

FactSage Solution – Introduction

Solution Introduction

This *Solution Introduction Slide Show* introduces users to the **Solution** module of **FactSage**. This is not the *Solution Slide Show* which appears in a different file.

These slides show you how to create a new solution file (*.soln.sln). The presentation is addressed to users who have already created their own solution databases in earlier versions of FactSage and wish to convert them into the new format and to users who wish to create new private databases.

The main reason for creating a private solution database is to employ the data in calculations involving **Equilib**, **Phase Diagram** and **View Data**. The slides show you how to make your private databases accessible to these modules. Note: **View Data** now provides useful tools for displaying the parameters that you have stored in your database. This is illustrated in Slides 8-10.

For defining a new phase and entering the data into a private solution database, see the **Solution** slide show.

Solution database files in FactSage 7.1, 7.2 and more recent

In **FactSage 6.4** (and prior versions) there were three different types of solution files :

1. *.dat file - private text data, e.g. [Solution.dat](#), [ExamSoln.dat](#)
2. *.sdb file - private binary data, e.g. [Userdata.sdb](#), [PrivSoln.sdb](#)
3. *.sda file - protected public data, e.g. [FTOxid53soln.sda](#) (FToxid)

In **FactSage 7.0 / 7.1** the solution file structures have been reformatted. The old solution files (*.dat, *.sdb, *.sda) have been replaced by two new files :

1. *soln.sln file - private text data, e.g. [Copsoln.sln](#), [Testsoln.sln](#)
2. *soln.sdc file - protected public data, e.g. [FTOxid53soln.sdc](#) (FToxid)

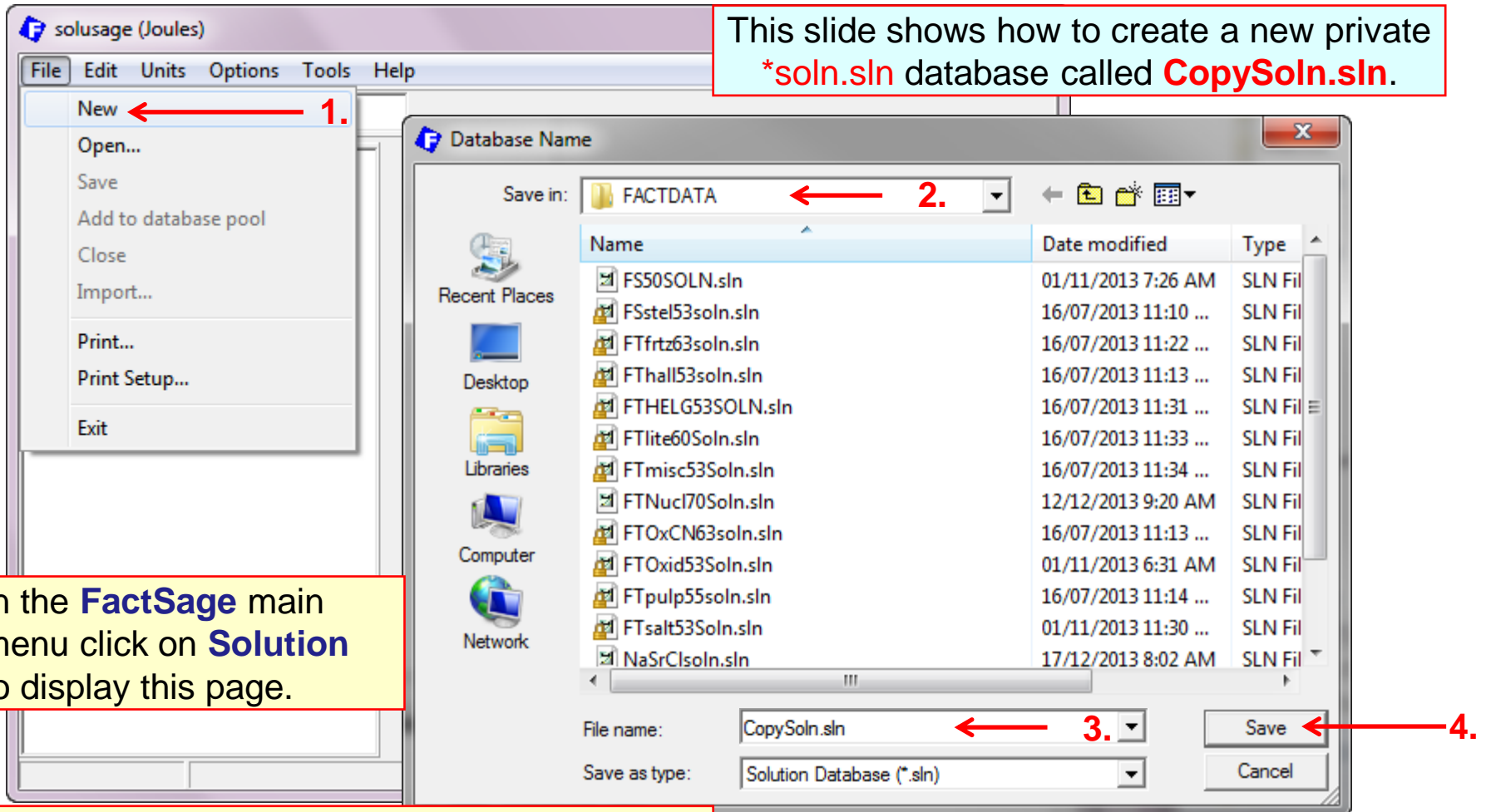
In **FactSage 7.1, 7.2** (and more recent) with the **Solution** module :

