FactSage 7.1 Solution – Introduction

Solution Introduction

This *Solution Introduction Slide Show* introduces users to the **Solution** module of **FactSage 7.1**. 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

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 The old solution files (*.dat, *.sdb, *.sda) have been replaced by two new files :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. Copysoln.sln, Testsoln.sln
2. *soln.sdc file - protected public data, e.g. FTOxid53soln.sdc (FToxid)

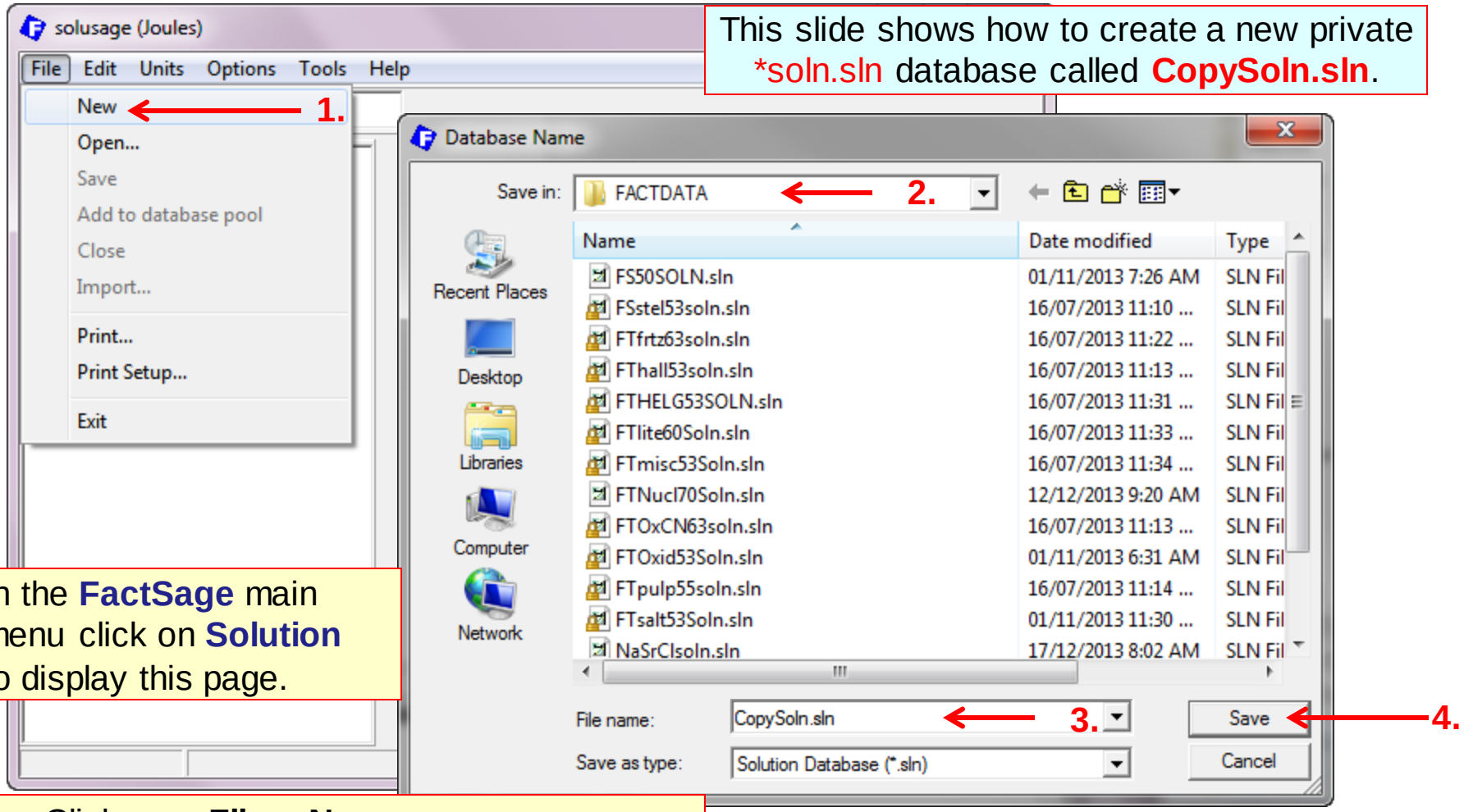
In **FactSage 7.1** with the **Solution** module :

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 *soln.sln database called **CopySoln.sln**.

