FactXML

Customizing the
Equilib results

The **FactXML** add-in

FactXML is an add-in to the ***Equilib*** program that enables you to edit the results of a calculation and save customized outputs as templates. There is no limitation to the number of templates.

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- **Set as Variable** and the **Formula** Feature
- **Draw Graph** and **Copy points**
- **Multiple lines** graph

Introduction

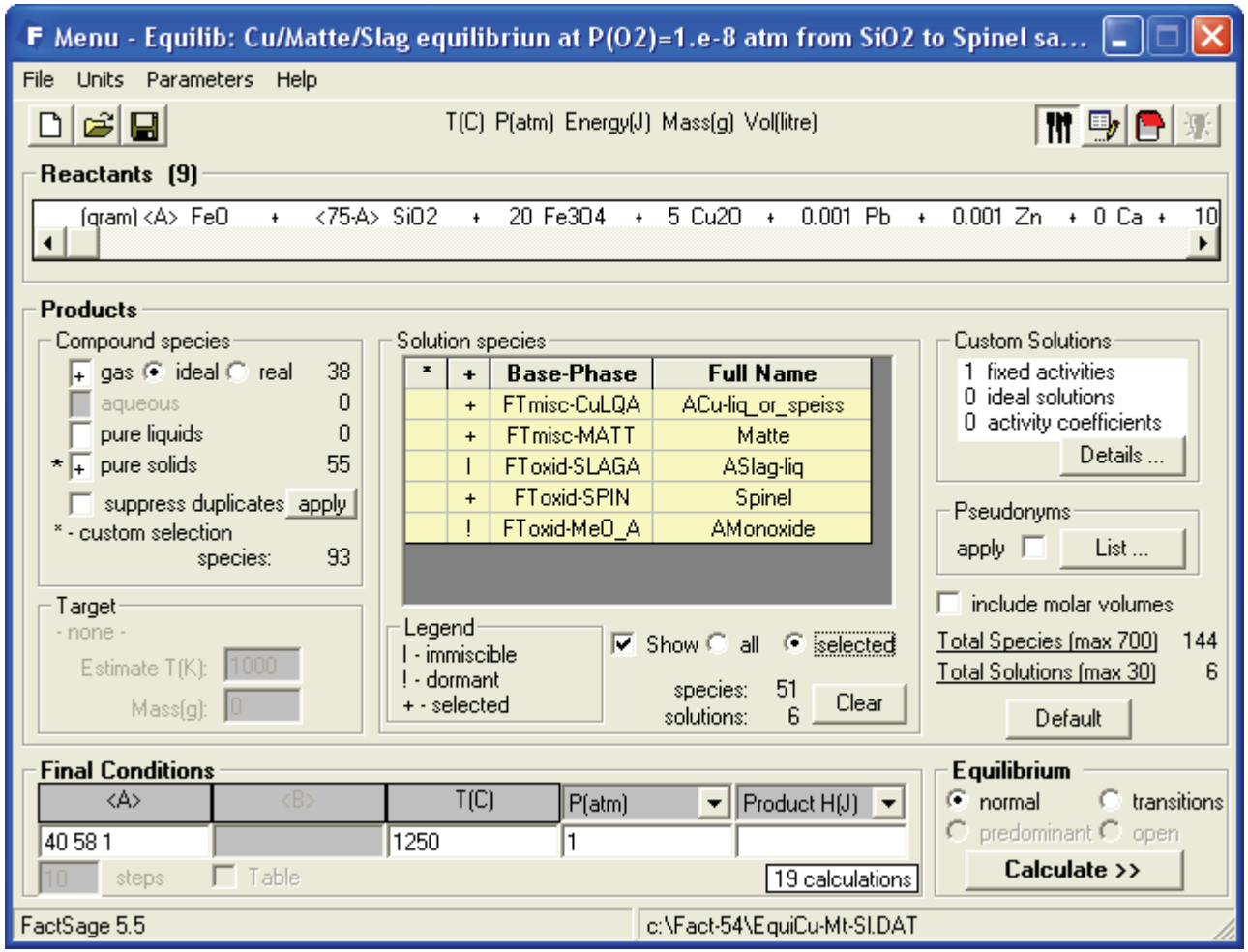
The following two slides show you how to access **FactXML**.

The starting point is an ***Equilib*** calculation of a slag-matte-metal equilibrium in a copper converter at 1250°C under a partial pressure of O_2 of 10^{-8} atm. It shows the effect of a variation in the composition of the slag from SiO_2 to spinel saturation.

Generating an *Equilib* output

The reaction is based on **100 grams of slag** + **100 grams of matte** and **100 g of metal**:

<A> FeO + <75-A> SiO_2 + 20 Fe_3O_4 + 5 Cu_2O + 100 Cu_2S + 0.001 Pb + 0.001 Zn + 0 Ca + 100 Cu



19 pages of results are generated with <A> varying from 40 to 58 in steps of 1

Accessing **FactXML**

This is the conventional **FACT** format output. Let us edit it with **FactXML**.

F Results - Equilib A=40 (page 1/19)

Output Edit Show Pages

T(C) P(atm) Energy(J) Mass(g) Vol(litre)

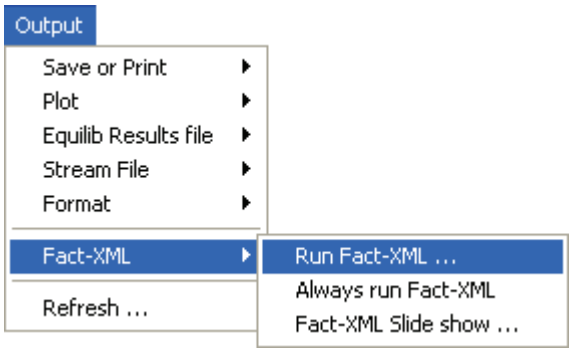
A=54 | A=55 | A=56 | A=57 | A=58 |

A=40 | A=41 | A=42 | A=43 | A=44 | A=45 | A=46 | A=47 | A=48 | A=49 | A=50 | A=51 | A=52 | A=53 |

```
(gram) <A> FeO +  <75-A> SiO2 +  20 Fe3O4 +  5 Cu2O +

(gram) 0.001 Pb +  0.001 Zn +  0 Ca +  100 Cu2S +

(gram) 100 Cu =

-  1.207     O2

   0.00000     litre (  0.55233     vol% SO2                          FACT53
                     +  0.27813E-02 vol% SO                           FACT53
                     +  0.11641E-02 vol% Cu                           FACT53
                     +  0.19754E-03 vol% S2                           FACT53)
                        (1250.00 C, 1 atm, gas_ideal, a=0.55659E-02)

+   108.75      gram  (  0.38518E-03 wt.% Pb                          FTmisc
                     +   98.088     wt.% Cu                           FTmisc
                     +  0.39541E-01 wt.% Fe                           FTmisc
                     +   1.8546     wt.% S                            FTmisc
                     +  0.17371E-01 wt.% O                            FTmisc)
                        (1250.00 C, 1 atm, ACu-liq_or_speiss)

+   93.395      gram  (   19.389     wt.% S                            FTmisc
                     +  0.57483     wt.% Fe                           FTmisc
                     +   80.036     wt.% Cu                           FTmisc
                     +  0.10390E-03 wt.% Pb                           FTmisc)
                        (1250.00 C, 1 atm, Matte)
```

Access **FactXML** using:

1. the Output menu



or:

2. by clicking on the **FactXML** button in the toolbar

The **FactXML** Viewer Window

The following five slides show you the **FactXML** editing features:

- The XML viewer graphic interface
- The menu bar
- The changing units capabilities
- The toolbar (including the searching options)
- The drop down menu.

