

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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Introduction

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

The starting point is an **Equilib** calculation of a slag-metal equilibrium in a copper converter at 1250°C under a partial pressure of O₂ of 10⁻⁸ atm. It shows the effect of a variation in the composition of the slag from SiO₂ 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> SiO₂ + 20 Fe₃O₄ + 5 Cu₂O + 100 Cu₂S + 0.001 Pb + 0.001 Zn + 0 Ca + 100 Cu

F Menu - Equilib: Cu/Matte/Slag equilibrium at P(O₂)=1.e-8 atm from SiO₂ to Spinel sa...

File Units Parameters Help

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

Reactants (9)

[gram] <A> FeO + <75-A> SiO₂ + 20 Fe₃O₄ + 5 Cu₂O + 0.001 Pb + 0.001 Zn + 0 Ca + 100

Products

Compound species: 38
+ gas ideal real
- aqueous 0
- pure liquids 0
* + pure solids 55
 suppress duplicates apply
* - custom selection species: 93

Target: none -
Estimate T(K): 1000
Mass(g): 0

Solution species

*	+	Base-Phase	Full Name
	+	FTmisc-CuLQA	ACu-liqu_or_speiss
	+	FTmisc-MATT	Matte
	!	FToxid-SLAGA	ASlag-liqu
	+	FToxid-SPIN	Spinel
	!	FToxid-MeO_A	AMonoxide

Legend:
! - immiscible
! - dormant
+ - selected

Custom Solutions:
1 fixed activities
0 ideal solutions
0 activity coefficients
Details ...

Pseudonyms:
apply List ...

include molar volumes
Total Species [max 700] 144
Total Solutions [max 30] 6
Default

Equilibrium
 normal transitions
 predominant open
Calculate >>

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
40 58 1		1250	1	

10 steps Table

19 calculations

c:\Fact-54\EquiCu-Mt-SLDAT

FactSage 5.5

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

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.

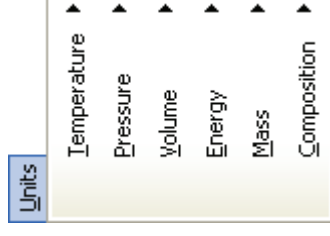
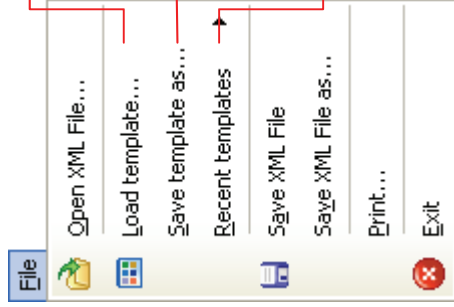
The Menu Bar

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.**).

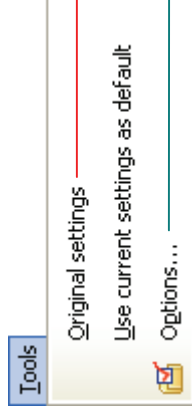
Lists up to the 5 last template files used.
Click on a template file to load it.



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](#))