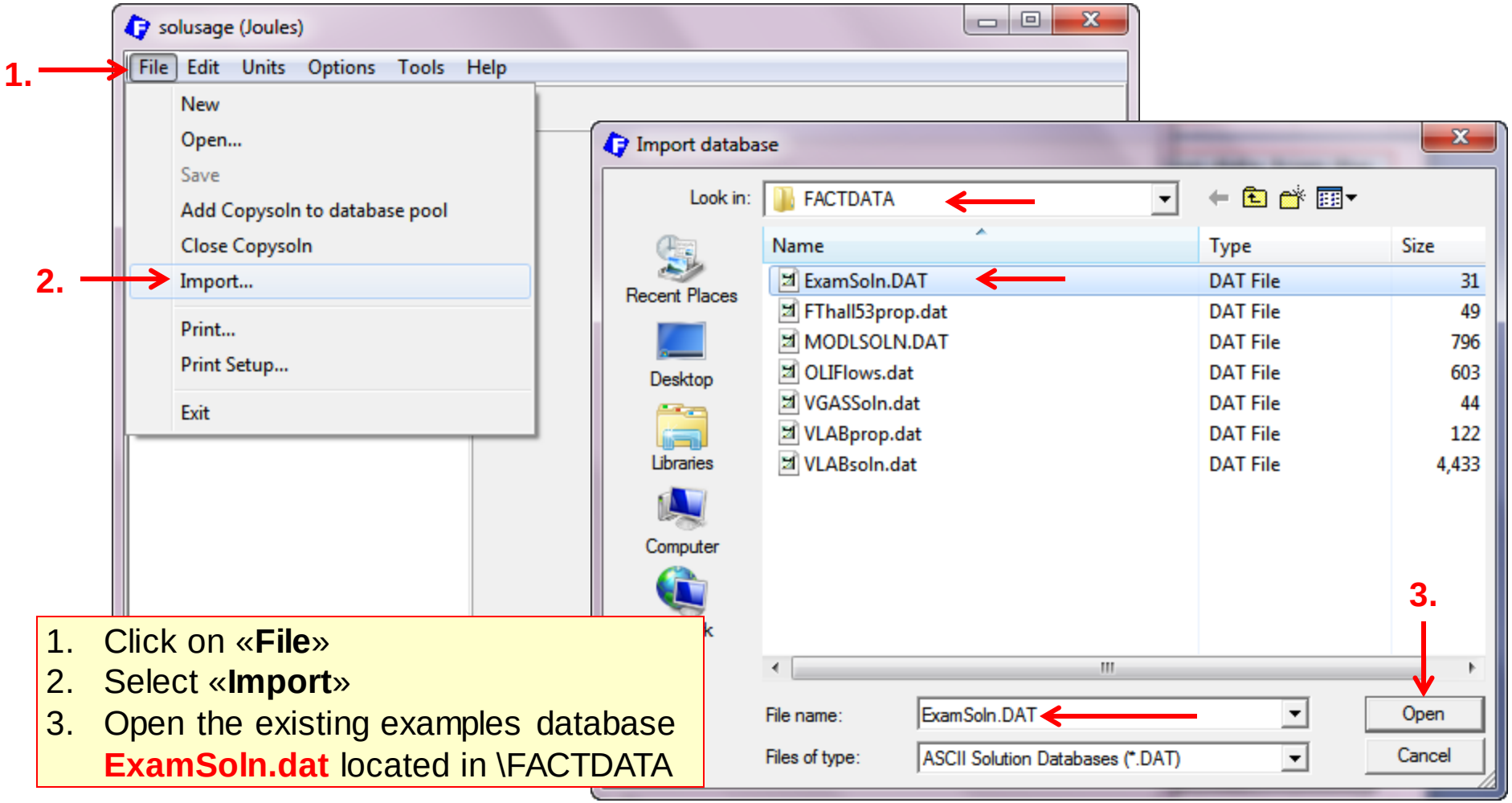


In the **FactSage** main menu click on **Solution** to display this page.

