The *Solution* module

Use ***Solution*** to enter non-ideal mixing properties in your private solution databases.

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(continued)

NOTE: Use the HOME/Pos1 button to return to the table of contents.

Table of Contents (continued)

NOTE: Use the HOME/Pos1 button to return to the table of contents.

The *Solution* module

Click on ***Solution*** in the main ***FactSage*** window.

Toolbars and menus

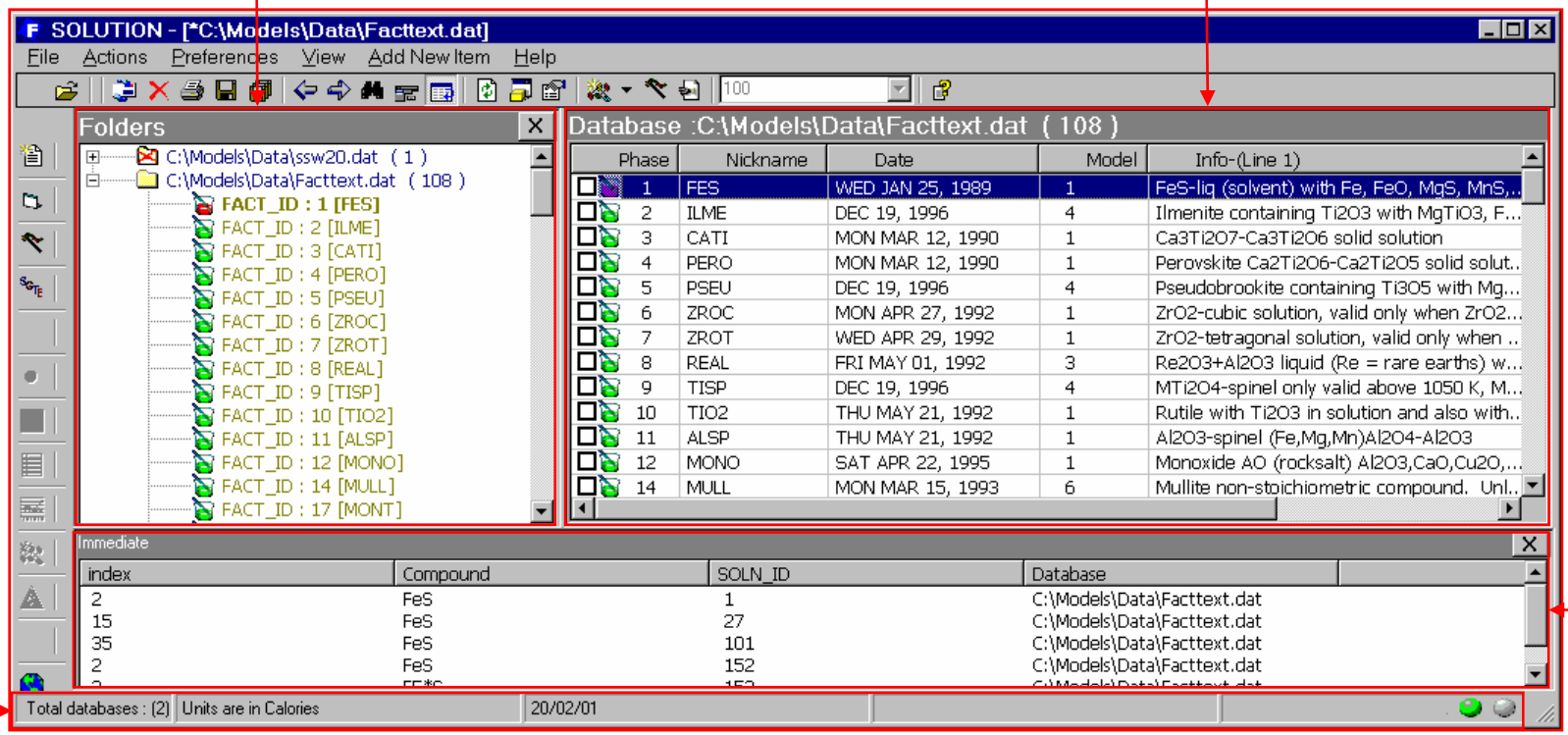
The following two slides explain the use of the ***Solution*** module from its Main window. There are three main sub-windows from which information on a the phase tree of a database, detailed information on particular data items, and results of data searches can be read.

Furthermore there are several option menus and toolbars available.

Solution Main Window

Treeview Window lists all the databases, solution phases and functions

Information Window provides detailed information on the current item selected in the Treeview Window

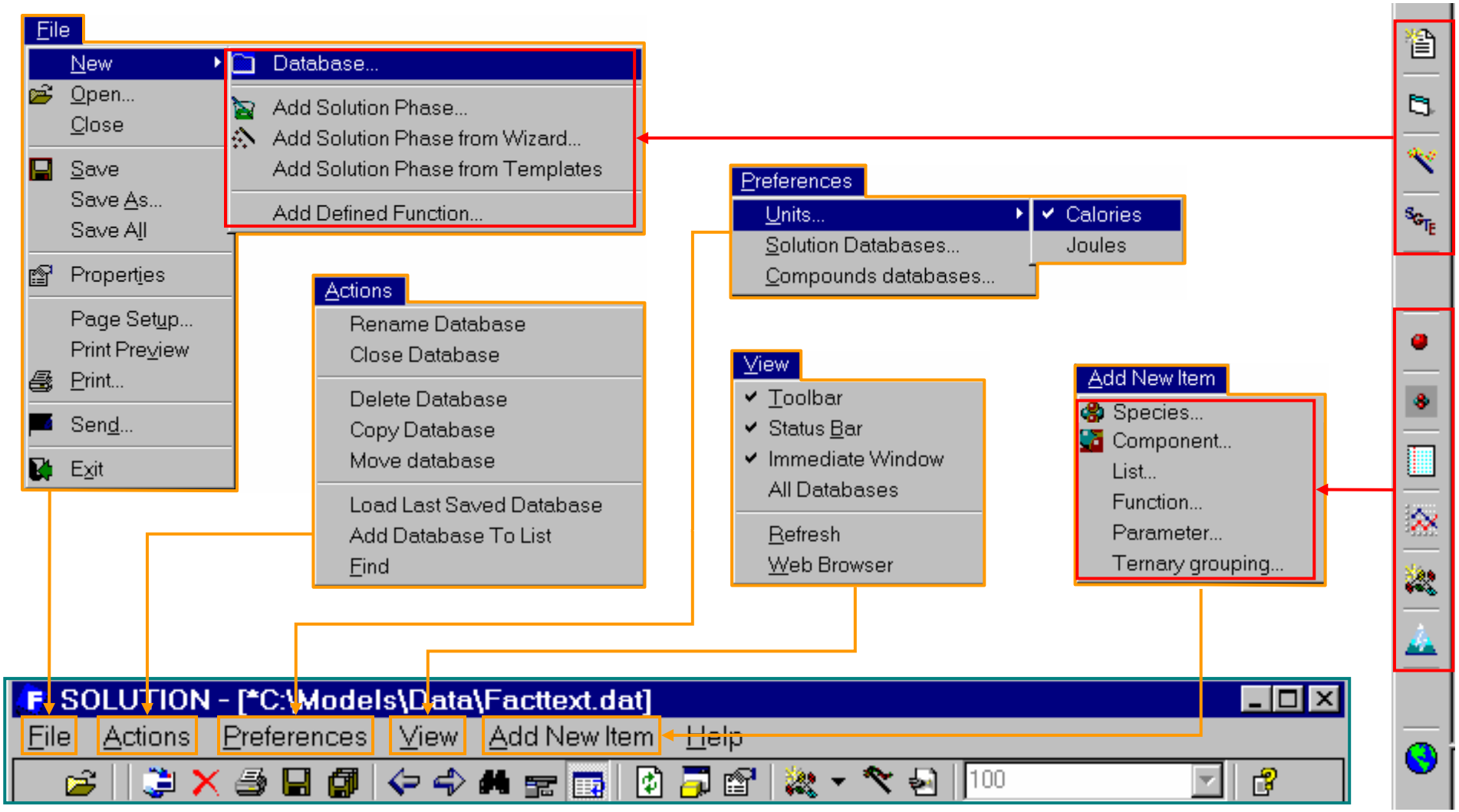


Status Bar: indicate the actual state of your session

Immediate Window displays search results, click on an item and the treeview jumps to it

The ***Solution*** program permits you to enter parameters defining the Gibbs Energy Surfaces of non-ideal solutions. (Data management: creating, listing, loading and modifying databases.)

Toolbars and menus



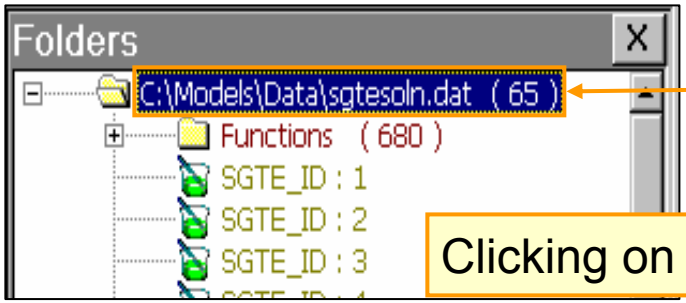
Features of the program are accessible through program menu at the top of the window, toolbars and also context menus available by right-clicking on various objects.

Obtaining information on an existing database

The following three slides show how information on a particular database that already exists can be obtained using the features of the ***Solution*** module.

As an example the **SGTE** solution database was used.

List of **Solution** Phases



To display the list of solution phases in the "SGTESOLN.dat" database, click on the specific database in the code explorer Treeview

Clicking on the column heading sorts the list on that field

Database :C:\Models\Data\sgtesoln.dat (65)

Phase	Nickname	Date	Model	Info-(Line 1)	Info-(Line 2)
1	<None>	MAY 28, 1998	20	FCC_A1	This is also the MC(1-x) carbide or nitride!
2	<None>	MAY 28, 1998	20	BCC_A2	
3	<None>	MAY 28, 1998	20	HCP_A3	o the M2C carbide and M2N nitride !
4	<None>	APR 23, 1998	20	CBCC_A12	-Mn phase !
5	<None>	APR 23, 1998	20	CUB_A13	-Mn phase !
6	<None>	APR 23, 1998	20	SIGMA	
7	<None>	APR 24, 1998	20	P_PHASE	
8	<None>	APR 24, 1998	20	MU_PHASE	
9	<None>	APR 24, 1998	20	R_PHASE	
10	<None>	APR 24, 1998	20		
11	<None>	APR 24, 1998	20		
12	<None>	APR 23, 1998	20		

Edit
View
Copy
Delete
Properties

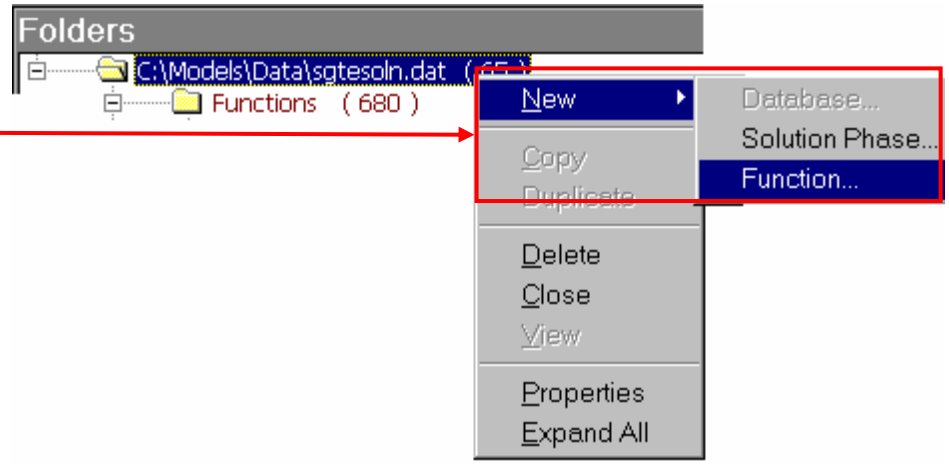
Right-click on an item for a context sensitive menu (other options if many items are selected)

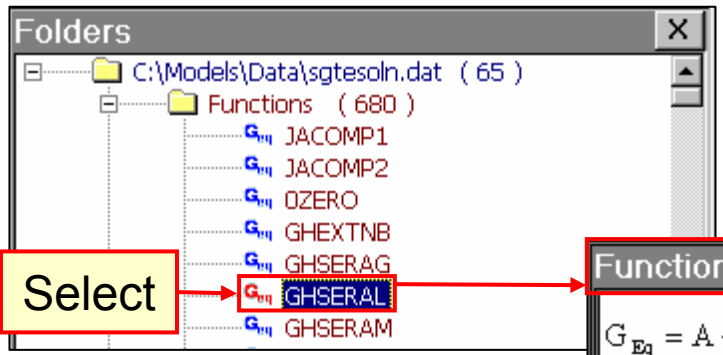
Columns displayed are:

- **Phase number**: becomes the solution phase number SOLN_N when the database is used by ***Equilib***;
- **Nickname**: appears when the database is used by ***Equilib***;
- **Date** of creation of the phase;
- Solution **model**: code number for the phase type (e.g., Compound Energy Model);
- **Two lines** of description.