1. you can create and edit private *.sln files using the common solution models ([Polynomial](#), [Redlich-Kister](#), [Muggianu](#), [Quasichemical](#), [Sublattice](#), [Compound Energy Formalism](#), etc.) . The program is [Windows 8](#) (Windows 7, Windows Vista) friendly.
2. you cannot edit old private solution files (e.g.. *.dat *.sdb) but you can import and convert them into the new *.sln format (but **not** convert *.sln back to the old format)
3. you can still access your old private *.dat and *.sdb solution databases in your calculations ([ViewData](#), [Equilib](#), [Phase Diagram](#))

Summary: You can access your old *.dat and *.sdb files from the Equilib and Phase Diagram modules just as before and change nothing. **Note** however, that in this case the program first automatically converts the files temporarily to *.sln format files internally which it then reads. You will not be aware that this is happening. However, the routine which reads the resultant *.sln files has a more rigorous error-checker than the previous FactSage 6.4 routine which read the old *.dat and *.sdb files. It is less forgiving of possible ambiguities and small errors. If it finds an error when reading the temporary files it may simply crash, giving no indication of why this happened. Therefore, we recommend that you first convert your old files to new *.sln files as described on the following pages. Any errors will be detected at this point and will be reported to you, thereby permitting you to correct them using the new Solution module. (Alternatively, you could correct the errors by editing the old *.dat and *.sdb files using the old 6.4 Solution module or a text editor and then converting them again to *.sln format.)

Create a new private solution database called CopySoln.sln

This slide shows how to create a new private *sln.sln database called **CopySoln.sln**.



In the **FactSage** main menu click on **Solution** to display this page.

1. Click on «**File > New**»
2. Open the «**FACTDATA**» subfolder or another folder if you prefer
3. Enter the new file name **CopySoln.sln**.
4. Click on «**Save**»

Note: the database name **CopySoln** must be **unique in the folder**. For example, there **cannot** be other files such as **CopySoln.dat** or **CopySoln.sdb** in the same folder.

Import an old private solution data file into the new CopySoln.sln

1. → File

2. → Import...

3. → Open

1. Click on «**File**»

2. Select «**Import**»

3. Open the existing examples database **ExamSoln.dat** located in \FACTDATA

Name	Type	Size
ExamSoln.DAT	DAT File	31
FTHall53prop.dat	DAT File	49
MODLSOLN.DAT	DAT File	796
OLIFlows.dat	DAT File	603
VGASSoln.dat	DAT File	44
VLABprop.dat	DAT File	122
VLABsoln.dat	DAT File	4,433

File name: ExamSoln.DAT

Files of type: ASCII Solution Databases (*.DAT)

This slide shows how to convert an old private solution data file (**ExamSoln.dat**) into the new format. This is done by *importing* **ExamSoln.dat** into the new private database **CopySoln.sln**.