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

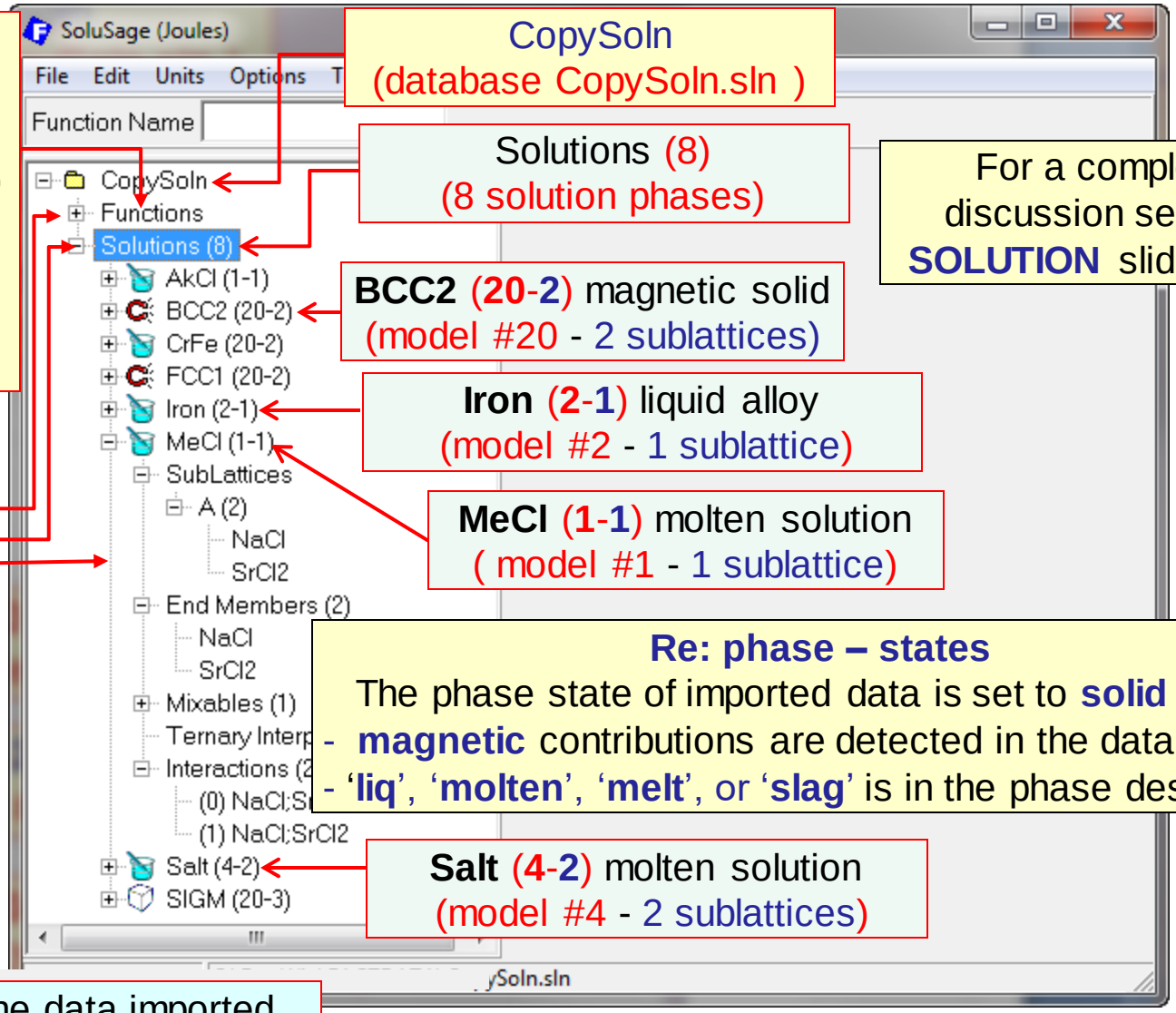


1. Click on «**File**»
2. Select «**Import**»
3. Open the existing examples database **ExamSoln.dat** located in \FACTDATA

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)

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

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)