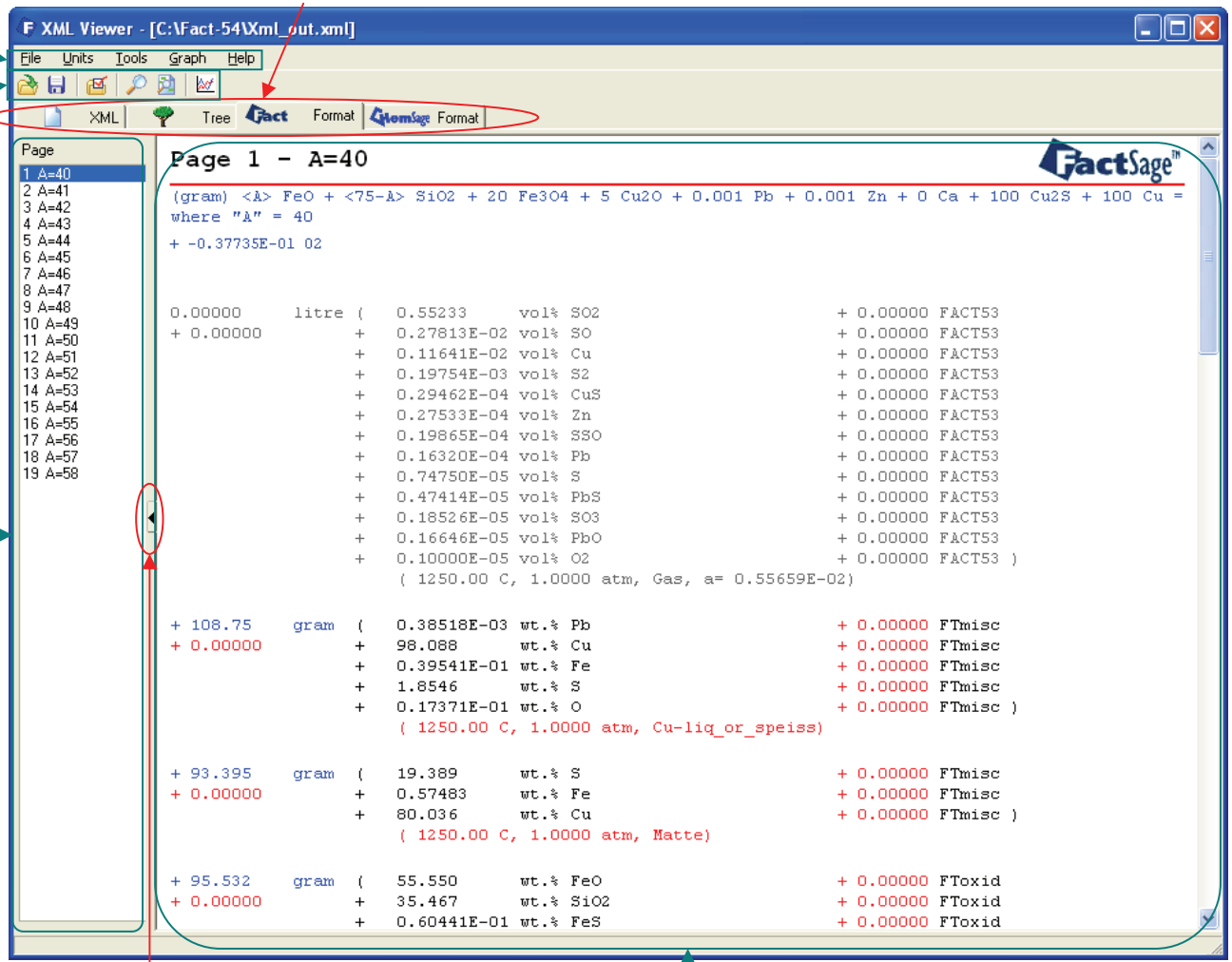
The **Options** and the **Graph Setup** editing features are shown in detail in sections 4 and 5.

The **XML Viewer** Window

Tabs including **Fact** format and **ChemSage** format

Menu bar

Tool bar



Page pane. Click on a page to display it.

Click on the triangle to open/close the page pane

Results pane. A right-click opens a drop-down menu.

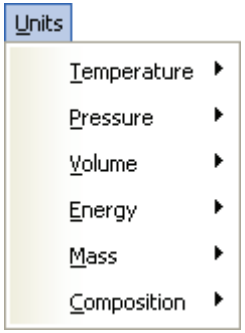
The Menu Bar

File Units Tools Graph Help

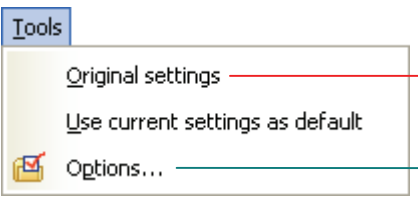
Opens the Load template… dialog box
Select your FactXML template to load it.

Saves a template file that contains all your current settings **(font, colors, units, etc.)**.

Lists up to the 5 last template files used.
Click on a template file to load it.

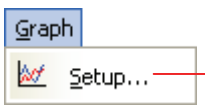


See next slide for more details



Returns to the output original settings defined in ***Equilib***

Opens the Options… dialog box (see slide 4.1)