List of Gibbs Energy Expression of **GHSERAL** Function

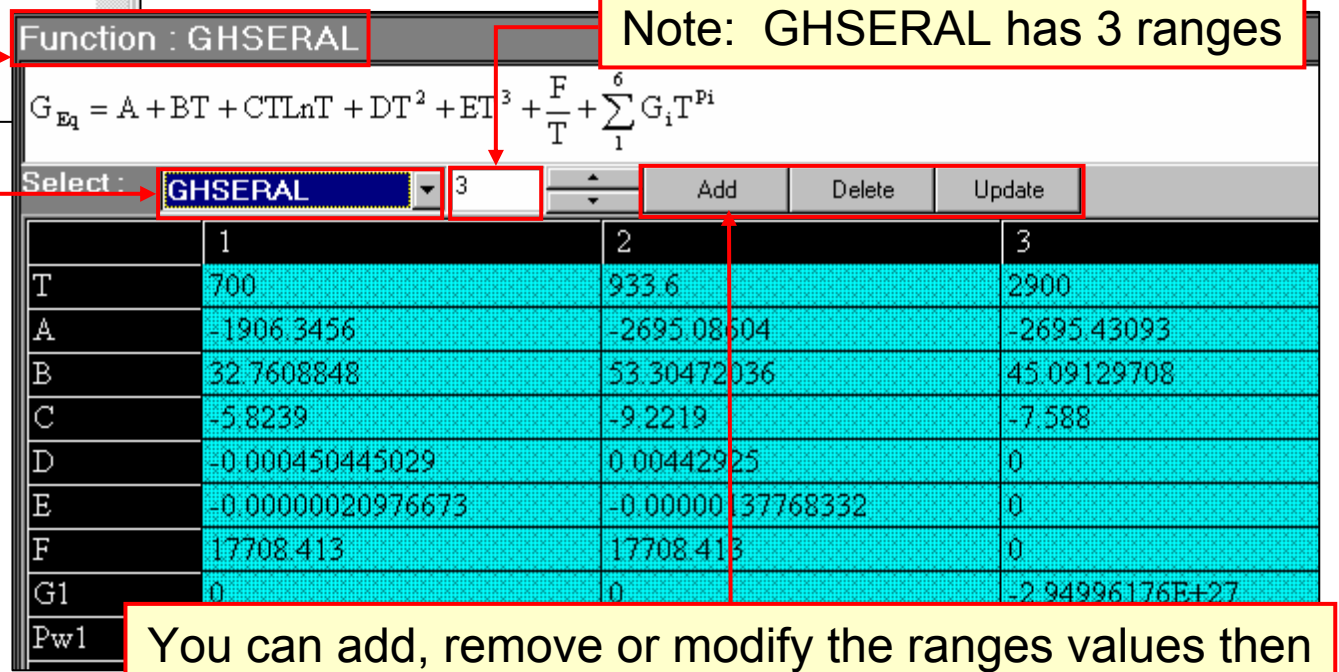
Context sensitive menu:
Entry of a new function can be done by right-click on the corresponding database.
Click on «New» and «Function».



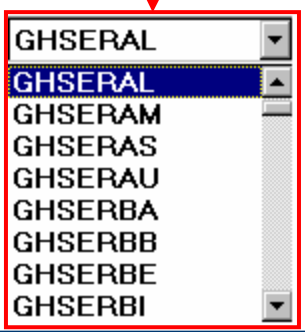


Select

Note: GHSERAL has 3 ranges

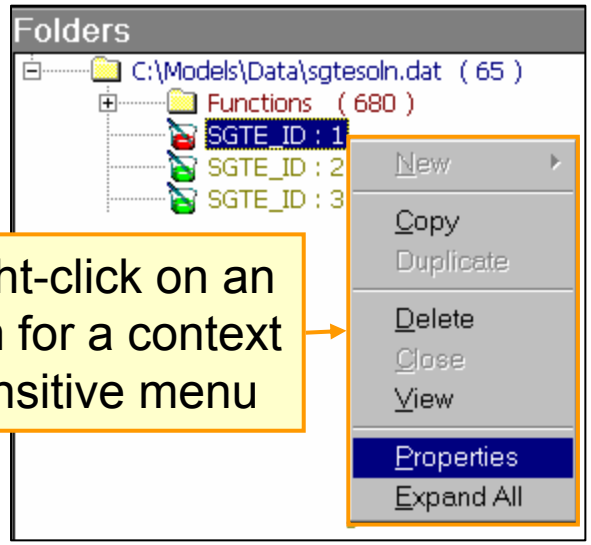


You can scroll for other functions



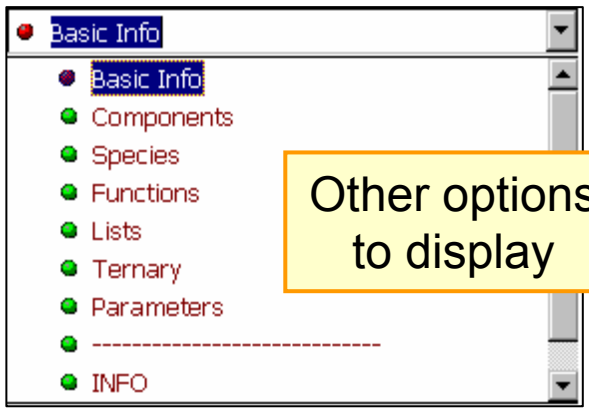
You can add, remove or modify the ranges values then press on the update button to save all modifications.

Inspection of the phase SGTE_1 alias FCC_A1

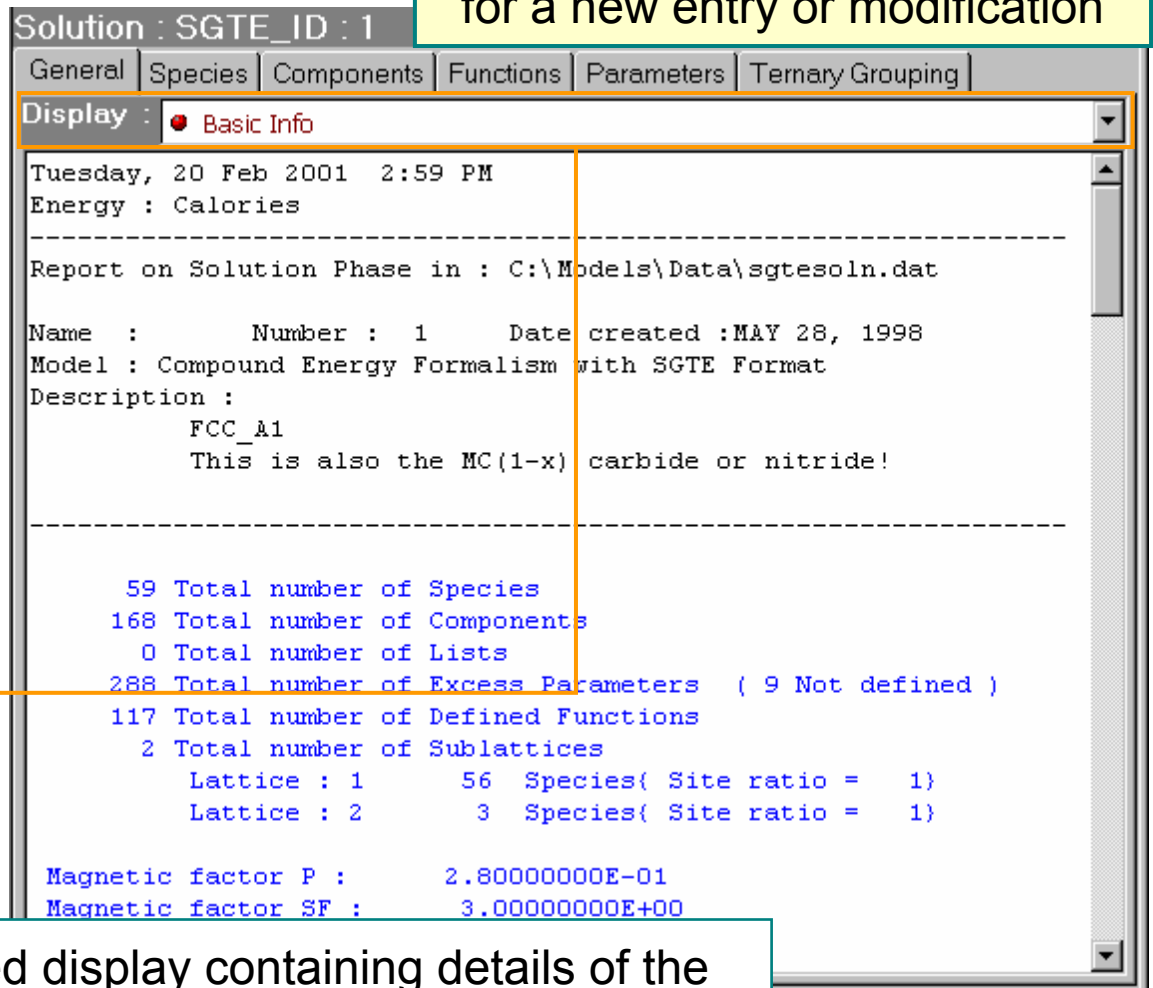


Right-click on an item for a context sensitive menu

Your solution phase is now ready for a new entry or modification



Other options to display



The information window is a tabbed display containing details of the currently selected phase in the Treeview Window. Number of tabs displayed and their contents depend upon the solution model chosen.

Generation of a database (Example: $NaCl\text{-}SrCl_2$ liquid)

The following fourteen slides show how a private solution database is built.

As an example the entry of the data for the liquid phase in the $NaCl\text{-}SrCl_2$ system are used.

The basic data that need to be stored are explained first and in the following thirteen slides the entry of each data item is shown in detail.

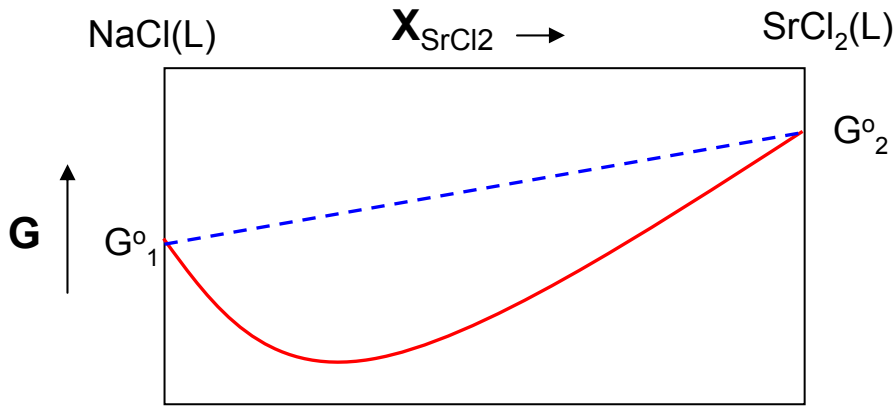
(This phase has also already been stored in Factdata/Examsoln.dat under the phasename LIQS. You may open and edit this file.)