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**

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

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
Exss BGP A0A1
```

WIN INS Tab: 9 Col: 1 Ln: 1

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.

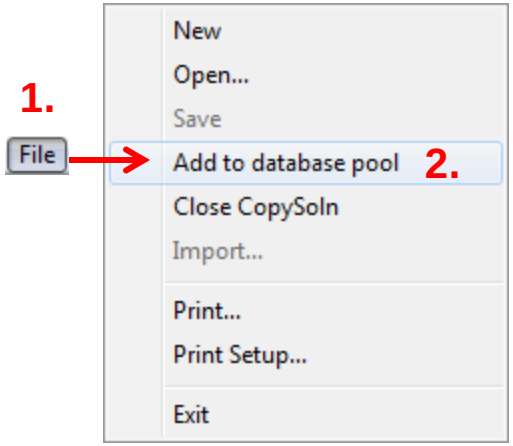
You can use a text editor to edit and save the file contents. But be careful - there is no error checking when you use a text editor ! Therefore, we suggest that you use the **Solution** module for editing.

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 >>.

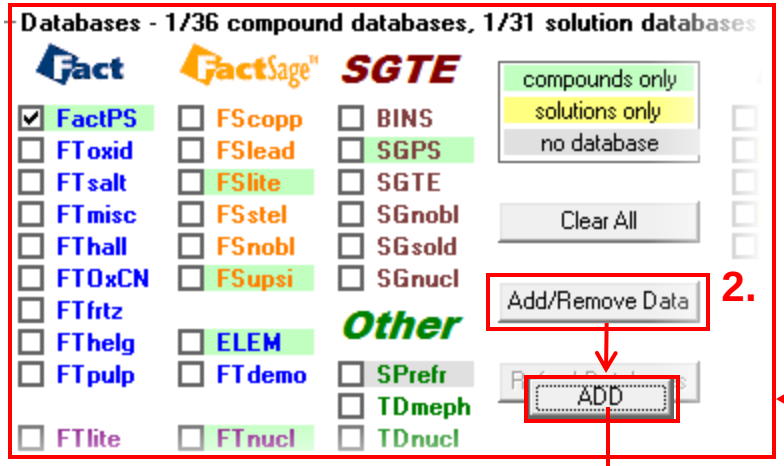
1. Click on «**File**»
2. Select «**Add to database pool**»