Display of data imported into CopySoln.sln

The end-member properties are stored in a separate "Functions" file called CopySoln.fdb created at the same time as you created CopySoln.sln. See the **SOLUTION** slide show

CopySoln
(database CopySoln.sln)

Solutions (8)
(8 solution phases)

BCC2 (20-2) magnetic solid
(model #20 - 2 sublattices)

Iron (2-1) liquid alloy
(model #2 - 1 sublattice)

MeCl (1-1) molten solution
(model #1 - 1 sublattice)

Salt (4-2) molten solution
(model #4 - 2 sublattices)




Treeview contents:
CopySoln
+ Functions
+ Solutions (8)
+ AkCl (1-1)
+ BCC2 (20-2)
+ CrFe (20-2)
+ FCC1 (20-2)
+ Iron (2-1)
+ MeCl (1-1)
- SubLattices
 - A (2)
 - NaCl
 - SrCl2
- End Members (2)
 - NaCl
 - SrCl2
+ Mixables (1)
- Ternary Interp
- Interactions (2)
 (0) NaCl,SrCl2
 (1) NaCl,SrCl2
+ Salt (4-2)
+ SIGM (20-3)

For a complete discussion see the **SOLUTION** slide show

Click on +/- to expand/collapse the treeview

Re: phase – states
The phase state of imported data is set to **solid** unless
- **magnetic** contributions are detected in the data, or
- 'liq', 'molten', 'melt', or 'slag' is in the phase description

Phase - states

-  – solid
-  – magnetic
-  – liquid

This slide shows the data imported from the old **ExamSoln.dat** database.

When finished click on «**File > Save**»

View the contents of CopySoln.sln

This slide displays the contents of the text file `CopySoln.sln`

```
CopySoln.sln - win32pad
File Edit View Favorites Tools Help
Base Copy Copy
Date Created: 2014/04/18 Modified: 2014/04/18
Vers 7.00
Desc Data imported from old ExamSoln.dat file
SolB AkCl 1 1 Polynomial
SlnO 2
Stat Liquid 0
Date Created: 2014/04/18 Modified: 2014/04/18
Name LiqLiKCsCl
Desc LiqLiKCsCl - liquid LiCl-KCl-CsCl
SubL A 3
Spec A0 1 LiCl
SpId A0 1
Spec A1 1 KCl
SpId A1 2
Spec A2 1 CsCl
SpId A2 3
EndM 0 A0 ClLi
EMid 1 2
Zeds 1
Amnt 1
Name LiCl
CpXp ClLi#AkCl_0000
VExp ClLi#AkCl_0000
EndM 0 A1 KCl
EMid 2 2
Zeds 1
Amnt 1
Name KCl
CpXp KCl#AkCl_0001 +KCl#AkCl_0001A
VExp KCl#AkCl_0001
EndM 0 A2 CsCl
EMid 3 2
Zeds 1
Amnt 1
Name CsCl
CpXp CsCl#AkCl_0002
VExp CsCl#AkCl_0002
List A0A1A2
Fxcs BCP A0A1
```

You can use a text editor to view the contents of `CopySoln.sln`

Each line starts with a 4-character identification (**Base**, **Date**, **Vers**, **Desc**, ...) The rest of the line is in free format.

By comparing the lines here with the expanded treeview display (see previous slide) it is straightforward to isolate the lines associate with a particular phase and property.

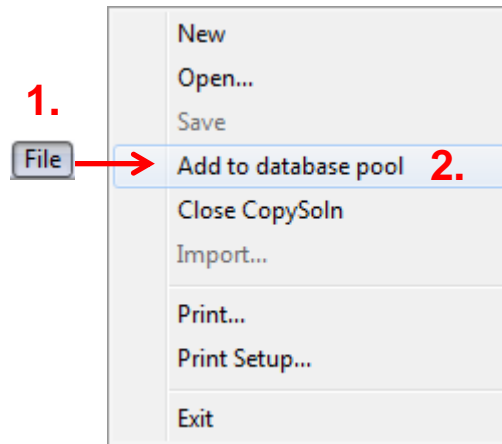
You can use a text editor to edit and save the file contents. But be careful - there is no error checking when you use a text editor ! Therefore, we suggest that you use the **Solution** module for editing.