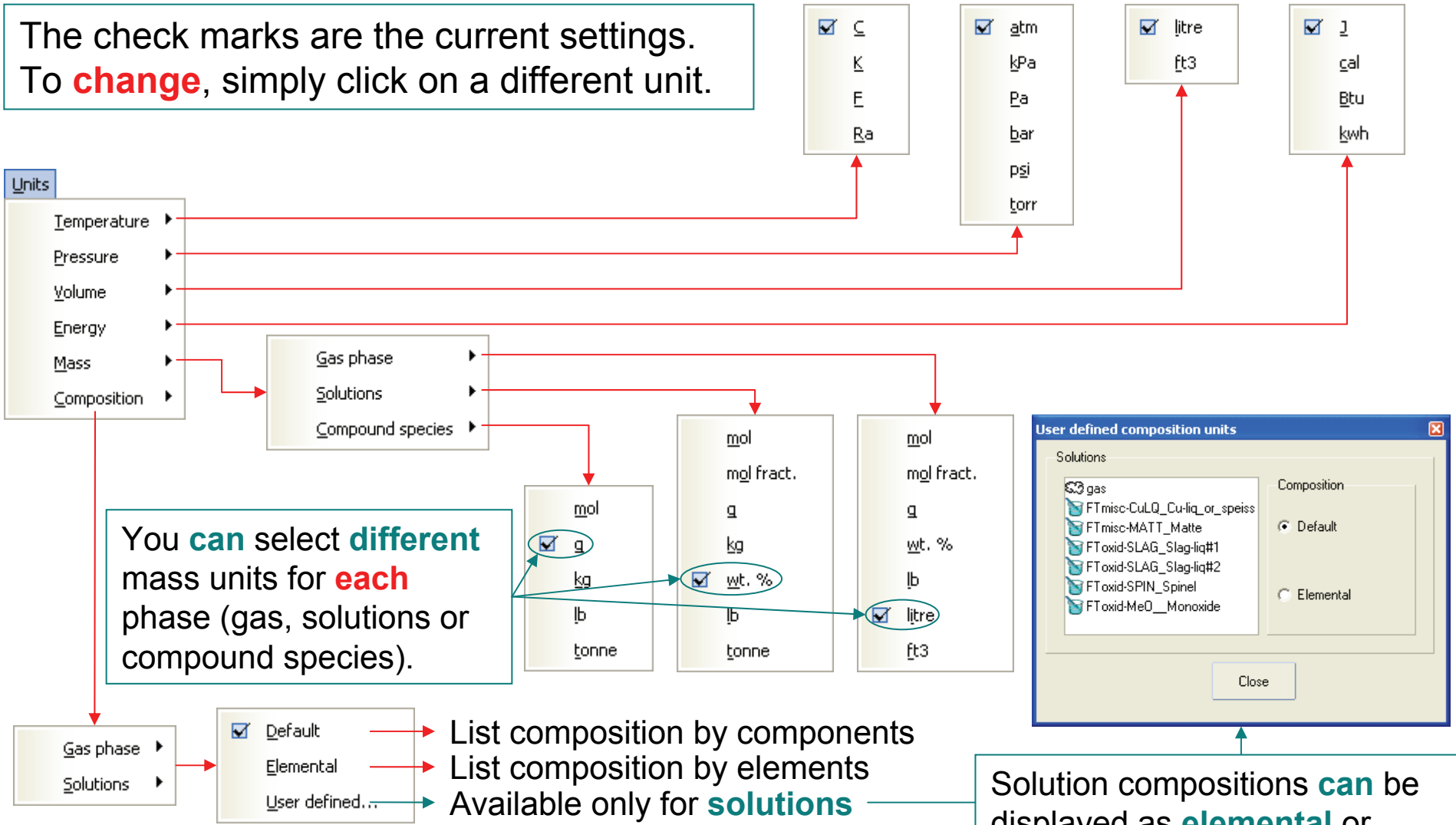


Opens the Set up Graph feature
(see slide 5.1)

Opens this slide show

Changing Units

The check marks are the current settings.
To **change**, simply click on a different unit.

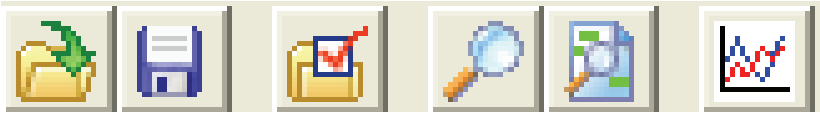


You **can** select **different** mass units for **each** phase (gas, solutions or compound species).

List composition by components
List composition by elements
Available only for **solutions**

Solution compositions **can** be displayed as **elemental** or **component** (default) values

The Toolbar



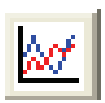
Open an XML file

Save an XML file

Options … : Opens Options dialog box (see slide 4.1)

Search: Opens the find dialog box

Search and Highlight: Opens the Search and Highlight dialog box



Graph: Opens the Graph Setup feature (see slide 5.1)

Drop-down Menu – Results Pane

A **right-click** in the **results pane** opens a **drop-down menu**

Access to the changing **units** feature (see slide 3.3 for details)

Only the stable phases are shown

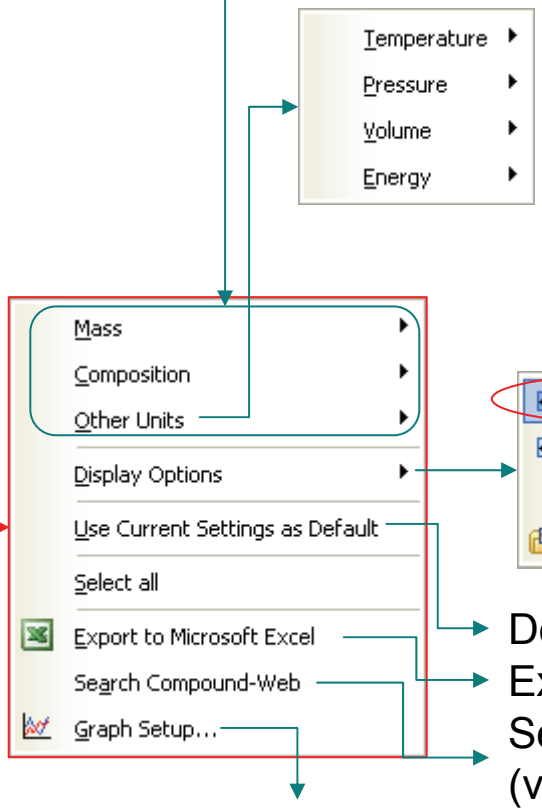
Access the **Options** window

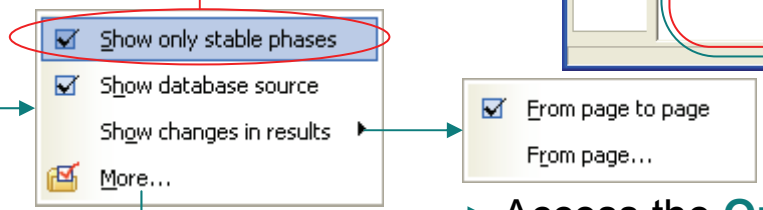
Define your current settings as default settings

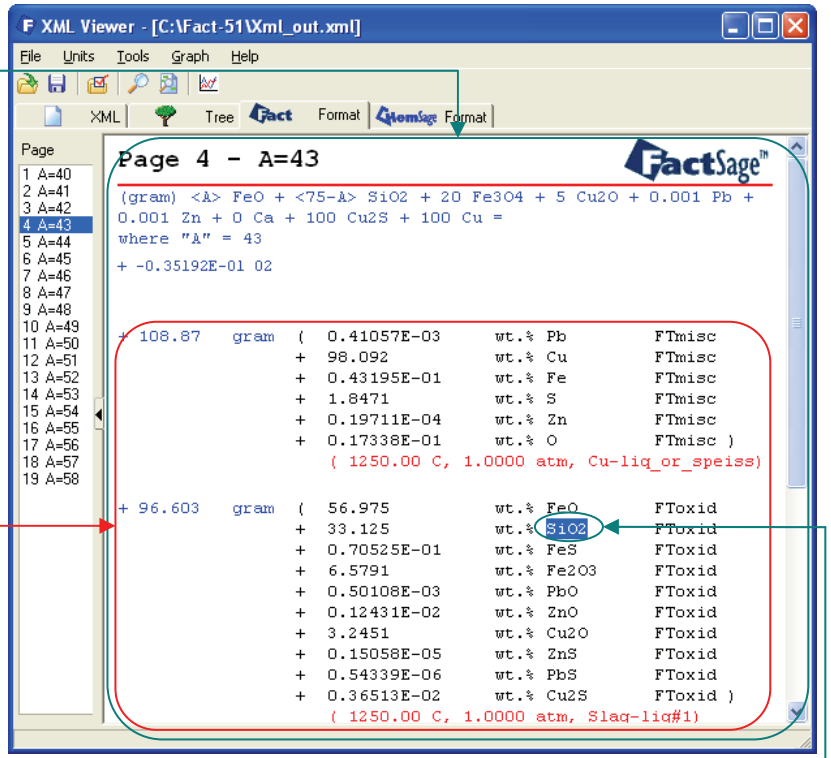
Export the current page to a Microsoft Excel spreadsheet

Search the **selected** compound in the Compound-Web database (via the Internet)

Opens the **Graph Setup** feature







Options features

Use the **Options…** dialog box, if you want to:

- Show
  - Only the stable phases
  - The database sources
  - The data changes: either incremental or cumulative
- Uses the pseudonyms defined previously in ***Equilib***
- Format font and colors
- Define and select a default template
- Set a different cut-off limit and the number of significant digits for each phase (gas, solutions and compound species)
- Set order, in each phase, by: name (alphabetical), composition (amount), activity, mass or reset to **FactXML** default values.
  For the solutions, you can also order the solution list.