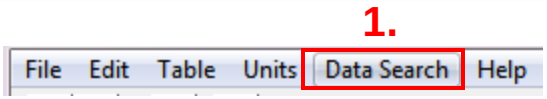


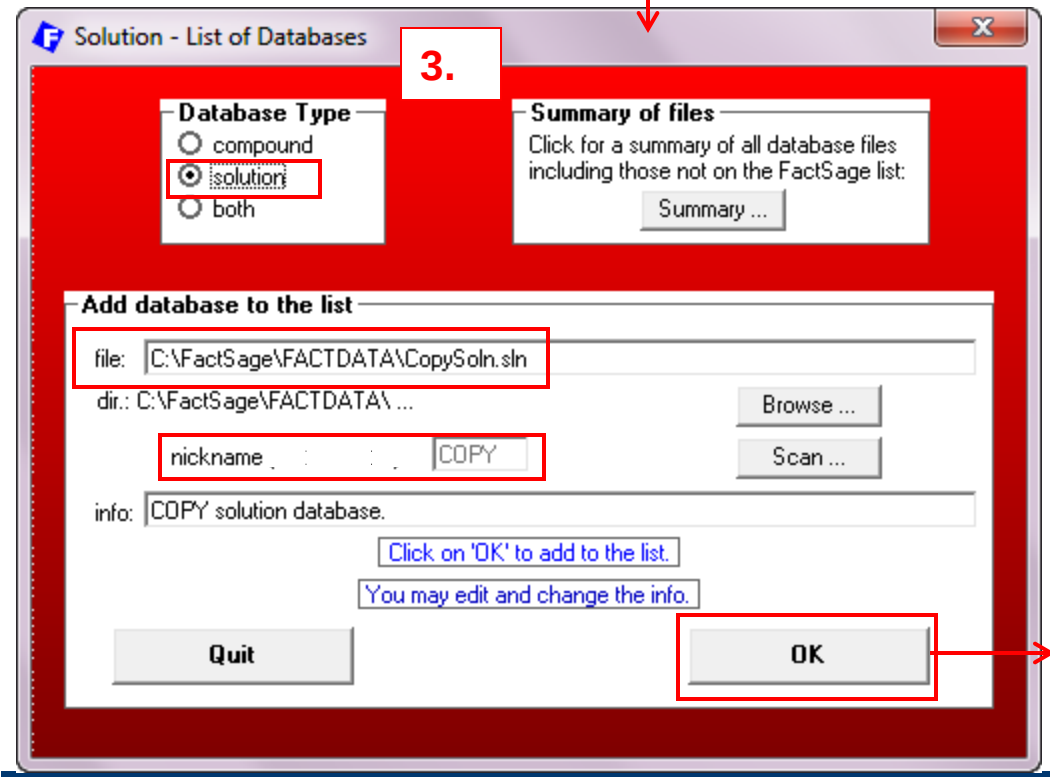
Include CopySoln.sln in **Equilib** Calculations – the old way

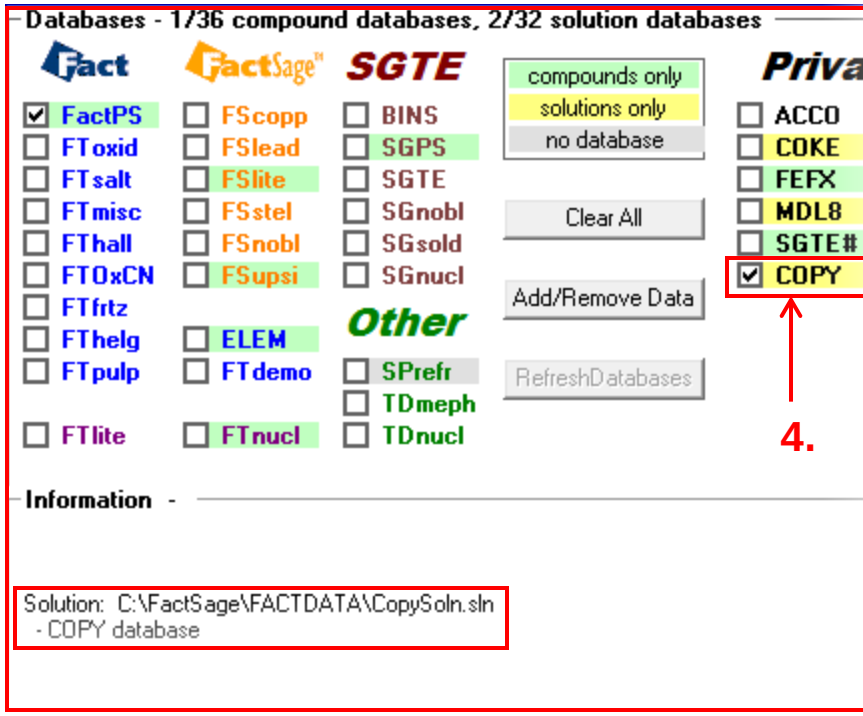
This is the "old" way of "adding" to the database list:

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

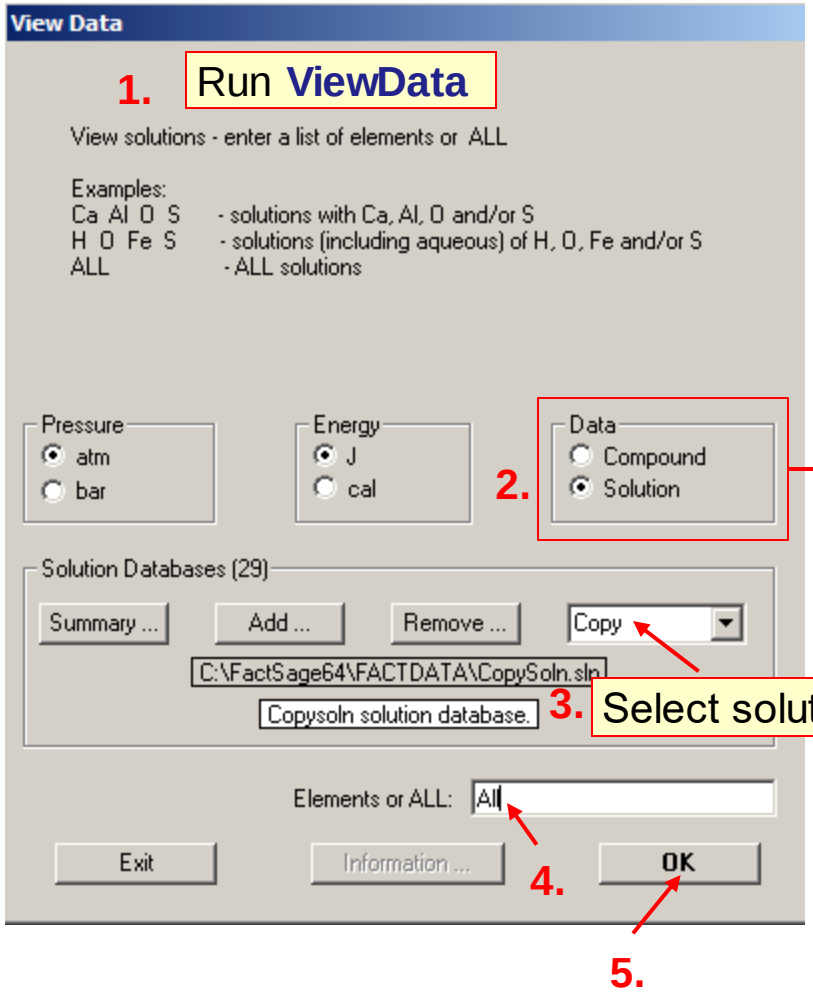




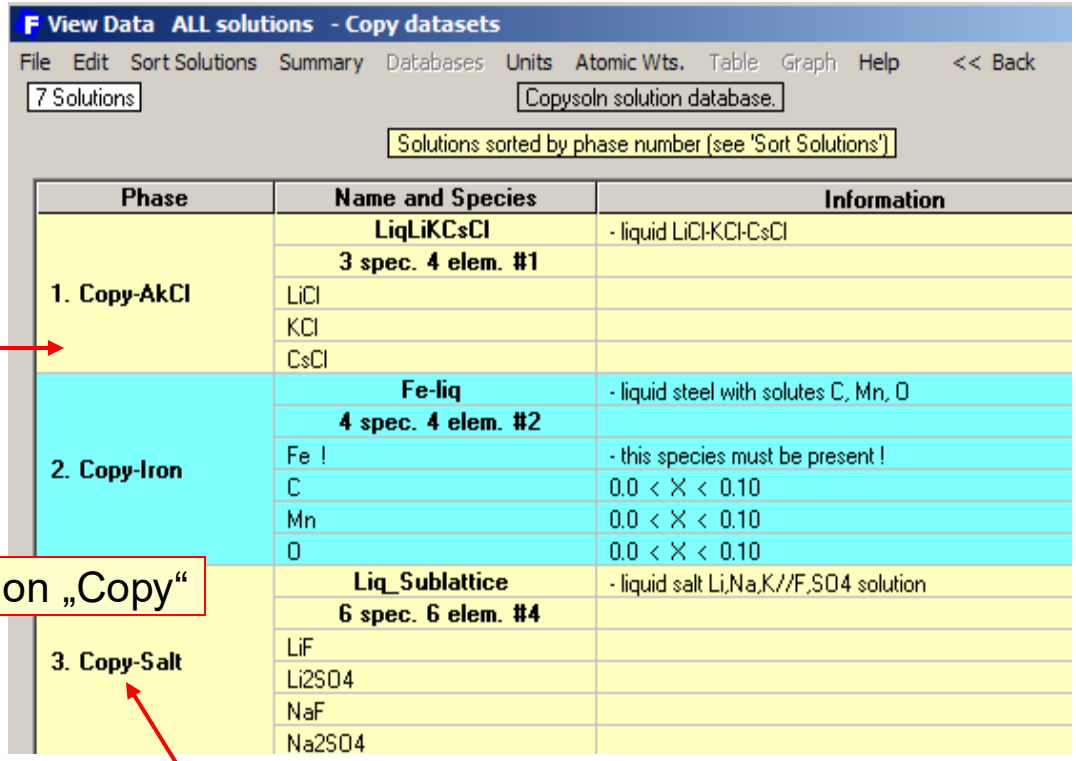




Displaying the solution data with **ViewData**



ViewData Summary of **Copy** solution database



Phase	Name and Species	Information
1. Copy-AkCl	LiqLiKCsCl	- liquid LiCl-KCl-CsCl
	3 spec. 4 elem. #1	
	LiCl	
	KCl	
	CsCl	
2. Copy-Iron	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