Example of use of *Solution* program Parameter Entry for a simple **Type-1 Polynomial Solution**

Description: Thermodynamic data for binary liquid NaCl-$SrCl_2$ phase

Entry: Joules **Model:** Polynomial

Components	Index	G^o
NaCl	1	L From FACTBASE
SrCl2	2	L From FACTBASE



Gibbs energy: $G = (X_1G^o_1 + X_2G^o_2) + RT(X_1\ln(X_1) + X_2\ln(X_2)) + G^E$

Binary Excess mixing terms

$$\Delta H = X_1X_2(-11128.649) + X_1^2X_2(-9547.7573)$$

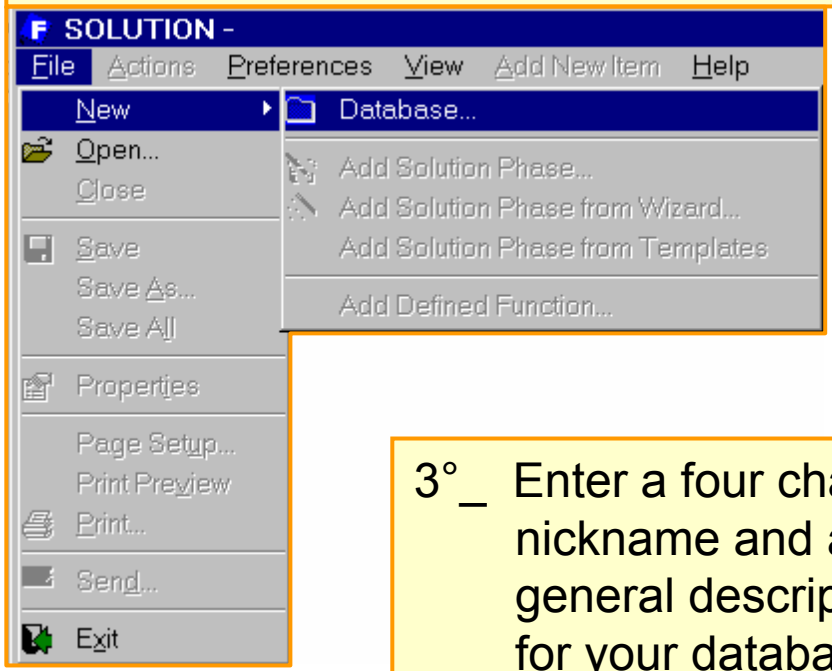
$$S^E = X_1X_2(-8.9242) + X_1^2X_2(-8.92971)$$

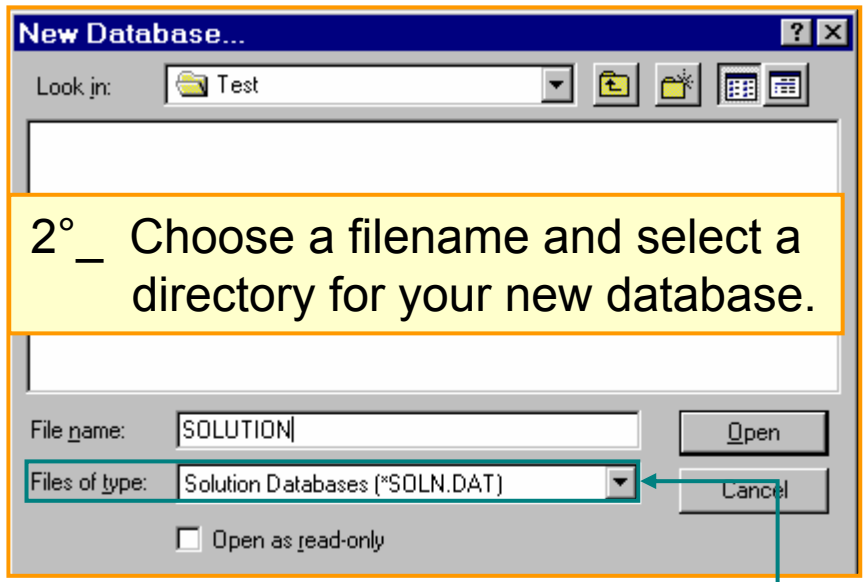
Hence:

$$G^E = X_1X_2(-11128.649 + 8.9242\,T) + X_1^2X_2(-9547.7573 + 8.92971\,T)$$

Creation of a Private Solution Database USERSOLN

1°_ Click on «New»; «Database…» from the «File» menu.

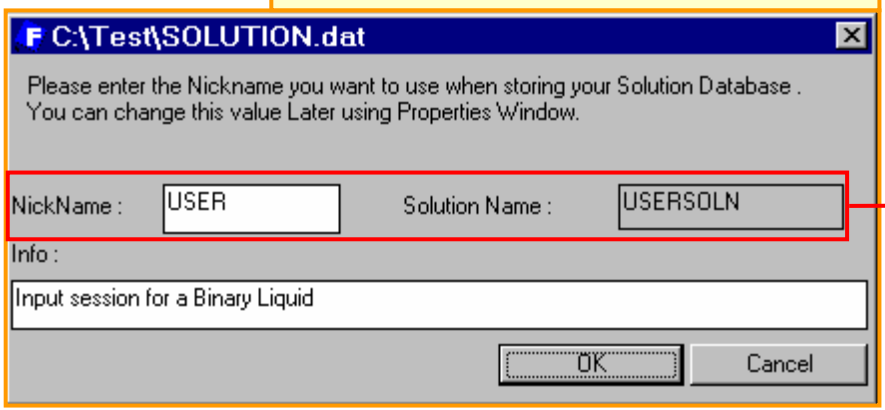


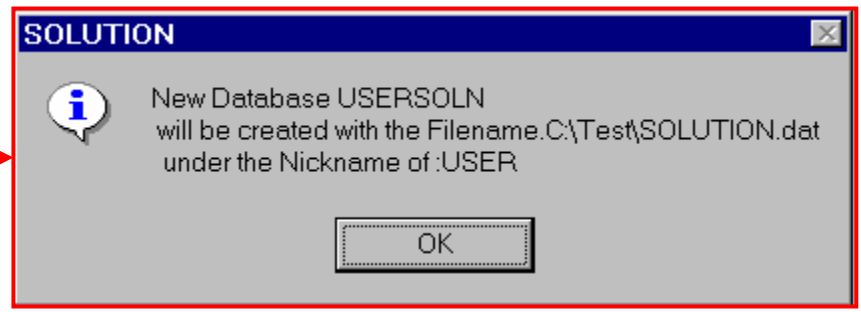


2°_ Choose a filename and select a directory for your new database.

Different database formats

3°_ Enter a four character nickname and a general description for your database (optional).

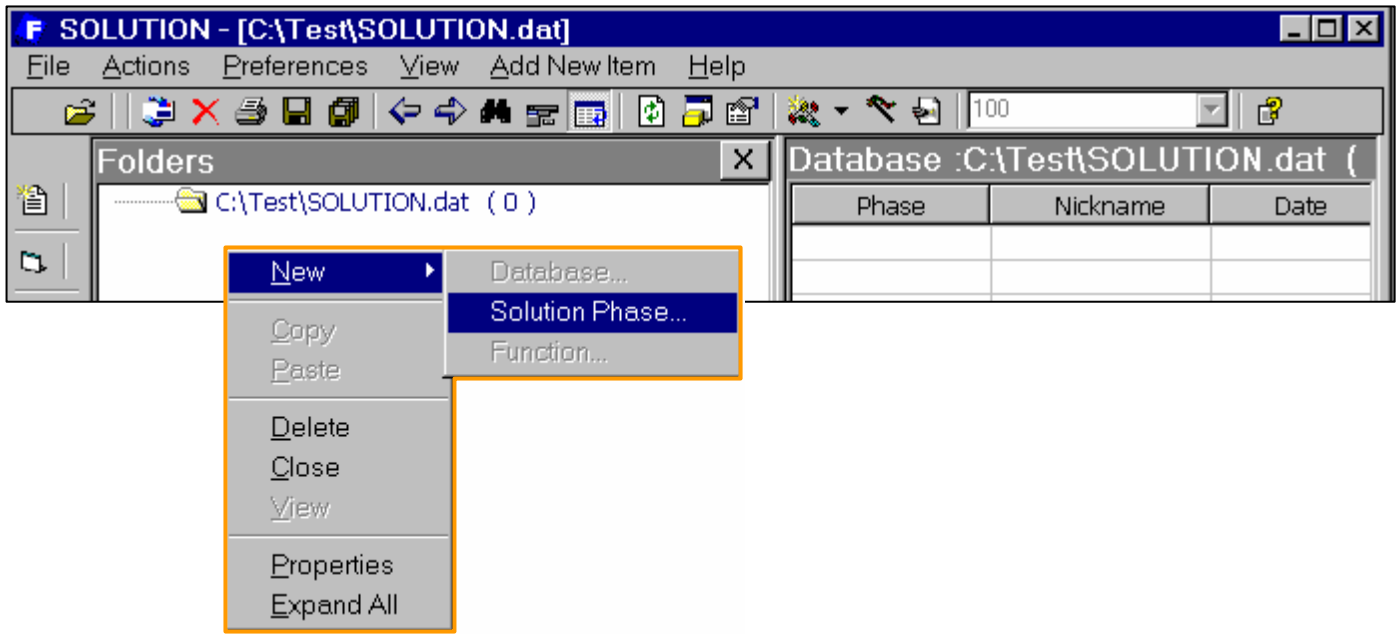




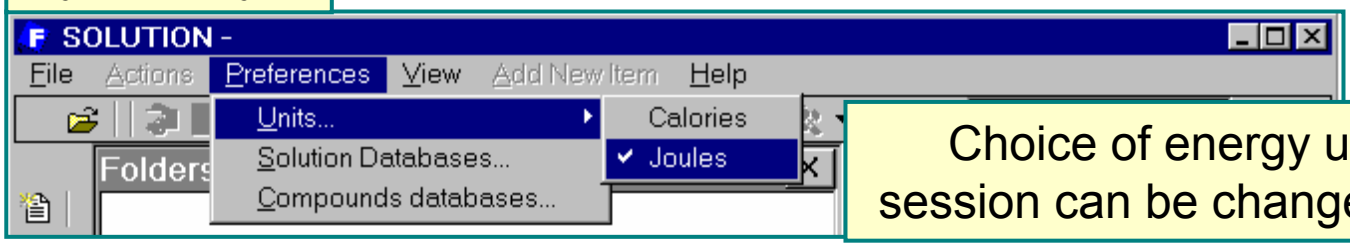
Creation of a **Solution Phase** (Entry for a Simple Polynomial Solution)

To create a solution phase:

1°_ Click on «New» and «Solution Phase…» from the «File» menu or the context sensitive menu