Include CopySoln.sln in Equilib / Phase Diagram Calculations

To include the new solution file **CopySoln.sln** in **FactSage** calculations (e.g. **Equilib / Phase Diagram**) the database must be “added to the List” of accessible **FactSage** databases (i.e. you must tell **FactSage** what the database is and where it is stored). There are 2 ways to do this:

- Select «**Add to database pool**» in the **Solution** «**File**» dropdown menu.
- Or, at any time you can use the **Equilib, Phase Diagram** or **ViewData** modules as before to “**Add**” a database to the list – How to do this is shown in the slide on the following page >>.

1. Click on «**File**»
2. Select «**Add to database pool**»



Include CopySoln.sln in Equilib Calculations – the old way

Databases - 1/36 compound databases, 1/31 solution databases

<input checked="" type="checkbox"/> FactPS	<input type="checkbox"/> FSscopp	<input type="checkbox"/> BINS
<input type="checkbox"/> FToxid	<input type="checkbox"/> FSlead	<input checked="" type="checkbox"/> SGPS
<input type="checkbox"/> FTsalt	<input checked="" type="checkbox"/> FSlite	<input type="checkbox"/> SGTE
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl
<input type="checkbox"/> FTball	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGsold
<input type="checkbox"/> FT0xCN	<input checked="" type="checkbox"/> FSupsi	<input type="checkbox"/> SGnucl
<input type="checkbox"/> FTfrtz		
<input type="checkbox"/> FThelg	<input checked="" type="checkbox"/> ELEM	Other
<input type="checkbox"/> FTpulp	<input type="checkbox"/> FTdemo	<input type="checkbox"/> SPrefr
		<input type="checkbox"/> TDmeph
<input type="checkbox"/> FTlite	<input type="checkbox"/> FTnucl	<input type="checkbox"/> TDnucl

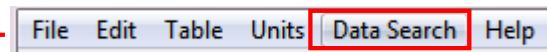
compounds only
solutions only
no database

Clear All

Add/Remove Data

ADD

- This is the “old“ way of “adding“ to the database list:
1. Open «Data Search» in Equilib/Phase Diagram
 2. Click on «Add/Remove Data > ADD».
 3. Select «Solution» and enter the full file name of the «COPY» database and save «OK»
 4. Select «COPY» in «Data Search» Window



Solution - List of Databases

3.

Database Type

compound

solution

both

Summary of files

Click for a summary of all database files including those not on the FactSage list.

Summary ...

Add database to the list

file: C:\FactSage\FACTDATA\COPYSoln.sln

dir.: C:\FactSage\FACTDATA\ ...

Browse ...

Scan ...

nickname: COPY

info: COPY solution database.

Click on 'OK' to add to the list.

You may edit and change the info.

Quit

OK

Databases - 1/36 compound databases, 2/32 solution databases

<input checked="" type="checkbox"/> FactPS	<input type="checkbox"/> FSscopp	<input type="checkbox"/> BINS	compounds only	
<input type="checkbox"/> FToxid	<input type="checkbox"/> FSlead	<input checked="" type="checkbox"/> SGPS	solutions only	<input type="checkbox"/> ACCO
<input type="checkbox"/> FTsalt	<input checked="" type="checkbox"/> FSlite	<input type="checkbox"/> SGTE	no database	<input type="checkbox"/> COKE
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl		<input type="checkbox"/> FEFX
<input type="checkbox"/> FTball	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGsold	Clear All	<input type="checkbox"/> MDL8
<input type="checkbox"/> FT0xCN	<input checked="" type="checkbox"/> FSupsi	<input type="checkbox"/> SGnucl	Add/Remove Data	<input checked="" type="checkbox"/> SGTE#
<input type="checkbox"/> FTfrtz				
<input type="checkbox"/> FThelg	<input checked="" type="checkbox"/> ELEM	Other		
<input type="checkbox"/> FTpulp	<input type="checkbox"/> FTdemo	<input type="checkbox"/> SPrefr	RefreshDatabases	
		<input type="checkbox"/> TDmeph		
<input type="checkbox"/> FTlite	<input type="checkbox"/> FTnucl	<input type="checkbox"/> TDnucl		