Options… General Tab

Uses the pseudonyms defined previously in ***Equilib***

Opens a dialog box for the selection of another template

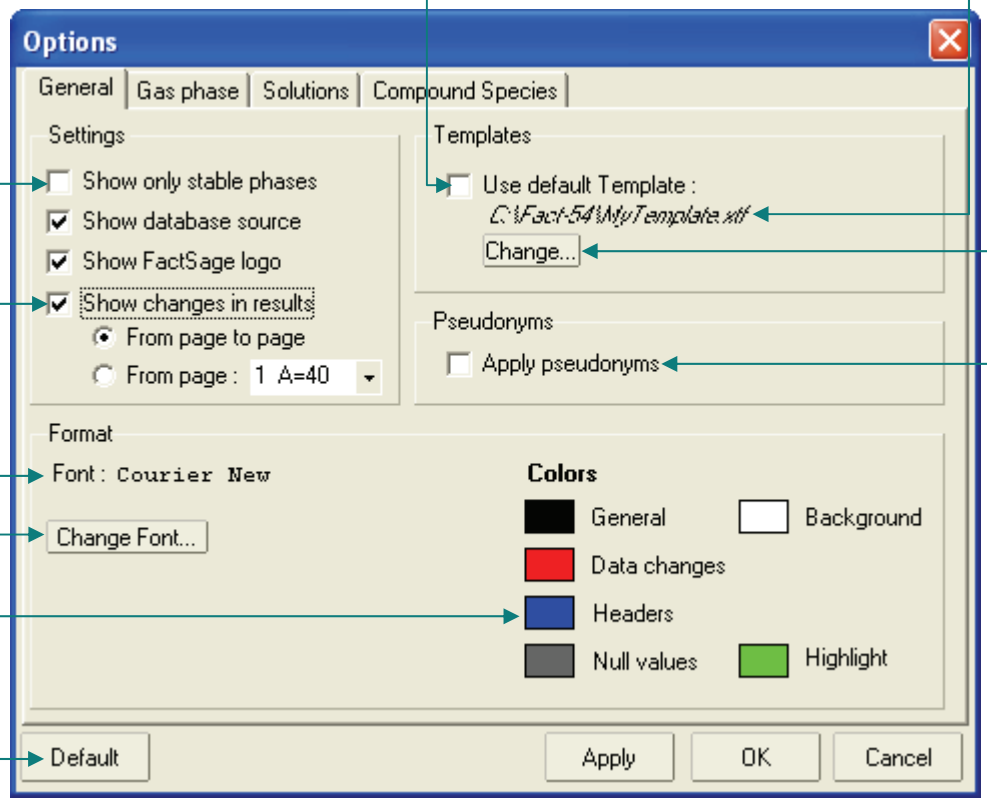
Location of the default XML template file

Check to use the following XML Template File as default

Select « **Show only stable phases** » to hide the products that have activities less than 1.

Select « **Show changes in results** »

1. « **From page to page** » to view the **incremental** changes in the output from the previous page (see slide 4.2);
2. « **From page: #** *page* » to view the **cumulative** changes in the output from the *selected page* (see slide 4.3).



Current font used

Opens the Font dialog box

Click on the color rectangle to open the Color dialog box

Click to restore original default FactXML values.

Options… General Tab / Settings and Colors

Settings

- [ ] Show only stable phases
- [x] Show database source
- [x] Show FactSage logo
- [x] Show changes in results
  - (•) From page to page
  - ( ) From page : 1 A=40

Incremental changes from **page 2 A=41**

XML Viewer - [C:\Fact-54\Xml_out.xml]

File Units Tools Graph Help

XML | Tree | Fact Format | GlobSage Format

Page
1 A=40
2 A=41
3 A=42
4 A=43
5 A=44
6 A=45
7 A=46
8 A=47
9 A=48
10 A=49
11 A=50
12 A=51
13 A=52
14 A=53
15 A=54
16 A=55
17 A=56
18 A=57
19 A=58

Page 3 - A=42

```
(gram) <A> FeO + <75-A> SiO2 + 20 Fe3O4 + 5 Cu2O + 0.001 Pb + 0.001 Zn + 0 Ca + 100 Cu2S + 100 Cu =
where "A" = 42
+ -0.36256E-01 02

0.00000      litre (   0.55184     vol% SO2                    - 0.38610E-03 FACT53
+ 0.00000          +   0.27788E-02 vol% SO                     - 0.19440E-05 FACT53
                   +   0.11641E-02 vol% Cu                     + 0.90000E-08 FACT53
                   +   0.19718E-03 vol% S2                     - 0.27600E-06 FACT53
                   +   0.29536E-04 vol% Zn                     + 0.18180E-05 FACT53
                   +   0.29436E-04 vol% CuS                    - 0.20370E-07 FACT53
                   +   0.19830E-04 vol% SSO                    - 0.27750E-07 FACT53
                   +   0.16911E-04 vol% Pb                     + 0.52759E-06 FACT53
                   +   0.74683E-05 vol% S                      - 0.52250E-08 FACT53
                   +   0.49087E-05 vol% PbS                    + 0.14982E-06 FACT53
                   +   0.18510E-05 vol% SO3                    - 0.12940E-08 FACT53
                   +   0.17249E-05 vol% PbO                    + 0.53813E-07 FACT53
                   +   0.10000E-05 vol% O2                     + 0.00000     FACT53 )
                       ( 1250.00 C, 1.0000 atm, Gas, a= 0.55609E-02)

+ 108.80     gram (   98.090      wt.% Cu                     + 0.16800E-02 FTmisc
+ 0.69200E-01     +   1.8504       wt.% S                      - 0.32530E-02 FTmisc
                   +   0.41578E-01 wt.% Fe                     + 0.15803E-02 FTmisc
                   +   0.17353E-01 wt.% O                      - 0.14200E-04 FTmisc
                   +   0.39872E-03 wt.% Pb                     + 0.12126E-04 FTmisc )
                       ( 1250.00 C, 1.0000 atm, Cu-liq_or_speiss)

+ 96.636     gram (   56.384      wt.% FeO                    + 0.63733     FToxid
- 0.44490E-01      +   34.149       wt.% SiO2                   - 1.0186      FToxid
                   +   6.0949       wt.% Fe2O3                  + 0.43998     FToxid
                   +   3.3008       wt.% Cu2O                   - 0.63134E-01 FToxid
                   +   0.66015E-01 wt.% FeS                    + 0.43343E-02 FToxid
                   +   0.35129E-02 wt.% Cu2S                   + 0.12962E-03 FToxid
                   +   0.12455E-02 wt.% ZnO                    - 0.20570E-05 FToxid
                   +   0.51880E-03 wt.% PbO                    - 0.18066E-04 FToxid )
                       ( 1250.00 C, 1.0000 atm, Slag-liq#1)
```

Colors

- General
- Background
- Data changes
- Headers
- Null values
- Highlight

Options… Show cumulative changes

Settings

- [ ] Show only stable phases
- [x] Show database source
- [x] Show FactSage logo
- [x] Show changes in results
  - ( ) From page to page
  - (•) From page : 1 A=40

Cumulative changes from **page 1 A = 40** to **page 3 A = 42** (compare with the previous slide)

XML Viewer - [C:\Fact-54\Xml_out.xml]