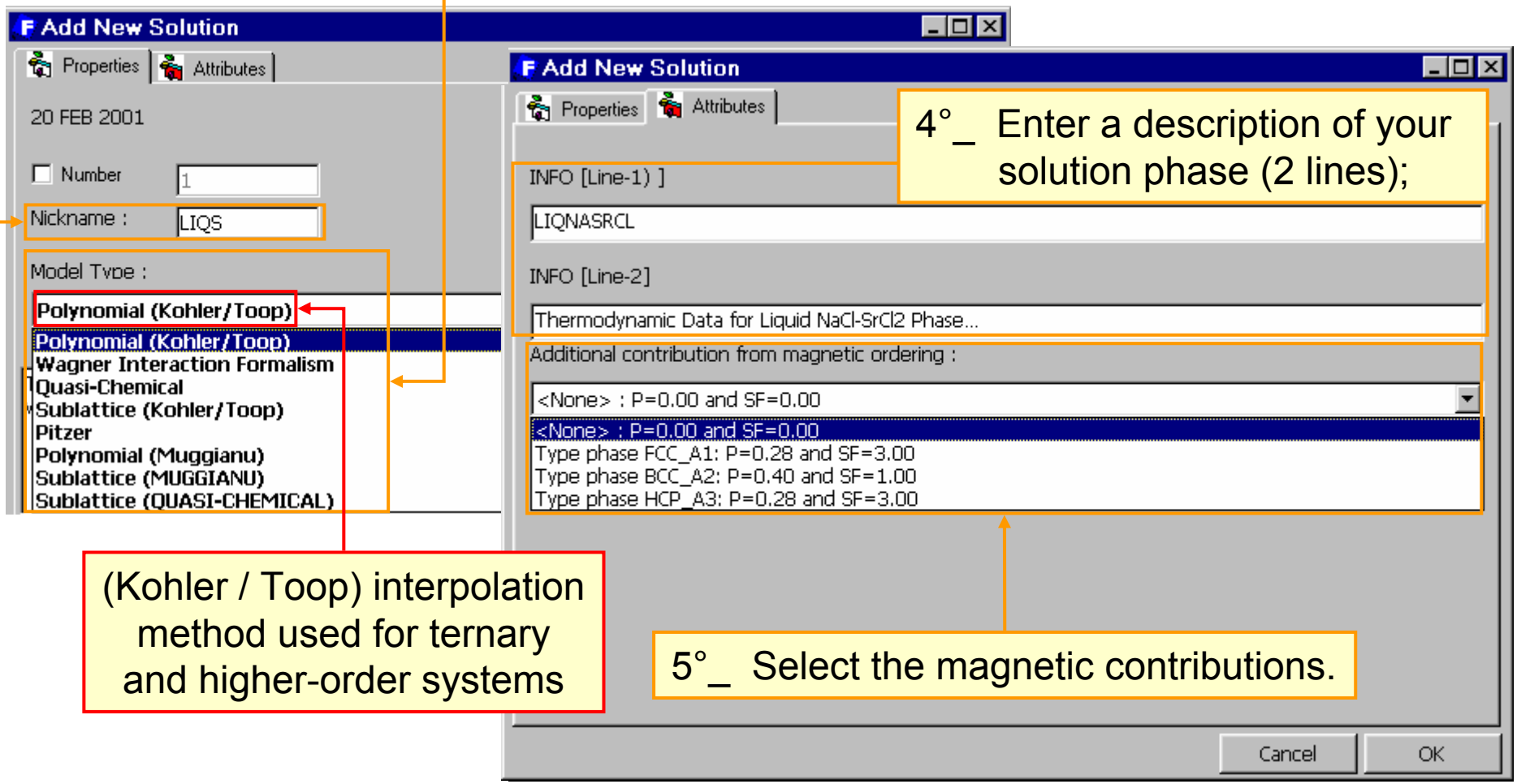
By the way…



Choice of energy units for the session can be changed at any time

…To create a solution phase:
2°_ Enter a four-character nicknamefor your new solution phase;

3°_ Select / Identify the solution model;

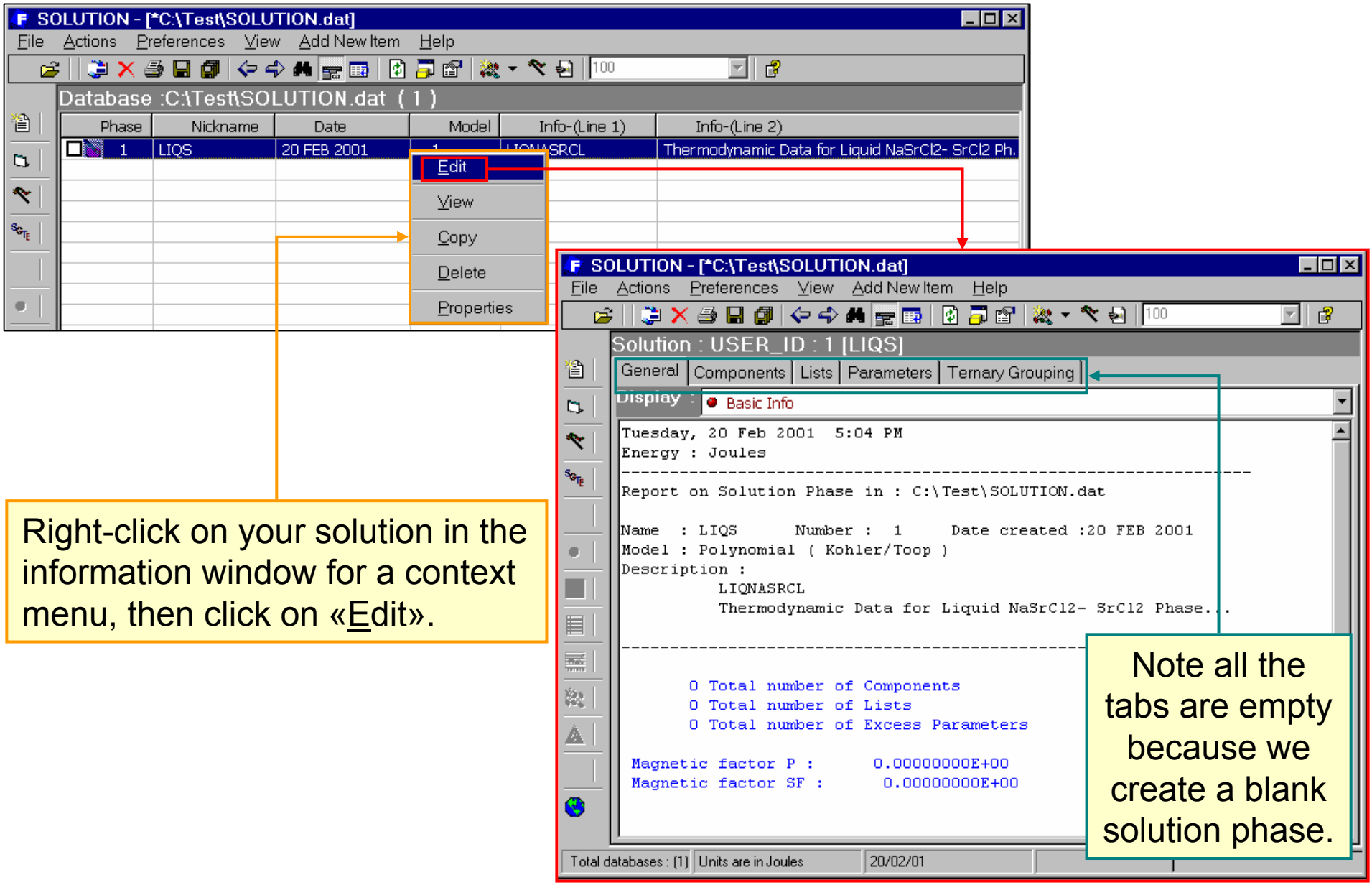


4°_ Enter a description of your solution phase (2 lines);

(Kohler / Toop) interpolation method used for ternary and higher-order systems

5°_ Select the magnetic contributions.

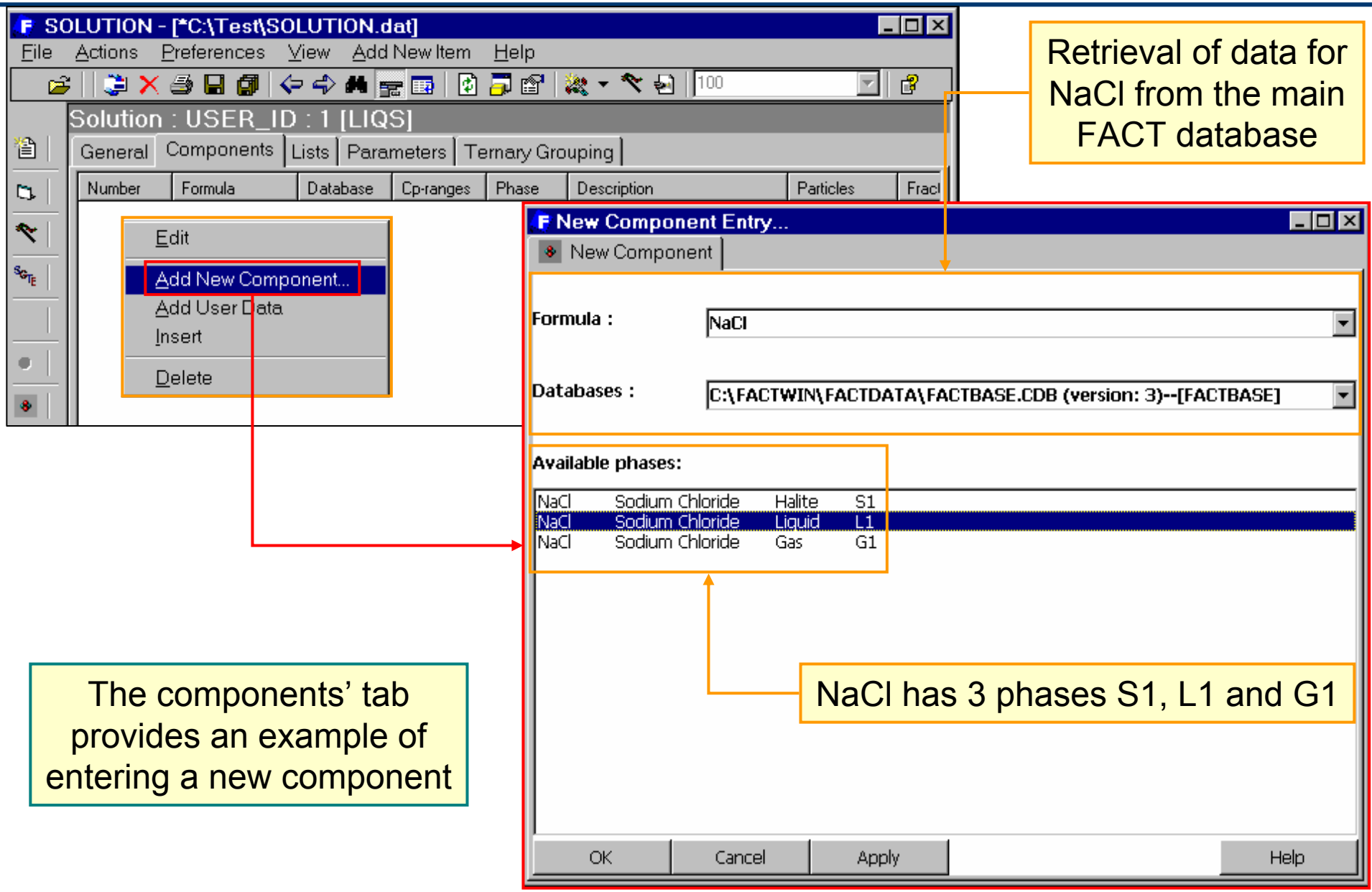
Basics of Entering Components, Lists and Parameters



Right-click on your solution in the information window for a context menu, then click on «Edit».

Note all the tabs are empty because we create a blank solution phase.