Information -

Solution: C:\FactSage\FACTDATA\COPYSoln.sln
- COPY database

4.

Displaying the solution data with ViewData

1. Run ViewData

View solutions - enter a list of elements or ALL

Examples:

Ca Al O S - solutions with Ca, Al, O and/or S
H O Fe S - solutions (including aqueous) of H, O, Fe and/or S
ALL - ALL solutions

Pressure

atm
 bar

Energy

J
 cal

2.

Data
 Compound
 Solution

Solution Databases (29)

Summary ...

Add ...

Remove ...

Copy

C:\FactSage64\FACTDATA\Copysoln.sln

Copysoln solution database.

3. Select solution „Copy“

Elements or ALL: All

4.

5.

OK

ViewData Summary of Copy solution database

F View Data ALL solutions - Copy datasets

File Edit Sort Solutions Summary Databases Units Atomic Wts. Table Graph Help << Back

7 Solutions

Copysoln solution database.

Solutions sorted by phase number (see 'Sort Solutions')

Phase	Name and Species	Information
1. Copy-AkCl	LiqLiKCsCl	- liquid LiCl-KCl-CsCl
	3 spec. 4 elem. #1	
	LiCl	
	KCl	
2. Copy-Iron	CsCl	
	Fe-liq	- liquid steel with solutes C, Mn, O
	4 spec. 4 elem. #2	
	Fe !	- this species must be present !
	C	0.0 < X < 0.10
3. Copy-Salt	Mn	0.0 < X < 0.10
	O	0.0 < X < 0.10
	Liq_Sublattice	- liquid salt Li,Na,K//F,S04 solution
	6 spec. 6 elem. #4	
	LiF	
	Li2SO4	
	NaF	
	Na2SO4	

To list the interaction parameters in the "Salt" phase of Copysoln.sln, click on the name of the phase. → See next slide

Interaction parameters of the "Salt" phase of CopySoln.sln

- See previous slide for input

Private Solution Database Interactions - Copy-Salt				
Phase	{0 - 22}	Interaction	i j k	Expression
3. Copy-Salt	(0)	BGP - Li;Na // F	1 1	-7565.0000256 +1.60700000848*T
	(1)	BGP - Li;Na // F	1 2	-368.000000424 +1.1240000108*T
	(2)	BGP - Li;Na // SO4	1 1	-4247.0001616
	(3)	BGP - Li;Na // SO4	2 1	-1443.99998752
	(4)	BGP - Li;Na // F	1 1	-19250.9998896 +1.37500001176*T
	(5)	BGP - Li;K // F	1 2	-1204.99999144
	(6)	BGP - Li;K // F	1 3	4731.9998184
	(7)	BGP - Li;K // F	2 1	3.1460000172*T
	(8)	BGP - Li;K // SO4	1 1	-7565.0000256 +1.60700000848*T
	(9)	BGP - Li;K // SO4	2 1	-3891.00000288 -1.00000001616*T
	(10)	BGP - Na;K // F	1 1	-335.000001648 +2.54100001872*T
	(11)	BGP - Na;K // SO4	1 1	-2196.9999904
	(12)	BGR - Li // F,SO4	0	-988.00001128 -2.35199999416*T
	(13)	BGR - Li // F,SO4	1	358.999998856
	(14)	BGR - Na // F,SO4	0	55.999999064 -1.21399998464*T
	(15)	BGR - Na // F,SO4	1	217.00000108 -2.04399998048*T
	(16)	BGR - K // F,SO4	0	-1262.99998016 -1.52199999832*T
	(17)	BGR - K // F,SO4	1	-486.00000936
	(18)	BGP - Li;Na;K // F	1 1 1	-300.000000664
	(19)	BGP - Li;Na;K // SO4	1 1 2	399.999998096
	(20)	BGP - Li;Na // F,SO4	1 1 1	-8483.0001688 +3.0689999824*T
	(21)	BGP - Li;K // F,SO4	1 1 1	-29893.000124 +14.0169999856*T
(22)	BGP - Na;K // F,SO4	1 1 1	-6338.0001856 +3.58799999472*T	

