the number of unnecessary duplicate species has been decreased.
3. Further supporting data, such as structural formulae, chemical names, common names, CAS numbers, melting points, boiling points, etc. have been added to the database.
4. HSC 4 uses the same database format as HSC 3, therefore, the user's own databases can also be used with the new HSC 4.0.
5. The search procedure for species in "Database Editor" and "Show Database" windows has been improved. The species lists now show the location of the closest match if the given formula is not found in the database.
6. A direct link to the graphics module has been added to the Cp data-fitting option. This allows the easy comparison of experimental and fitted data.
7. **Important Note**: The main reason for the small differences with HSC 3 and 4 calculation results is the new data in the HSC 4 database.

General improvements

The graphics, printing and format properties as well as resizing capabilities of the table forms have been improved in most calculation modules. This makes it easier to produce high quality hard copies of the results.

Numerous minor improvements and adjustments have been made which are not always visible. However, they will make the life of the HSC user easier. This work has been based mainly on feedback from HSC users.