For **NaCl** we enter the **standard Gibbs energy** of the liquid from the **FACT** Compound database

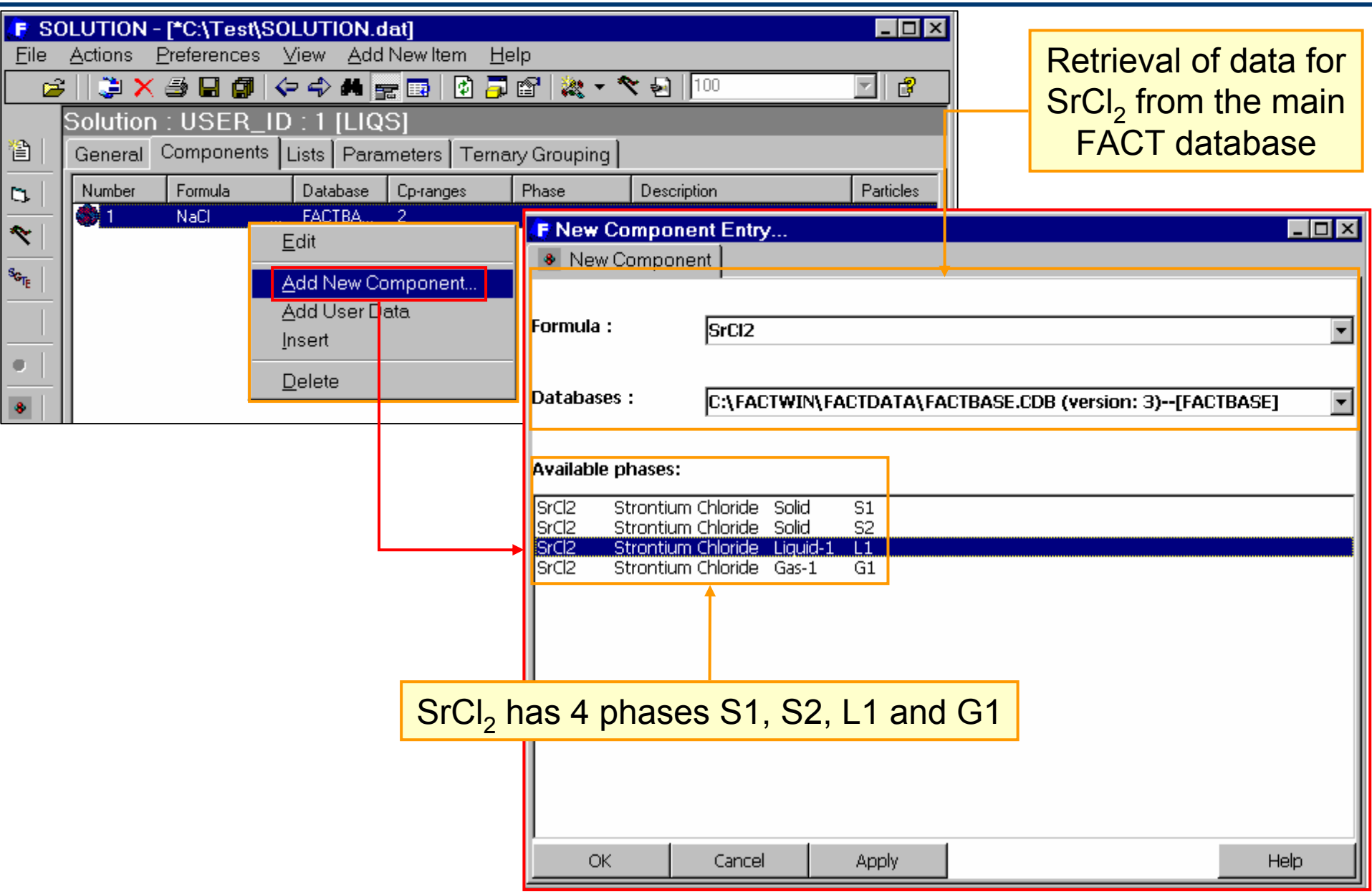


Retrieval of data for NaCl from the main FACT database

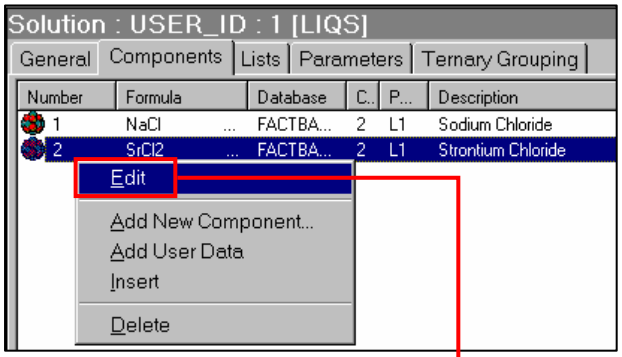
The components' tab provides an example of entering a new component

NaCl has 3 phases S1, L1 and G1

For $SrCl_2$ we enter the **standard Gibbs energy** of the liquid from the **FACT** Compound database

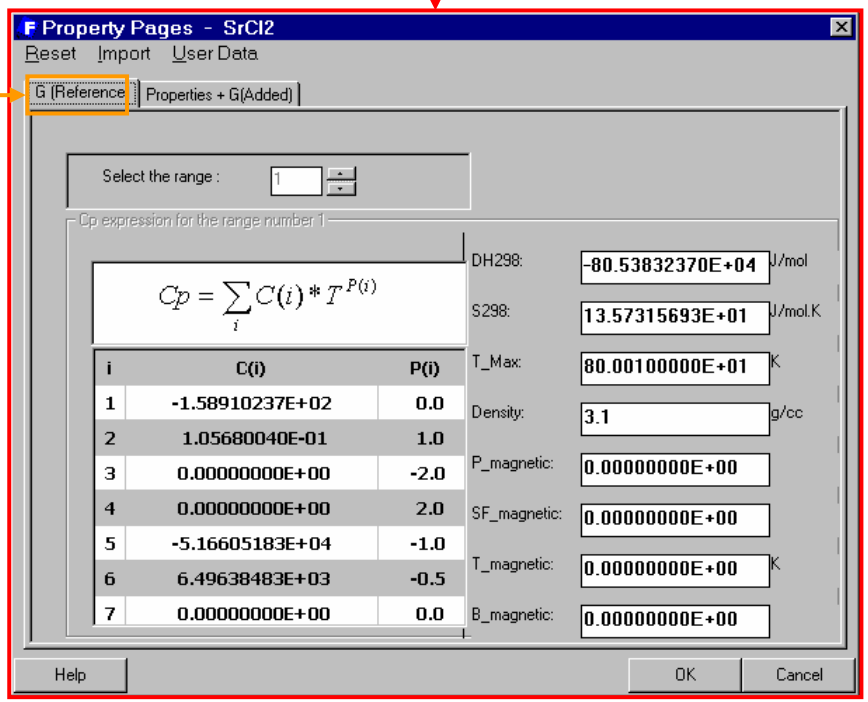


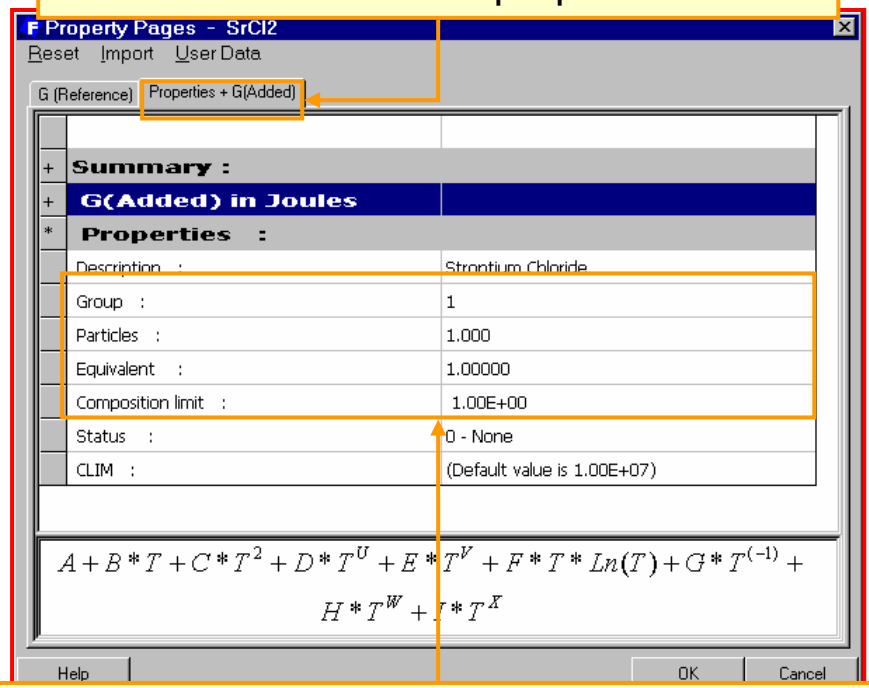
Alternate way to enter thermodynamic data



If $G°_{(added)}$ is defined then: $G°_{SrCl_2} = G°_{ref}$ (L1) + $G°_{(added)}$
(If $G°_{ref} = 0$, you must respect the convention that $H°_{298} = 0$ for elements).

The Properties + G(Added) tab displays certain variables for the component and some advanced properties.

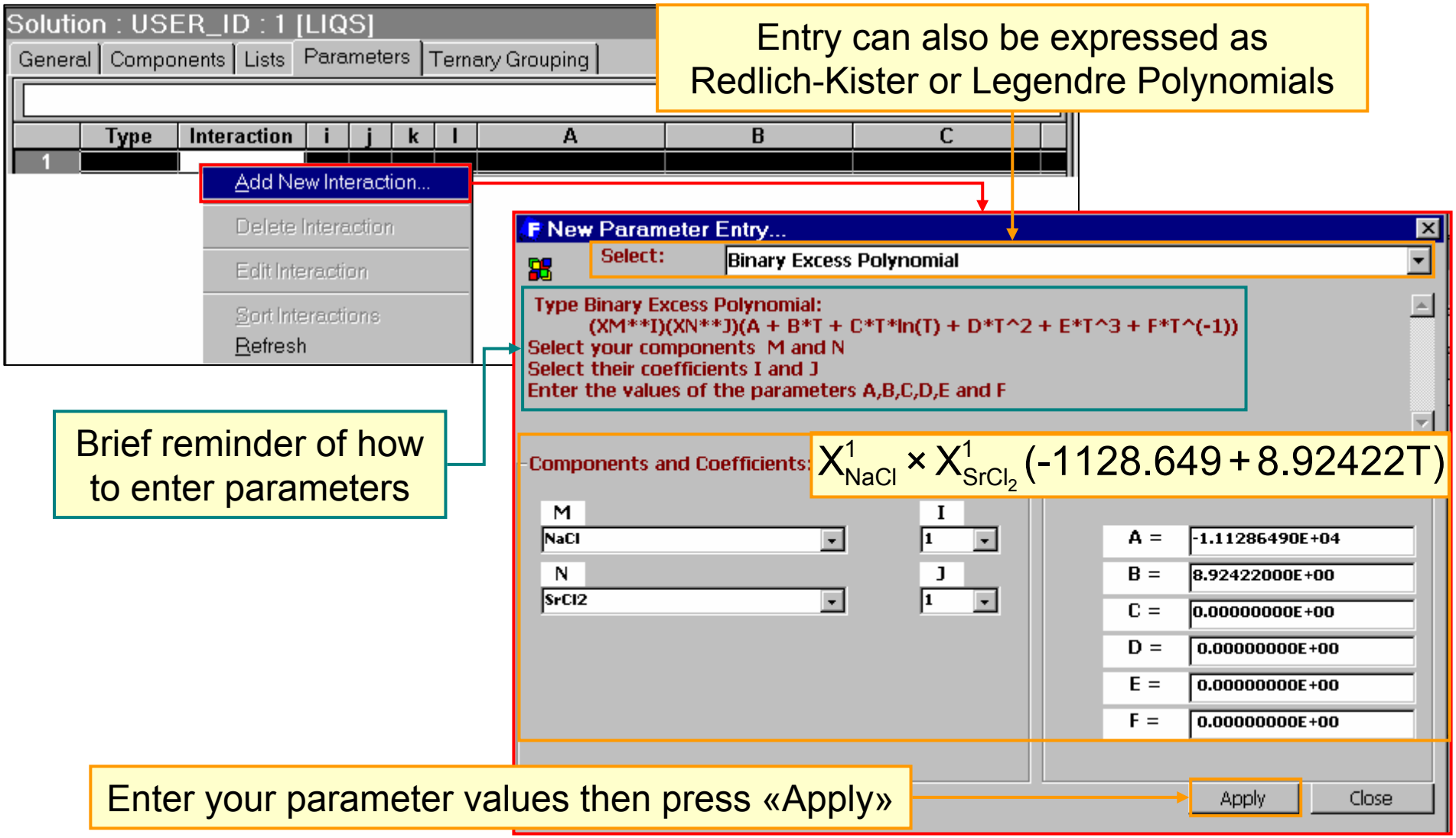




The G(Reference) tab displays C_p values and other «extended properties»