Displaying the interaction parameters for all the phases stored in

CopySoln.sln

1. Click on Sort Solutions

F View Data ALL solutions - Copy datasets
File Edit Sort Solutions Summary Databases Units Atomic Wts. Table Graph Help << Back
7 Solutions Copysoln solution database.
Solutions sorted by phase number [see 'Sort Solutions']

Phase	Name and Species	Information
1. Copy-AkCl	LiqLiKCsCl	- liquid LiCl-KCl-CsCl
	3 spec. 4 elem. #1	
	LiCl	
	KCl	
2. Copy-Iron	Fe-liq	- liquid steel with sol
	4 spec. 4 elem. #2	
	Fe l	- this species must b
	C	0.0 < X < 0.10
Mn	0.0 < X < 0.10	

Sort Solutions Summary Database
 by phase number
 by alphabet
 by number of species
 by number of elements
 by solution model #
 list all the species
 do not list all the species
List all solution interactions ...

2. Click on „List all“

F Private Solution Database Interactions - all phases
File Edit

Phase (7)	(0 - 22)	Interaction	i j k	Expression
1. Copy-AkCl	(0)	BGP - LiCl;KCl	1 1	-17570.0000672 +7.2670000648*T
	(1)		2 1	-377.000001992 -4.9579998336*T
	(2)		1 1	-19455.6 +20.5409998912*T
	(3)	BGP - LiCl;CsCl	2 1	-7447.52 -3.28499998656*T
	(4)		2 2	-9079.28
	(5)	BGP - KCl;CsCl	1 1	794.99999904
	(6)	BGP - LiCl;KCl;CsCl	1 1 1	-19999.9999048
2. Copy-Iron	(0)	BGP - C	1	17235.97923 -14.35915877*T
	(1)	BGP - Mn	1	5587.35072
	(2)	BGP - O	1	-117118.18786 +24.51117548*T
	(3)	BGP - C	2	199332.06274
	(4)	BGP - C;Mn	1 1	-29117.41402
	(5)	BGP - C;O	1 1	-317689.11259
	(6)	BGP - Mn;O	1 1	-73192.63153
3. Copy-Salt	(0)	BGP - Li;Na // F	1 1	-7565.0000256 +1.60700000848*T
	(1)		1 2	-368.000000424 +1.1240000108*T
	(2)	BGP - Li;Na // SO4	1 1	-4247.0001616
	(3)		2 1	-1443.99998752
	(4)		1 1	-19250.9998896 +1.37500001176*T
	(5)	BGP - Li;K // F	1 2	-1204.99999144
	(6)		1 3	4731.9998184

Interacting with Equilib / Phase Diagram

Let us say you have stored a solution database (such as CopySoln.sln) and have added it to the database pool in **Equilib** or **Phase Diagram**.

Now you are using the **Solution** module to edit and make changes to the parameters and you wish to use the updated database immediately in **Equilib** (or **Phase Diagram**) calculations to see the effect of the changes.

Each time you save the changes in **Solution** you want the new data to be transmitted to **Equilib**.

In the **Equilib** «Data Search Window» (see Reactants Window) there is a «**Refresh databases**» button that causes the program to re-read the databases.

1. In **Solution** edit the data. Click on «**File > Save**»
2. In **Equilib** or **Phase Diagram** click on «**Data Search**» > «**Refresh databases**»

In **Equilib** and **Phase Diagram** when you click on «**Calculate ...**» the program automatically checks and re-reads the databases if they have been edited. That is, it is **NOT** necessary for you to «**Refresh databases**» - this is done for you.