File Units Tools Graph Help

XML | Tree | Fact Format | ChemSage Format

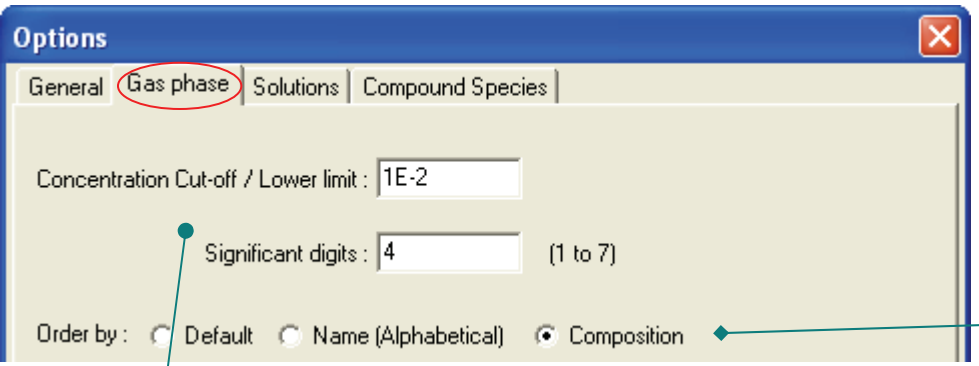
Page

1 A=40
2 A=41
3 A=42
4 A=43
5 A=44
6 A=45
7 A=46
8 A=47
9 A=48
10 A=49
11 A=50
12 A=51
13 A=52
14 A=53
15 A=54
16 A=55
17 A=56
18 A=57
19 A=58

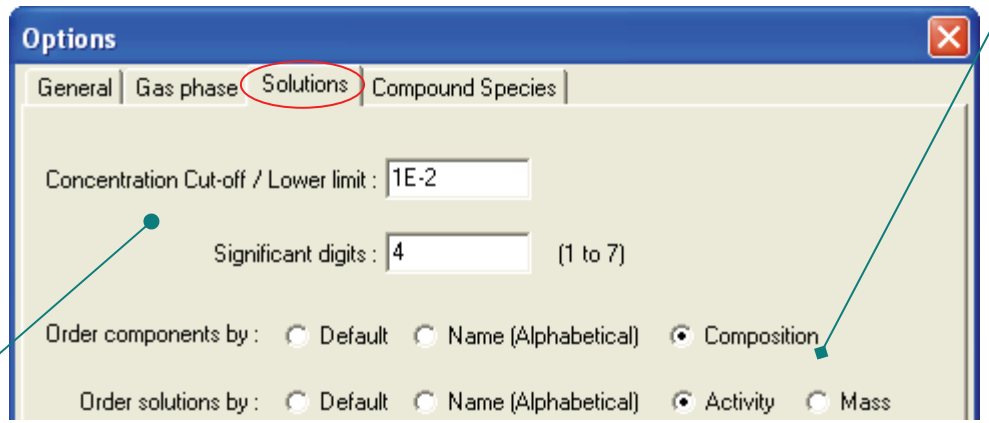
Page 3 - A=42

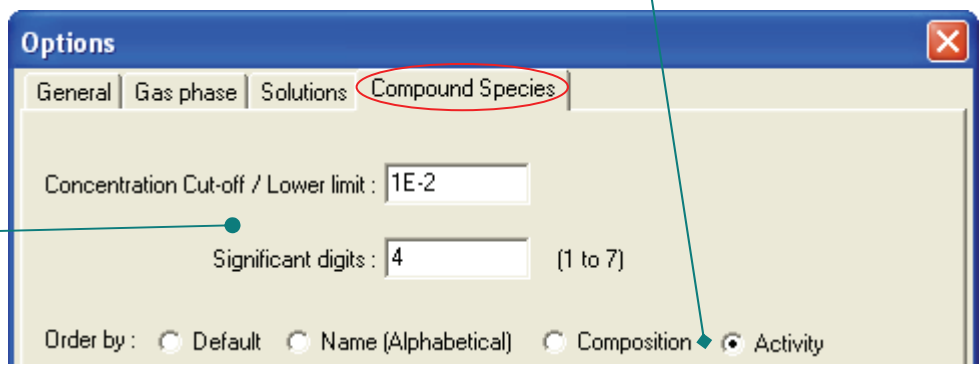
```
(gram) <A> FeO + <75-A> SiO2 + 20 Fe3O4 + 5 Cu2O + 0.001 Pb + 0.001 Zn + 0 Ca + 100 Cu2S + 100 Cu =
where "A" = 42
+ -0.36256E-01 O2

0.00000      litre (   0.55184      vol% SO2                    - 0.49830E-03 FACT53
+ 0.00000          +   0.27788E-02 vol% SO                     - 0.25090E-05 FACT53
                   +   0.11641E-02 vol% Cu                     + 0.12000E-07 FACT53
                   +   0.19718E-03 vol% S2                     - 0.35620E-06 FACT53
                   +   0.29536E-04 vol% Zn                     + 0.20032E-05 FACT53
                   +   0.29436E-04 vol% CuS                    - 0.26280E-07 FACT53
                   +   0.19830E-04 vol% SSO                    - 0.35820E-07 FACT53
                   +   0.16911E-04 vol% Pb                     + 0.59120E-06 FACT53
                   +   0.74683E-05 vol% S                      - 0.67430E-08 FACT53
                   +   0.49087E-05 vol% PbS                    + 0.16733E-06 FACT53
                   +   0.18510E-05 vol% SO3                    - 0.16710E-08 FACT53
                   +   0.17249E-05 vol% PbO                    + 0.60300E-07 FACT53
                   +   0.10000E-05 vol% O2                     + 0.00000     FACT53 )
                       ( 1250.00 C, 1.0000 atm, Gas, a= 0.55609E-02)

+ 108.80     gram  (   98.090      wt.% Cu                     + 0.21700E-02 FTmisc
+ 0.53400E-01      +   1.8504       wt.% S                      - 0.42020E-02 FTmisc
                   +   0.41578E-01 wt.% Fe                     + 0.20373E-02 FTmisc
                   +   0.17353E-01 wt.% O                      - 0.18340E-04 FTmisc
                   +   0.39872E-03 wt.% Pb                     + 0.13536E-04 FTmisc )
                       ( 1250.00 C, 1.0000 atm, Cu-liq_or_speiss)

+ 96.636     gram  (   56.384      wt.% FeO                    + 0.83399     FToxid
+ 1.1041           +   34.149       wt.% SiO2                   - 1.3181      FToxid
                   +   6.0949       wt.% Fe2O3                  + 0.56155     FToxid
                   +   3.3008       wt.% Cu2O                   - 0.83193E-01 FToxid
                   +   0.66015E-01 wt.% FeS                    + 0.55741E-02 FToxid
                   +   0.35129E-02 wt.% Cu2S                   + 0.16605E-03 FToxid
                   +   0.12455E-02 wt.% ZnO                    - 0.17337E-04 FToxid
                   +   0.51880E-03 wt.% PbO                    - 0.26560E-04 FToxid )
                       ( 1250.00 C, 1.0000 atm, Slag-liq#1)
```

Gas Phase, Solutions and Compound Species



Set order by: name (alphabetical), composition (amount), activity, mass or reset to FactXML default values.
For the solutions, you can also order the solution list.





A different cut-off limit and the number of significant digits can be set for each phase.

Graph Setup

The following seven slides show you how you can edit a graph with the **FactXML Graph Setup** feature.

Note:

1. the flexibility offered by the **Formula** feature where you can calculate a mathematical expression with variables previously defined in **Graph Setup** and use it as an axis variable.
2. The possibility to draw **multiple lines** with a few clicks.

The **Graph Setup** Dialog Box

Graph Axes Preview frame

Variables frame

Y-axis frame

Y-axis (**X-axis**) panel – the view may differ with the variable selected.