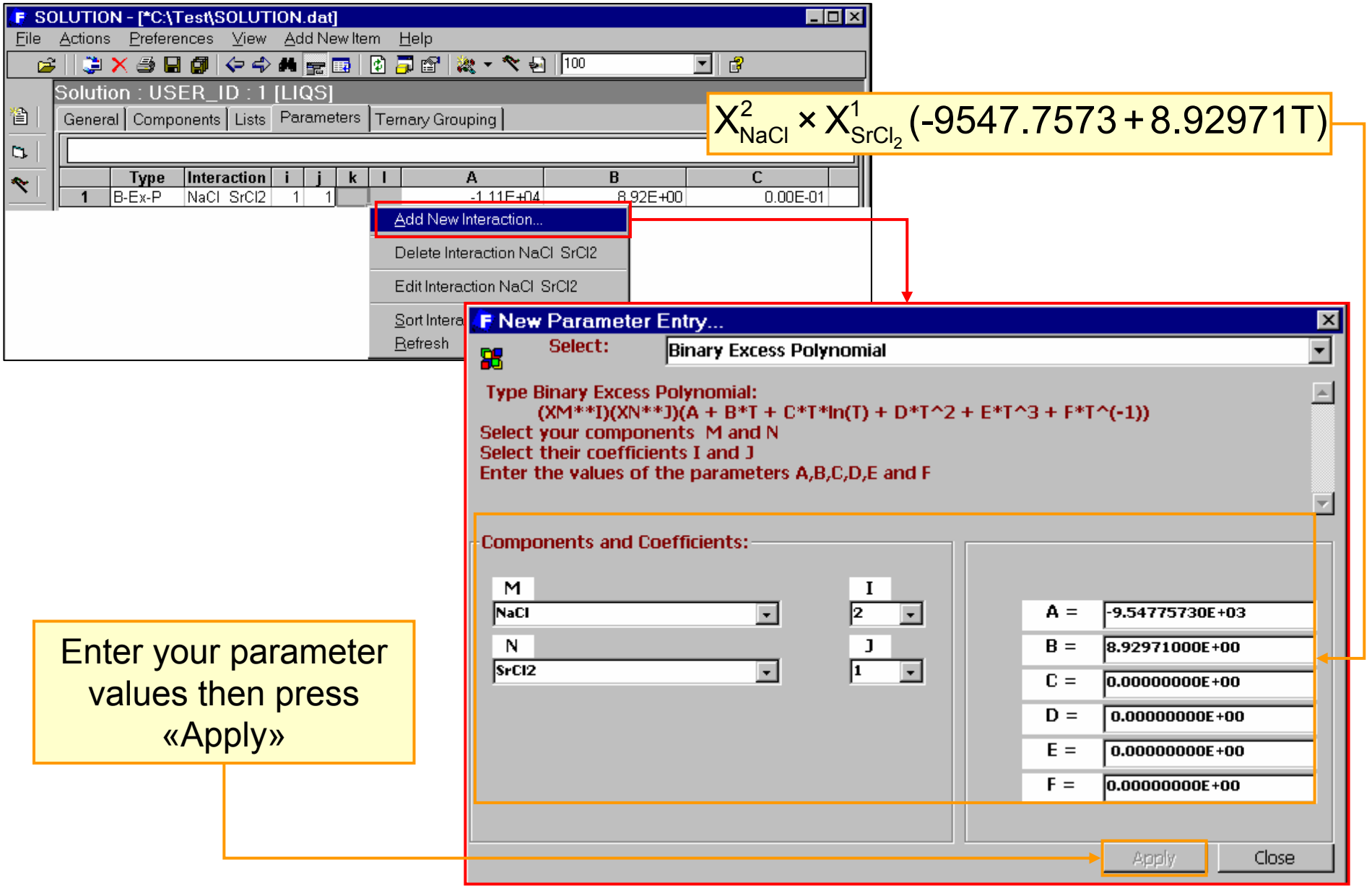
Default values are chosen regarding ”Particles”, “Equivalent”, “Composition limits” and “Acid/Base (Kohler-Toop)” groupings

Entry of Model Parameters for Excess Mixing Properties (Solution Polynomial)



The Gibbs energy of mixing is given by $\Delta G = RT (X_1 \ln X_1 + X_2 \ln X_2) + G^E$

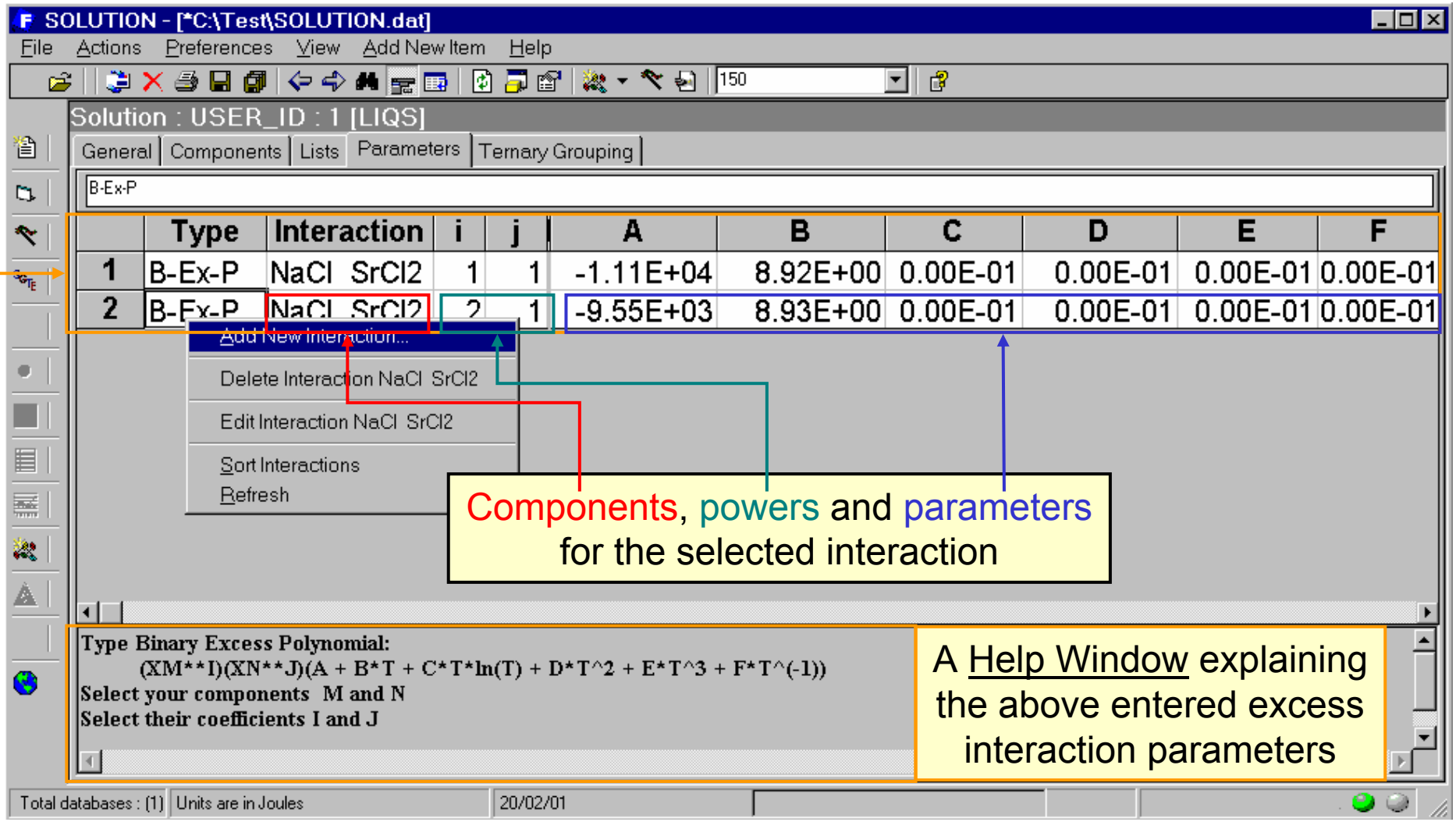
Entry of the Second Parameter for **Excess Mixing Properties** of the solution



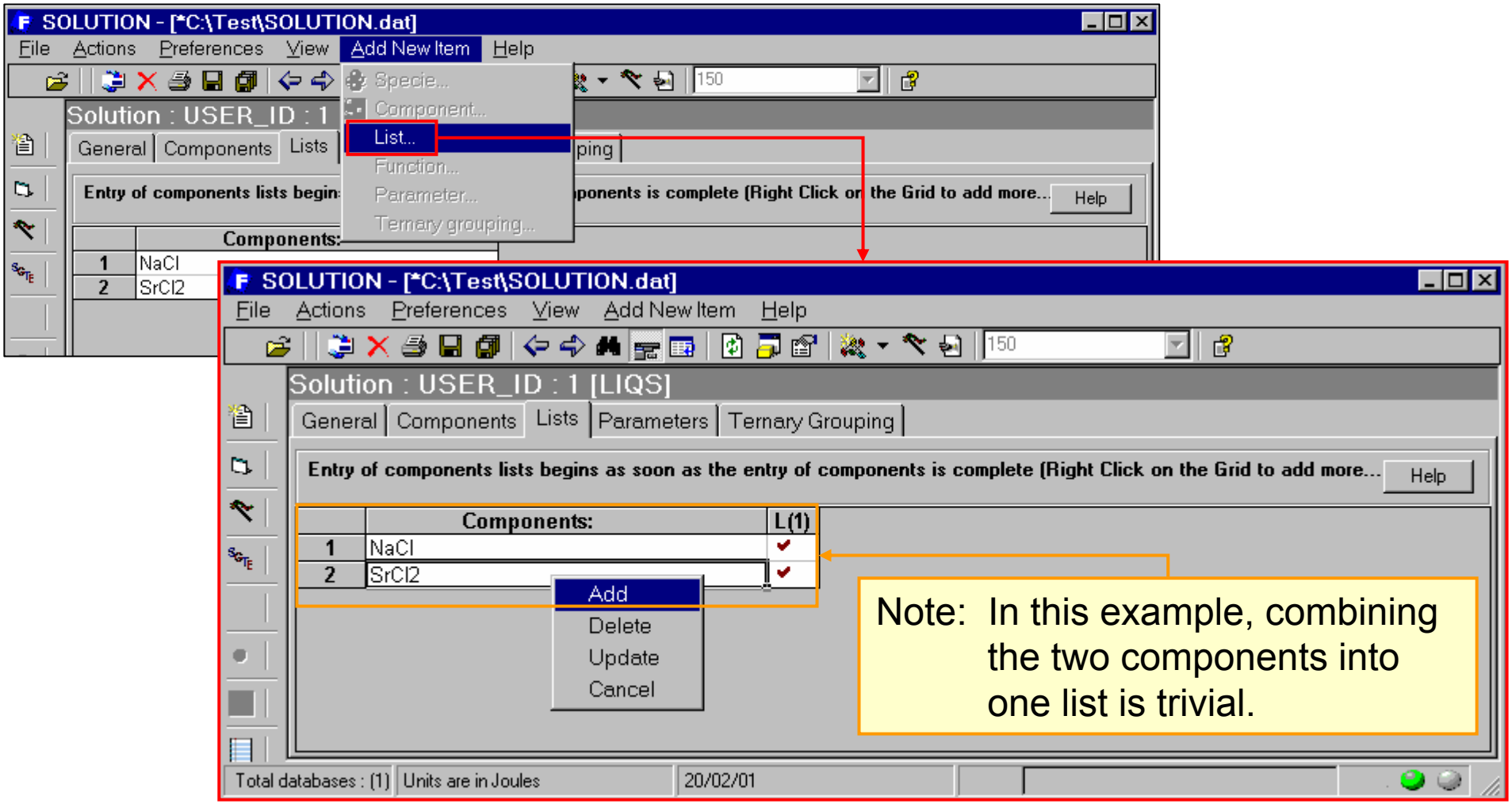
Enter your parameter values then press «Apply»