	Mn	0.0 < X < 0.10
	O	0.0 < X < 0.10
3. Copy-Salt	Liq_Sublattice	- liquid salt Li,Na,K//F,SO4 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

File Edit

Phase	(0 - 22)	Interaction	i j k	Expression
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)	BGP - Li;K // F	1 1	-19250.9998896 +1.37500001176*T
	(5)		1 2	-1204.99999144
	(6)		1 3	4731.9998184
	(7)		2 1	3.1460000172*T
	(8)	BGP - Li;K // SO4	1 1	-7565.0000256 +1.60700000848*T
	(9)		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)		1	358.999998856
	(14)	BGR - Na // F,SO4	0	55.999999064 -1.21399998464*T
	(15)		1	217.00000108 -2.04399998048*T
	(16)	BGR - K // F,SO4	0	-1262.99998016 -1.52199999832*T
	(17)		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 1	-8483.0001688 +3.0689999824*T
	(21)	BGP - Li;K // F,SO4	1 1 1 1	-29893.000124 +14.0169999856*T
	(22)	BGP - Na;K // F,SO4	1 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	
	CsCl	
2. Copy-Iron	Fe-liq	- liquid steel with solu
	4 spec. 4 elem. #2	
	Fe !	- this species must be
	C	0.0 < X < 0.10
	Mn	0.0 < X < 0.10

Sort Solutions | Summary | Databases

- ✔ 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)	BGP - LiCl;CsCl	1 1	-19455.6 +20.5409998912*T
	(3)		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)	BGP - Li;K // F	1 1	-19250.9998896 +1.37500001176*T
	(5)		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.