Figure Settings frame

X-axis frame

Command frame

Graph - Setup

Favorites

Variables
clear
a
b
c

1
Activity
0
1
19
Page #

Figure Settings
Font size : 12
labels per line : 5
line colors...
Full Screen

Y-Axis
Activity
Y
+ variable
Formula :
MIN 0
MAX 1
STEP 0.01
Label every 0.1

X-Axis
Page #
X
+ variable
Formula :
MIN 1
MAX 19
STEP 0.18
Label every 1.8

Y X
Species/phases:

	Species	Phase	DB	Activity	MIN	MAX	Pseudonym
	O	Gas	FACT53	5.493E-10	5.493E-10	5.493E-10	
	O2	Gas	FACT53	1.000E-08	1.000E-08	1.000E-08	
	O3	Gas	FACT53	3.360E-21	3.360E-21	3.360E-21	
	Si	Gas	FACT53	1.947E-22	7.169E-23	1.947E-22	
	Si2	Gas	FACT53	3.199E-39	4.338E-40	3.199E-39	
	Si3	Gas	FACT53	6.609E-54	3.300E-55	6.609E-54	

Clear
mol mol fract. gram kg lb

Copy points
Draw >>
Cancel

Axis Frames and panels: selection of variables and scale

Click on the **down arrow** to access the variables menu.
Point and click on a variable to select it.
Some **variables** may require an additional selection in the axis **panel**.

Selection of the axis **scale**

Y
1/Y
ln(Y)
log10(Y)
exp(Y)

Y-Axis
Activity
Y
+ variable
Formula :
MIN 0
MAX 1
STEP 0.01
Label every 0.1

Set as **variable** button

Formula text box

Axis **settings**

Activity
Alpha <A>
Amount
Amount changes
Formula
Page #
Pressure
Temperature
Volume
Thermodynamic Properties

Cp
Cpint
Cppar
G
Gint
Gint (xs)
Gpar
Gpar (xs)
H
Hint
Hint (xs)
Hpar
Hpar (xs)
S
Sint
Sint (xs)
Spar
Spar (xs)
V
Vint

Y X
Species/phases:

Species	Phase	DB	Activity	MIN	MAX	Pseudonym
O	Gas	FACT53	5.493E-10	5.493E-10	5.493E-10	
O2	Gas	FACT53	1.000E-08	1.000E-08	1.000E-08	
O3	Gas	FACT53	3.360E-21	3.360E-21	3.360E-21	
Si	Gas	FACT53	1.947E-22	7.169E-23	1.947E-22	
Si2	Gas	FACT53	3.199E-39	4.338E-40	3.199E-39	
Si3	Gas	FACT53	6.609E-54	3.300E-55	6.609E-54	
SiO	Gas	FACT53	7.836E-11	2.886E-11	7.836E-11	

Clear mol mol fract. gram kg lb

Species panel

Click to **select** the species or the phases

Y X
Species/phases:

Species	Phase	DB	Sint (xs)	MIN	MAX	Pseudonym
Gas	-		-2.868E-01	-2.882E-01	-2.868E-01	
Cu-liq...	-	FTmisc	-3.533E-02	-3.533E-02	-3.155E-02	
Matte	-	FTmisc	-2.626E+00	-2.626E+00	-2.623E+00	
Slag-li...	-	FToxid	-7.054E-01	-1.335E+00	-7.054E-01	
Slag-li...	-	FToxid	-1.103E+00	-1.920E+00	-9.751E-01	
Spinel	-	FToxid	5.122E+00	5.122E+00	5.122E+00	
Mono...	-	FToxid	4.355E+00	4.355E+00	4.355E+00	

Clear mol mol fract. gram kg lb

Phases panel

Note: The same selections are possible with the X-axis

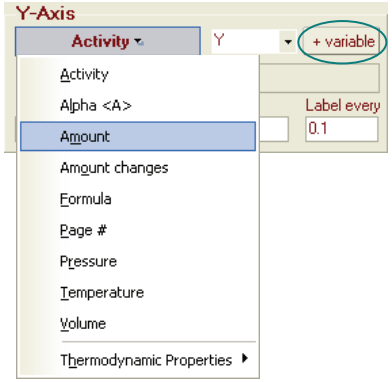
Set as variable and the Formula feature

For example, we wish to plot the Fe^{2+}/Fe^{3+} ratio in the slag vs Alpha <A>. The ratio is:

$$\frac{Fe^{2+}}{Fe^{3+}} = \frac{X_{FeO} + X_{FeS}}{2\,X_{Fe_2O_3}}$$

where X_c is the mole fraction of the compound c in the slag.

In order to use the Formula feature, we must select the variables: X_{FeO}, X_{FeS} and X_{Fe2O3} in the slag.



Selection of variables in the axis frame (either Y or X)

The general procedure is:

- Click on the dropdown arrow to access the variables list.
- Point and click to select the variable.
- Click on the **«+ variable»** button.

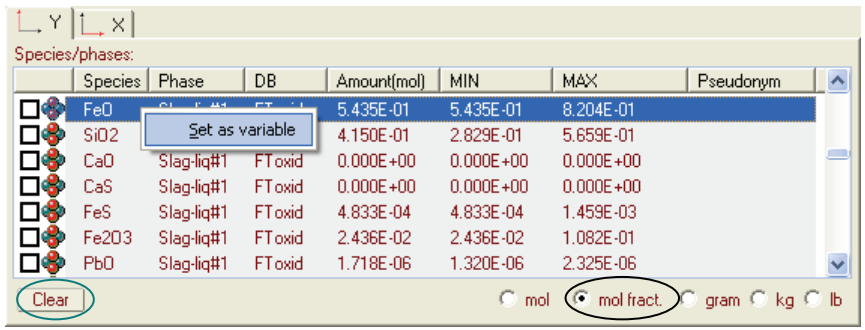
Note: In this case, the selection of Amount displays the Species list in the axis panel and so we also have to select the species and their units (here the **mol fract.** radio button is selected) to use in our formula. After step 2, we can select the variables by one of two methods:

A. First method:

1. Right click on the line to select a species – this opens a popup menu.
2. Click on **«Set as variable»** in the popup menu.
3. Repeat steps 1 and 2 for the other two variables.

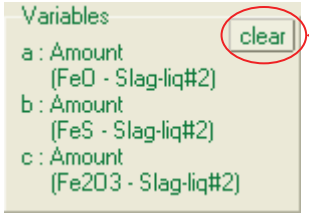
B. Second method:

1. Click in the check box to select a species.
2. Click on the **«+ variable»** button in the axis frame.
3. Click on the **clear** button in the Axis panel.
4. Repeat steps 1 to 3 for the other two variables.