Summarize, Edit and View the Excess Parameters

A grid showing the existing excess interactions



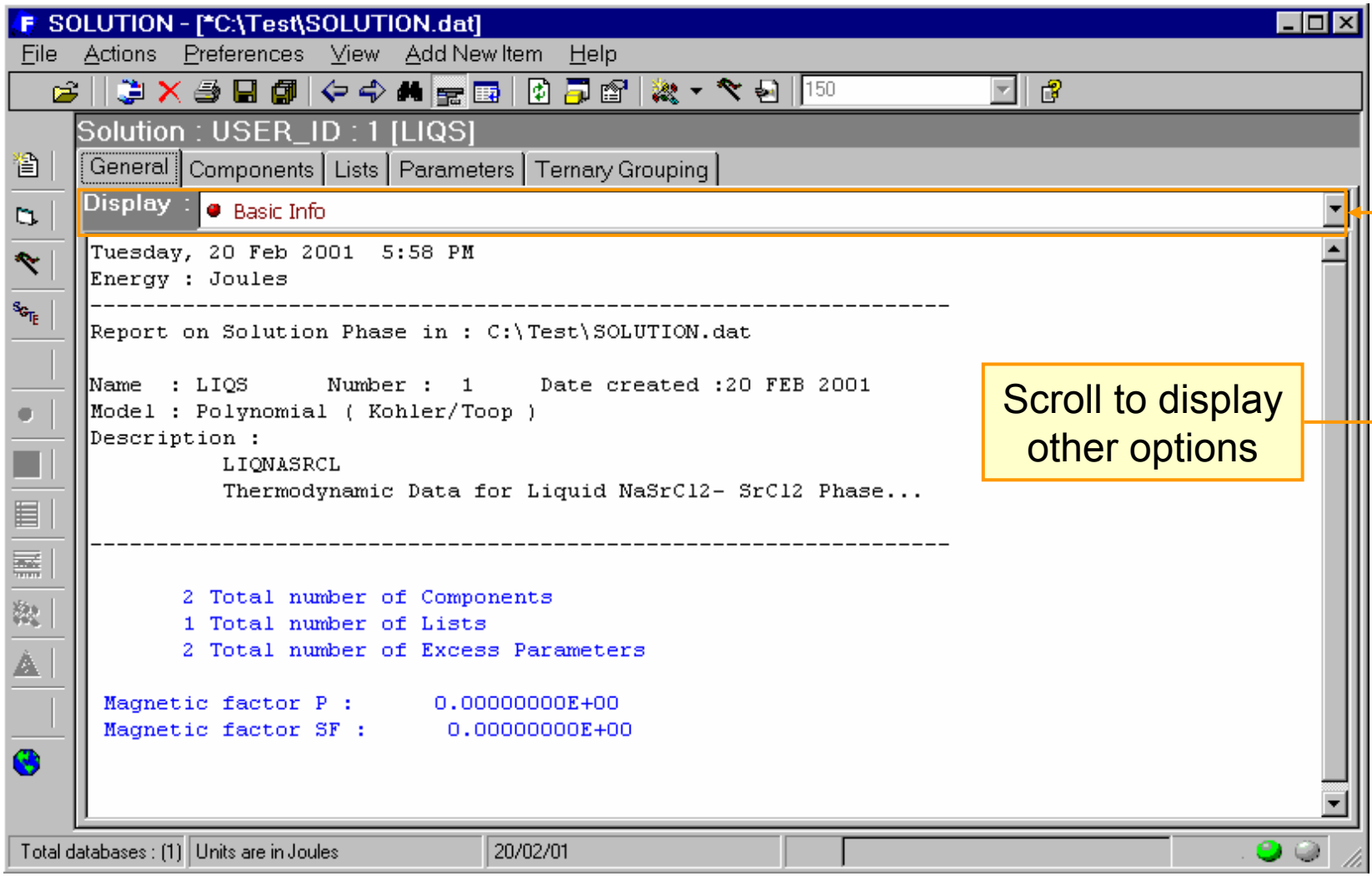
Entry of Component Lists



A solution phase may contain one or more lists of components which have been assessed together to form a multi-component solution. Only the use of such combinations is safe (in ***Equilib***).

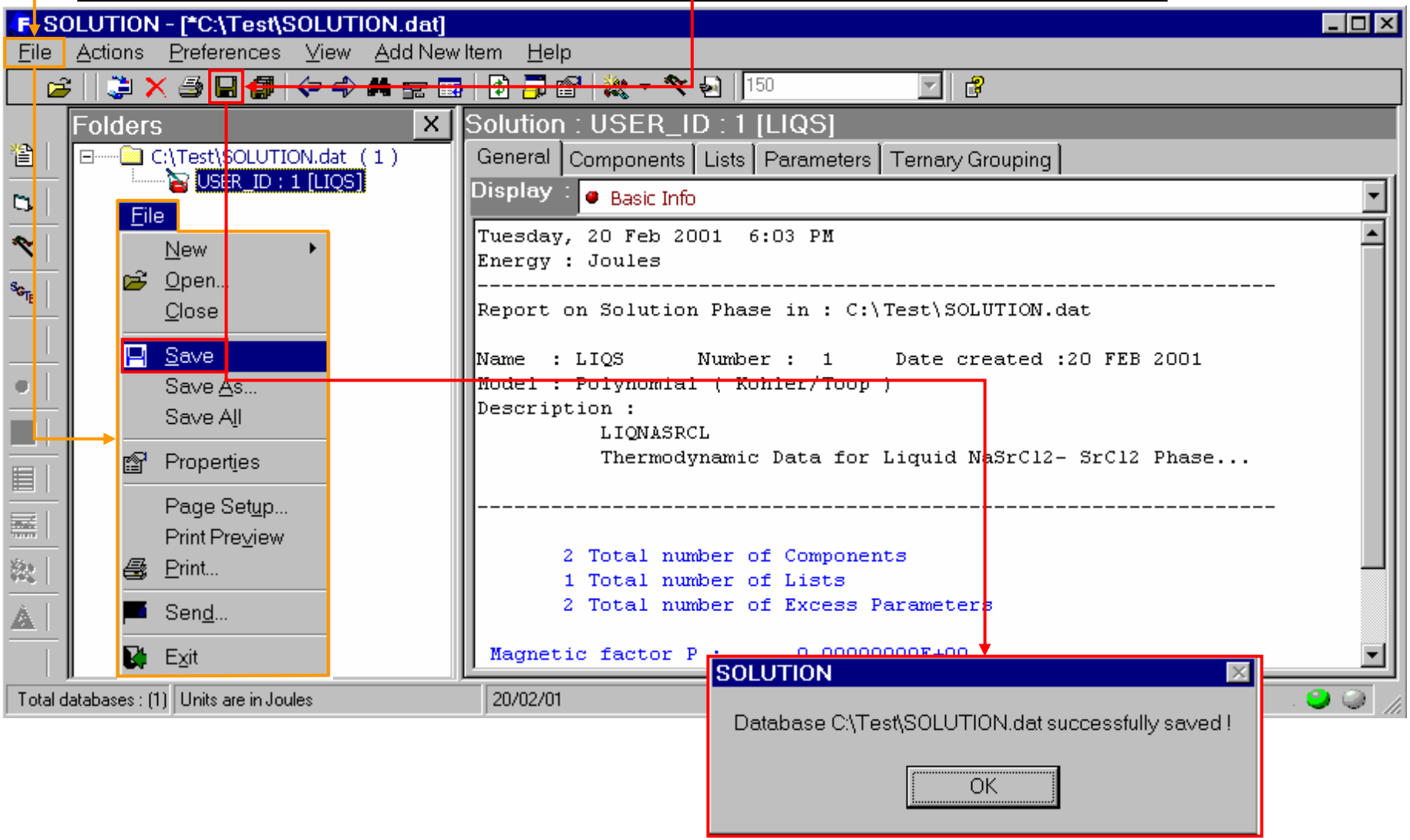
Inspecting the Solution File

Note that the parameters ($H°_{298}$, $S°_{298}$, C_P) in the expression for $G°_{(ref)}$, $G_{(added)}$ and $G_{(excess)}$ can also be displayed using other display options.



Saving Solution Database

Saving a database can be done by clicking on «Save» from the «File» menu or by pressing the «Save» button.



Examples of data entries in solution database

The following 11 slides show 4 different examples of the data needed to describe non-ideal solutions according to different Gibbs energy models.

These files are stored in your Factdata directory in Examsoln.dat. You can open this file using the ***Solution*** module in order to see how the data have been entered.

The first example shows the data for a simple substitutional solution treated with polynomials in the mole fractions and using the Kohler method for extrapolation into the ternary, here the **Liquid LiCl-KCl-CsCl Phase**.

The phase name used in the Factdata/Examsoln.dat database is AkCl.

First example from Factdata/Examsoln.dat

Thermodynamic Data for **Liquid LiCl-KCl-CsCl Phase**

Phase Nickname: **AkCl**

Entry in joules
Kohler interpolation method

	Component No.	G°
LiCl	1	L from FACT database
KCl	2	S1 from FACT database + ΔG^{o}_{fusion} where: $\Delta G^{o}_{fusion} = 26284 - 25.176\,T$
CsCl	3	L from FACT database

Binary excess mixing terms:

LiCl-KCl system: $\Delta H = X_1X_2(-17570 - 377X_1)$

$S^E = X_1X_2(-7.627 - 4.958X_1)$

Hence: $G^E = X_2X_1(-17570 + 7.267T) + X_2X_1^2(-377 - 4.958T)$

LiCl-CsCl system: $\Delta H = X_1X_3(-19456 - 7448X_1 - 9080X_1X_3)$

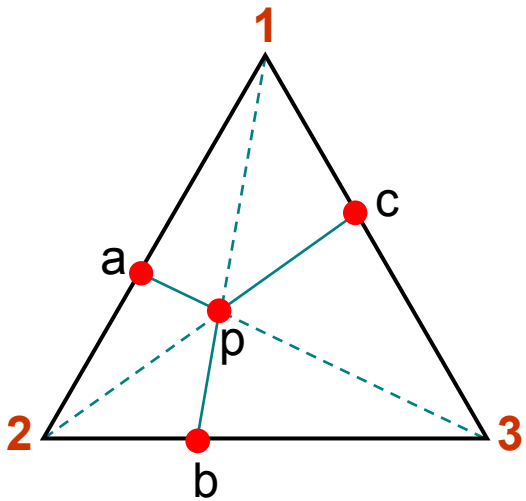
$S^E = X_1X_3(-20.541 + 3.285X_1)$

KCl-CsCl system: $G^E = X_2X_3(795)$

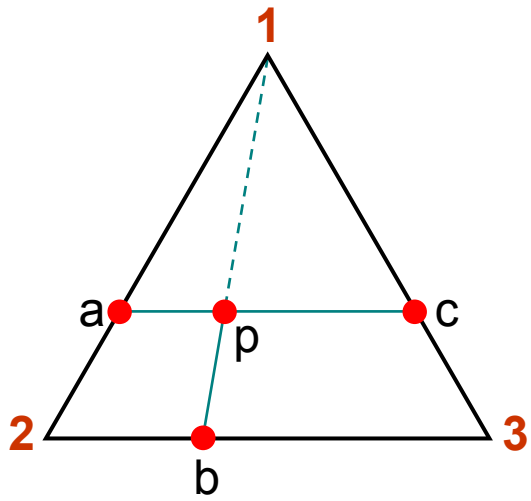
Ternary terms: $G^E = X_1X_2X_3(-20000)$

Kohler, Toop and Muggianu interpolation methods

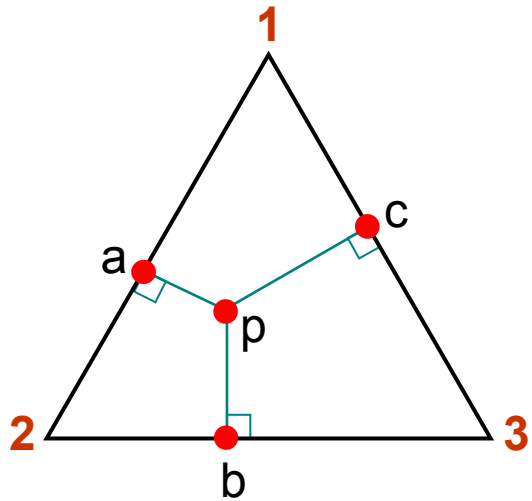
Kohler



Toop



Muggianu



Kohler, **Toop** and **Muggianu** methods of including binary polynomial terms in ternary **Gibbs** Energy Equations.