Writing a **formula** and selecting the axis variables

After setting the variables, the **Variables** frame looks like:

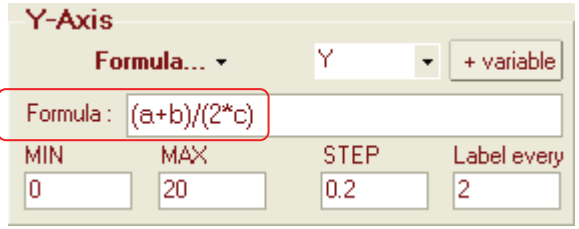


Use this button to **clear** the current variables selection

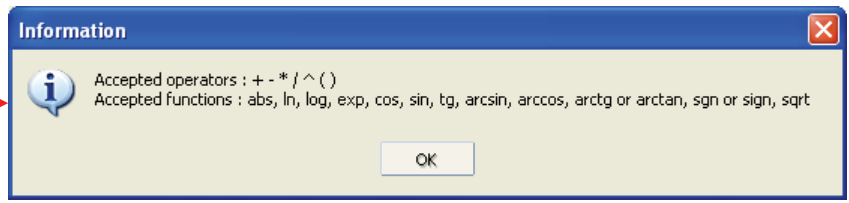
We can now translate the **equation**:

$$\frac{Fe^{2+}}{Fe^{3+}} = \frac{X_{FeO} + X_{FeS}}{2\,X_{Fe_2O_3}}$$

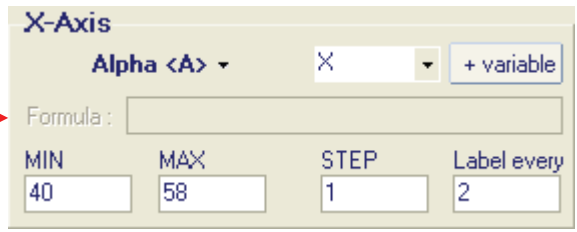
Into this **formula**:



A right click in the formula text box displays the **information**

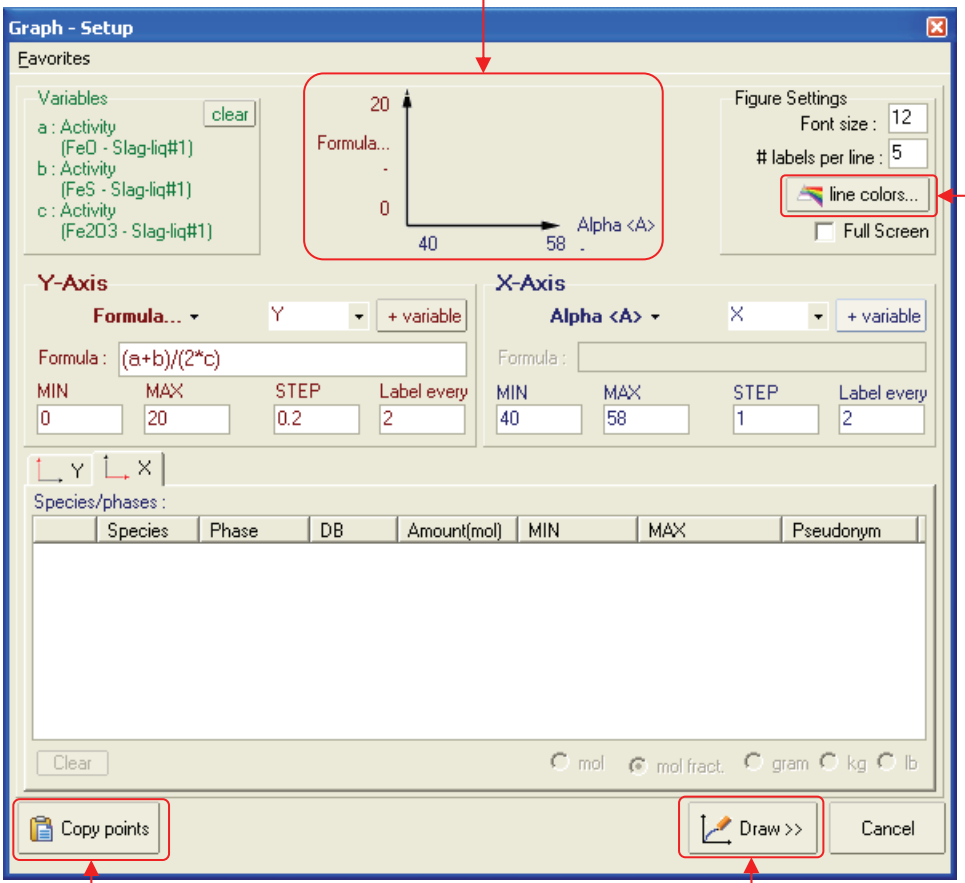


<A> is the **X-axis** variable and varies from **40** to **58**:

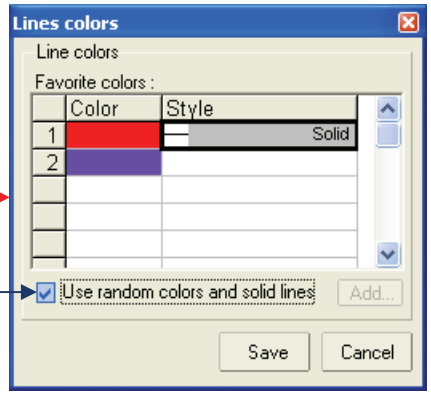


Draw graph and copy points

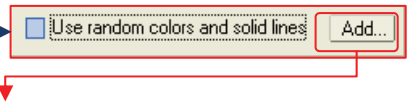
Graph Axes Preview frame



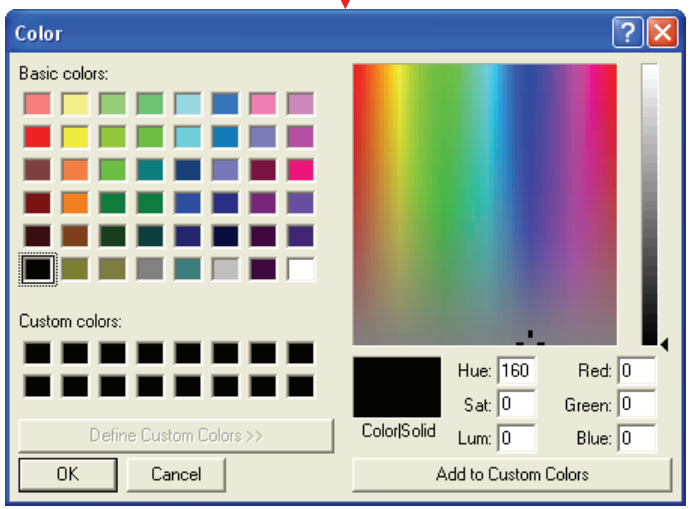
Opens the **Line Colors** dialog box



Uncheck to allow the manual selection of colors



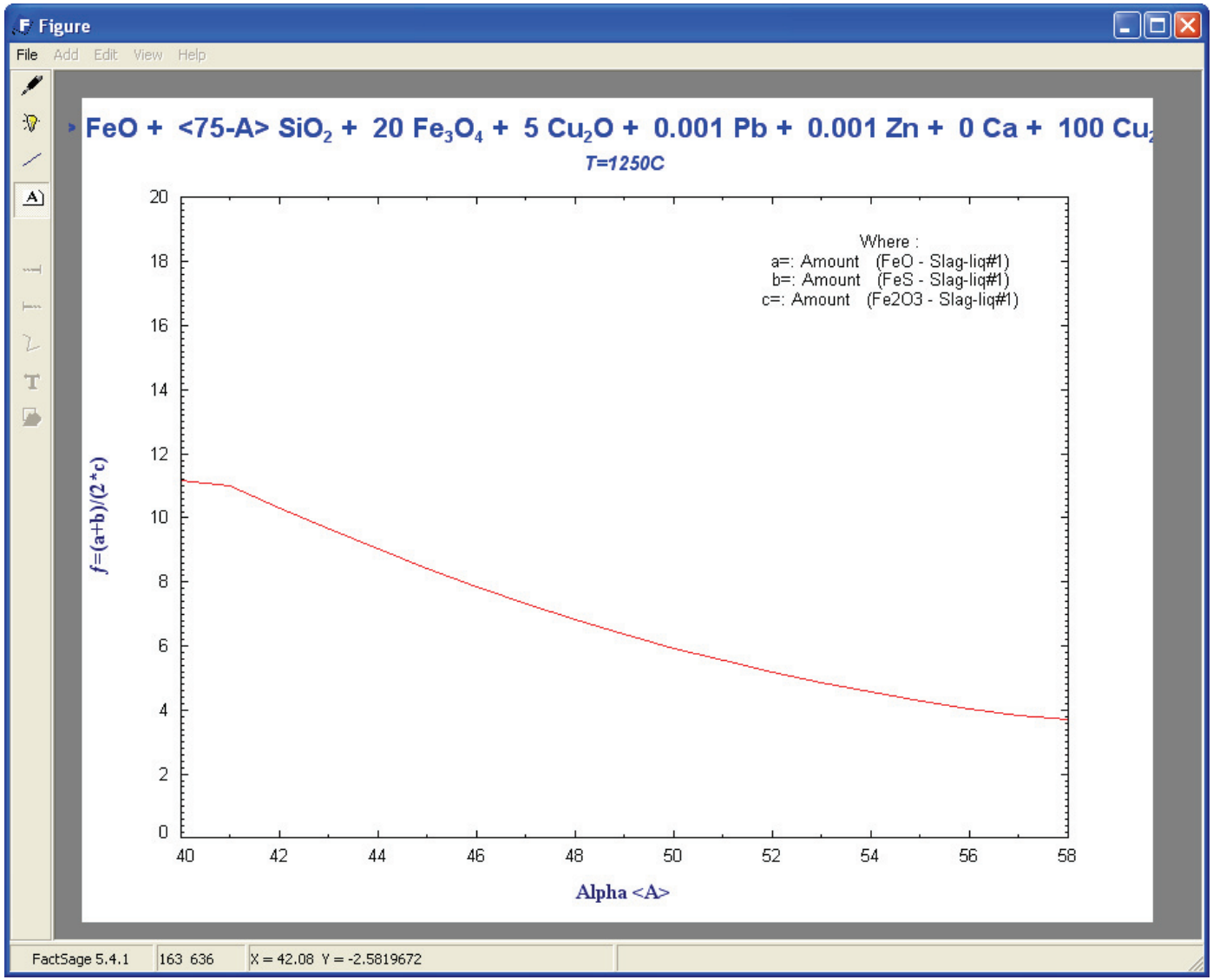
Add… opens the Windows **Color** dialog box



Copy points in the clipboard

Draw the graph in ***Figure***

Graph Setup and *Figure*



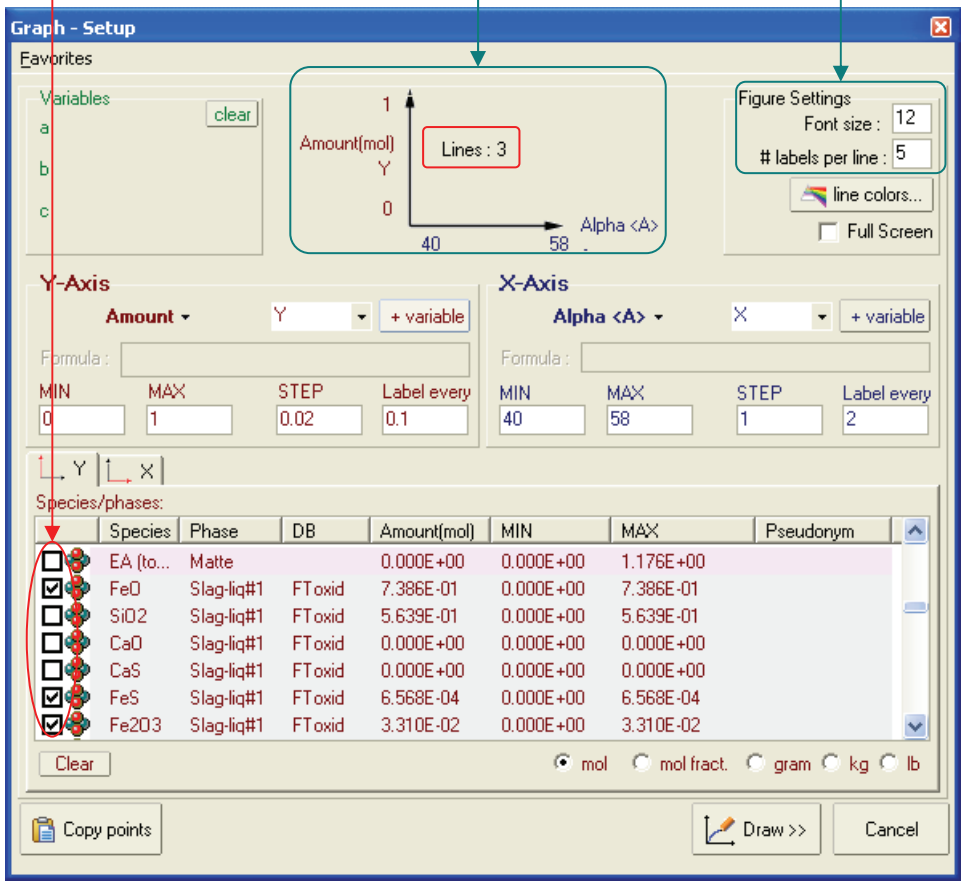
You can then edit the graph using the ***FactSage Figure*** module.

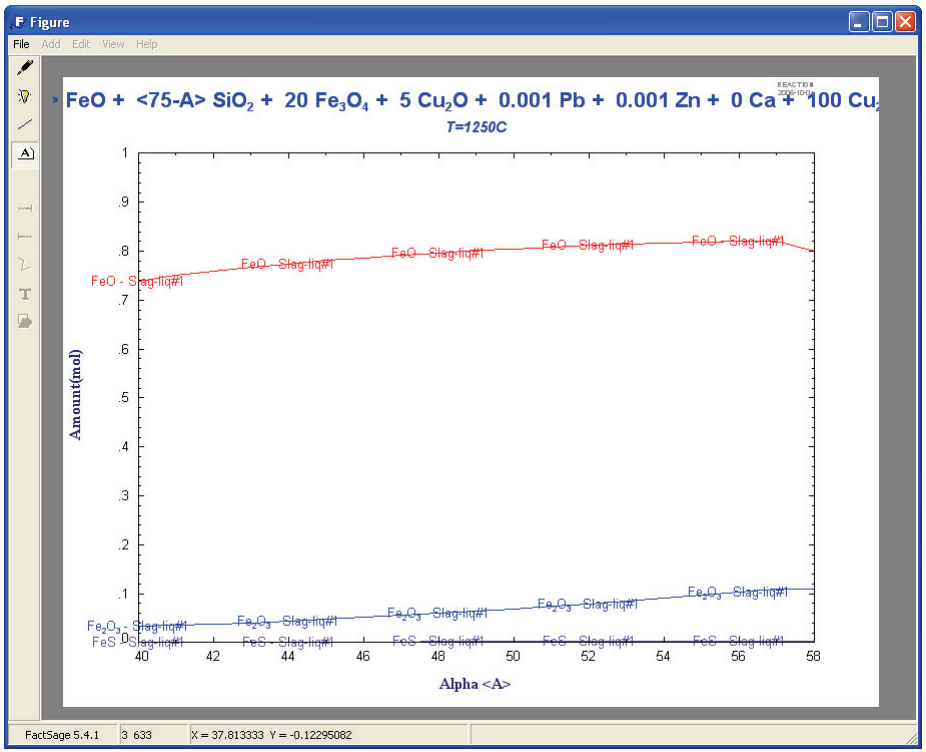
Multiple lines graph

Multiple lines can be drawn.
For example, the amount of **FeO**, **FeS** and **Fe_2O_3** in the slag.

A label in the **Graph Axes Preview** frame indicates the **number of lines**

You can specify the number of labels per line and their font size in the **figure settings** frame





You can then edit the graph using the ***FactSage Figure*** module.