Reference:
P. Chartrand and A.D. Pelton, «On the choice of "Geometric" Thermodynamic Models», J. Phase Equilibria, 21, 141-147 (2000).

Second example from Factdata/Examsoln.dat

The second example shows the data used for the description of a dilute metallic solution, here **Liquid Fe-C-Mn-O Solution.**

The phase name used in **Factdata/Examsoln.dat** is **IRON**.

Second example from Factdata/Examsoln.dat

Thermodynamic Data for **Liquid Fe-C-Mn-O Solution**

Phase Nickname: **IRON**

Entered Component	Component number	G° (ref)	N (Particles/mol)	Actual Component	Composition Limit (X)
Fe (solvent)	1	FACT L	1	Fe	–
C	2	FACT S1	1	C	0.1
Mn	3	FACT L	1	Mn	0.1
O_2	4	FACT G	2	O	0.1

Actual Component	i	$\ln \gamma_i^\circ$
C	2	2073/T – 1.727
Mn	3	672/T
O	4	-14086/T + 2.948

i	j	ε_{ij}
2	2	23974/T
2	3	-3502/T
2	4	-38209/T
3	4	-8803

Reference:**(Unified interaction parameter formalism)**
A.D. Pelton, «The Polynomial Representation of Thermodynamic Properties in Dilute Solutions», Met. Trans., 28B, 869-76 (1997).

Third example from Factdata/Examsoln.dat

The third example shows the data used for the description of the **Liquid Li, Na, K / F, SO_4 Solution.**

The dataset is given the name **SALT** in the **Factdata/Examsoln.dat** database.

Third example from Factdata/Examsoln.dat

Thermodynamic Data for **Liquid Li, Na, K / F, SO_4 Solution**

Phase Nickname: **SALT**

(Sublattice Model)

	Species Number	Lattice	Absolute Charge	Kohler/Toop Group
Li	1	cationic	1	1
Na	2	cationic	1	1
K	3	cationic	1	1
F	4	anionic	1	(1)
SO_4	5	anionic	2	(2)

G° of all liquid salts from FACT database

X_i = ionic site fractions:

$$X_{Li} = \frac{n_{Li}}{(n_{Li} + n_{Na} + n_K)} \quad \text{etc}$$

$$X_F = \frac{n_F}{(n_F + n_{SO_4})} \quad \text{etc}$$

Y_i = equivalent ionic fractions:

$$Y_{Li} = X_{Li} \quad \text{etc}$$

$$Y_F = \frac{n_F}{(n_F + 2n_{SO_4})}$$

$$Y_{SO_4} = \frac{2n_{SO_4}}{(n_F + 2n_{SO_4})}$$

References: **(Sublattice Model)**

A.D. Pelton «A Database and Sublattice Model for Molten Salt Solutions», Calphad J., 12, 127-142 (1988).

(Quasichemical Sublattice Model)

Y. Dessureault and A.D. Pelton, «Contribution to the Quasichemical Model of Reciprocal Molten Salt Solutions», J. Chim. Phys., 88, 1811-1830 (1991).

Excess terms (Joules/equivalent)

Binary Common-Anion Systems

LiF - NaF: $G^E = Y_1Y_2(-7565 + 1.607T) + Y_1Y_2^2(-368 + 1.124T)$

LiF - KF: $G^E = Y_1Y_3(-19251 + 1.375T) + Y_1Y_3^2(-1205) + Y_1Y_3^3(4732) + Y_1^2Y_3(3.146T)$

NaF - KF: $G^E = Y_2Y_3(-335 + 2.541T)$

$Li(SO_4)_{½}$ - $Na(SO_4)_{½}$: $G^E = Y_1Y_2(-4247) + Y_1^2Y_2(-1444)$

$Li(SO_4)_{½}$ - $K(SO_4)_{½}$: $G^E = Y_1Y_3(-10712 + 4.700T) + Y_1^2Y_3(-3891 - 1.000T)$

$Na(SO_4)_{½}$ - $K(SO_4)_{½}$: $G^E = Y_2Y_3(-2197)$

Binary Common-Cation Systems

LiF - $Li(SO_4)_{½}$: $G^E = Y_4Y_5(-988 - 2.352T) + Y_4Y_5(Y_5 - Y_4)(-359)$

NaF - $Na(SO_4)_{½}$: $G^E = Y_4Y_5(56 - 1.214T) + Y_4Y_5(Y_5 - Y_4)(-217 + 2.044T)$

KF - $K(SO_4)_{½}$: $G^E = Y_4Y_5(-1263 - 1.522T) + Y_4Y_5(Y_5 - Y_4)(486)$

Ternary Common-Anion Terms

LiF - NaF - KF: $Y_1Y_2Y_3(-300)$

$Li(SO_4)_{½}$ - $Na(SO_4)_{½}$ - $K(SO_4)_{½}$: $Y_1Y_2Y_3^2(400)$

Reciprocal Terms

$Y_1Y_2Y_4Y_5(-8483 + 3.069T)$

$Y_1Y_3Y_4Y_5(-29893 + 14.017T)$

$Y_2Y_3Y_4Y_5(-6338 + 3.588T)$

The fourth example shows the data stored for the Fe-Cr system. The data are given in the form that is used in the **SGTE** Solution database.

Functions are used to define the Gibbs energies of the components of the solution phases.

The excess Gibbs energy of liquid, FCC and BCC is treated with the Redlich-Kister polynomial.

For the SIGMA phase a three-sublattice ideal solution approach is used.

Fourth example from Factdata/Examsoln.dat

Thermodynamic properties of the **Cr-Fe System**

Entry in **joules**

Excess Model: Redlich-Kister-Muggianu

Phase	Nickname	Number of Sublattices	Sites	Constituents on sublattice numbers		
				1	2	3
LIQUID	LIQU	1	1	Cr, Fe	–	–
BCC_A2	BCC	2	1:3	Cr, Fe	Va	–
FCC_A1	FCC	2	1:1	Cr, Fe	Va	–
SIGMA	SIGM	3	8:4:18	Fe	Cr	Cr, Fe

Thermodynamic parameters of the elements and solution phases

LIQUID:

$${}^{o}G_{Cr}^{LIQUID} = \mathbf{LIQU015}$$

$${}^{o}G_{Fe}^{LIQUID} = \mathbf{GFELIQ}$$

$${}^{o}L_{Cr,Fe}^{LIQUID} = -14550 + 6.65T$$

BCC_A2 (Additional contribution from magnetic ordering):

$${}^{o}G_{Cr}^{BCC} = \mathbf{GHSERCR}$$

$${}^{o}G_{Fe}^{BCC} = \mathbf{GHSERFE}$$

$$T_C^{BCC} = -311.5y_{Cr} + 1043y_{Fe} + y_{Cr}y_{Fe}\left[1650 + 550\left(y_{Cr} - y_{Fe}\right)\right]$$

$$\beta^{BCC} = -0.01y_{Cr} + 2.22y_{Fe} - 0.85y_{Cr}y_{Fe}$$

$${}^{o}L_{Cr,Fe:Va}^{BCC} = 20500 - 9.68T$$

FCC_A1 (Additional contribution from magnetic ordering):

$${}^{o}G_{Cr}^{FCC} = \mathbf{GCRFCC}$$

$${}^{o}G_{Fe}^{FCC} = \mathbf{GFEFCC}$$

$$T_C^{FCC} = -1109y_{Cr} - 201y_{Fe}$$

$$\beta^{FCC} = -2.46y_{Cr} - 2.1y_{Fe}$$

$${}^{o}L_{Cr,Fe:Va}^{FCC} = 10833 - 7.477T$$

$${}^{1}L_{Cr,Fe:Va}^{FCC} = 1410$$

SIGMA:

$$G_{Fe:Cr:Cr}^{SIGMA} = 8\ \mathbf{GFEFCC} + 22\ \mathbf{GHSERCR} + \mathbf{SIGM034}$$

$$G_{Fe:Cr:Fe}^{SIGMA} = 8\ \mathbf{GFEFCC} + 4\ \mathbf{GHSERCR} + 18\ \mathbf{GHSERFE} + \mathbf{SIGM035}$$

$$\mathbf{LIQU015} = \begin{cases} \mathbf{GHSERCR} + 24339.955 - 11.420225T + 2.37615\times10^{-21}T^{7} & \text{for } T < 2180\,K \\ \mathbf{GHSERCR} + 18409.36 - 8.563683T + 2.88526\times10^{32}T^{-9} & \text{for } T > 2180\,K \end{cases}$$

$$\mathbf{GHSERCR} = \begin{cases} \left\{ \begin{array}{l} -8856.94 + 157.48T - 26.908T\ln T + 1.89435\times10^{-3}T^{2} \\ -1.47721\times10^{-6}T^{3} + 139250T^{-1} \end{array} \right\} & \text{for } T < 2180\,K \\ -34869.344 + 344.18T - 50T\ln T - 2.88526\times10^{32}T^{-9} & \text{for } T > 2180\,K \end{cases}$$

$$\mathbf{GHSERFE} = \begin{cases} \left\{ \begin{array}{l} 1225.7 + 124.34T - 23.5143T\ln T - 4.39752\times10^{-3}T^{2} \\ -5.8927\times10^{-8}T^{3} + 77359T^{-1} \end{array} \right\} & \text{for } T < 1811\,K \\ -25383.581 + 299.31255T - 46T\ln T + 2.29603\times10^{31}T^{-9} & \text{for } T > 1811\,K \end{cases}$$

$$\mathbf{GFELIQ} = \begin{cases} 12040.17 - 6.55843T - 3.6751551\times10^{-21}T^{7} + \mathbf{GHSERFE} & \text{for } T < 1811\,K \\ -10839.7 + 291.302T - 46T\ln T & \text{for } T > 1811\,K \end{cases}$$

$$\mathbf{GCRFCC} = 7284 + 0.163T + \mathbf{GHSERCR}$$

$$\mathbf{GFEFCC} = \begin{cases} -1462.4 + 8.282T - 1.15T\ln T + 6.4\times10^{-4}T^{2} + \mathbf{GHSERFE} & \text{for } T < 1811\,K \\ -27098.266 + 300.25256T - 46T\ln T + 2.78854\times10^{31}T^{-9} & \text{for } T > 1811\,K \end{cases}$$

$$\mathbf{SIGM034} = 92300 - 95.96T$$

$$\mathbf{SIGM035} = 117300 - 95.96T$$

References for the fourth example

- **Compound Energy Formalism**
  - M.Hillert and M.Jarl,Calphad Vol 2(1978) p 227-238
  - J.O. Anderson, A.Fernandez Guillermet, M.Hillert, B.Jansson, B.Sundman,Acta Metall., 34(1986) p 437-445.
- **Cr-Fe system**
  - Alan Dinsdale, SGTE Data for Pure Elements,Calphad Vol 15(1991) p 317-425.
  - J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92.