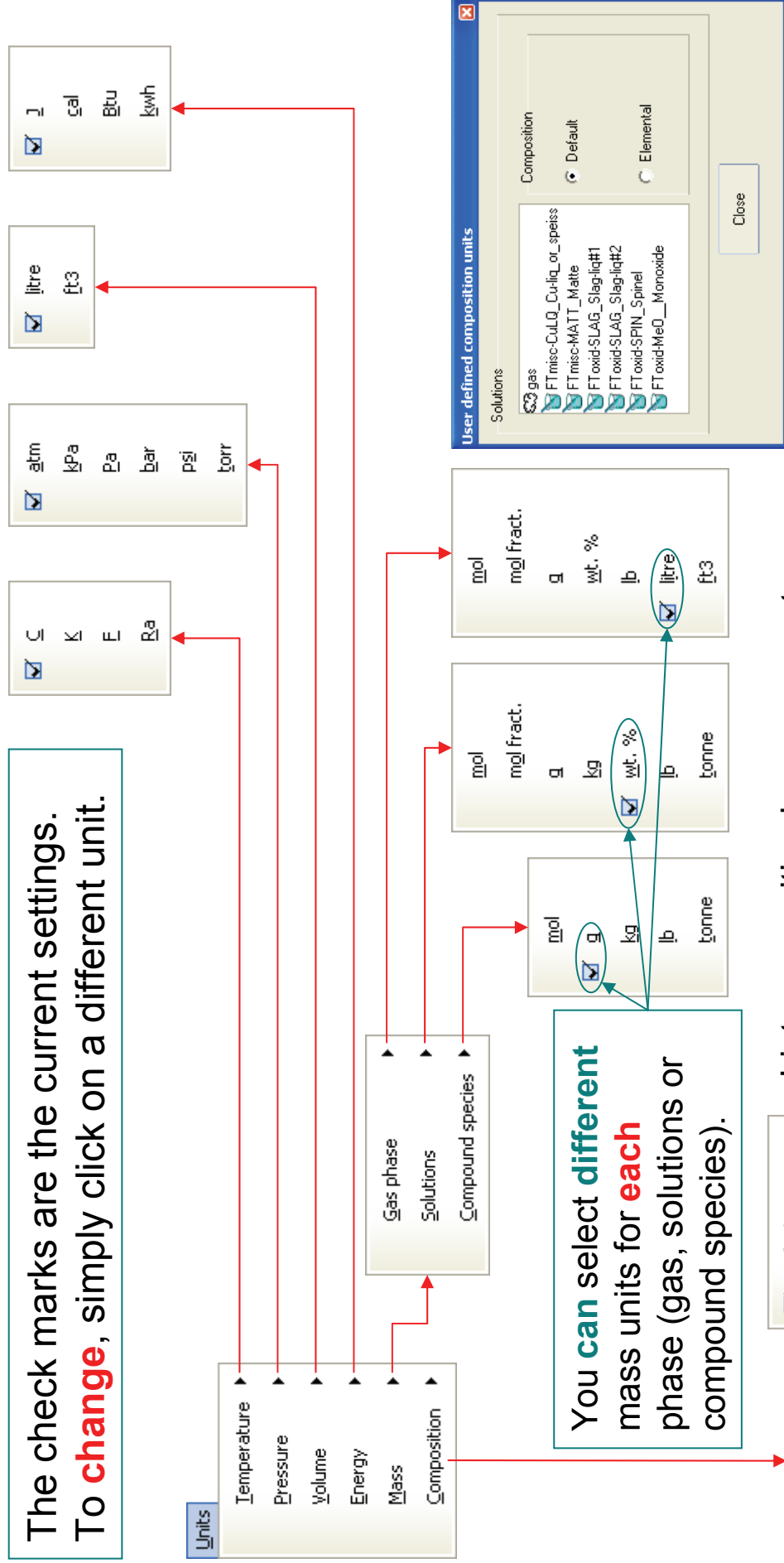


Opens this slide show



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

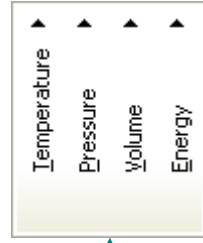
 Search and Highlight: Opens the Search and Highlight dialog box

 **Graph**: Opens the **Graph Setup feature** (see [slide 5.1](#))

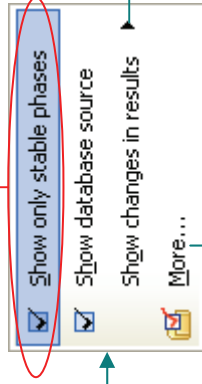
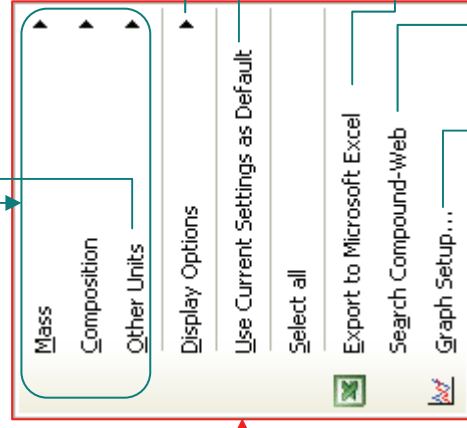
Drop-down Menu – Results Pane

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

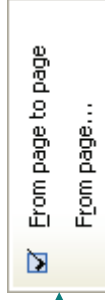


Access the **Options** window

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

Phase	wt. %	Phase	wt. %
FTmisc	0.41057E-03	FTmisc	0.001 Pb
FTmisc	98.092	FTmisc	0.001 Zn
FTmisc	0.43195E-01	FTmisc	0 Ca
FTmisc	1.8471	FTmisc	100 Cu2S
FTmisc	0.19711E-04	FTmisc	100 Cu
FTmisc	0.17338E-01	FTmisc	
FTmisc	(1250.00 C, 1.0000 atm, Cu-liq_or_speiss)		
FToxid	56.975	FToxid	
FToxid	33.125	FToxid	
FToxid	0.70525E-01	FToxid	
FToxid	6.5791	FToxid	
FToxid	0.50108E-03	FToxid	
FToxid	0.12431E-02	FToxid	
FToxid	3.2451	FToxid	
FToxid	0.15058E-05	FToxid	
FToxid	0.54339E-06	FToxid	
FToxid	0.36513E-02	FToxid	
FToxid	(1250.00 C, 1.0000 atm, Siqr-liq#1)		



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.

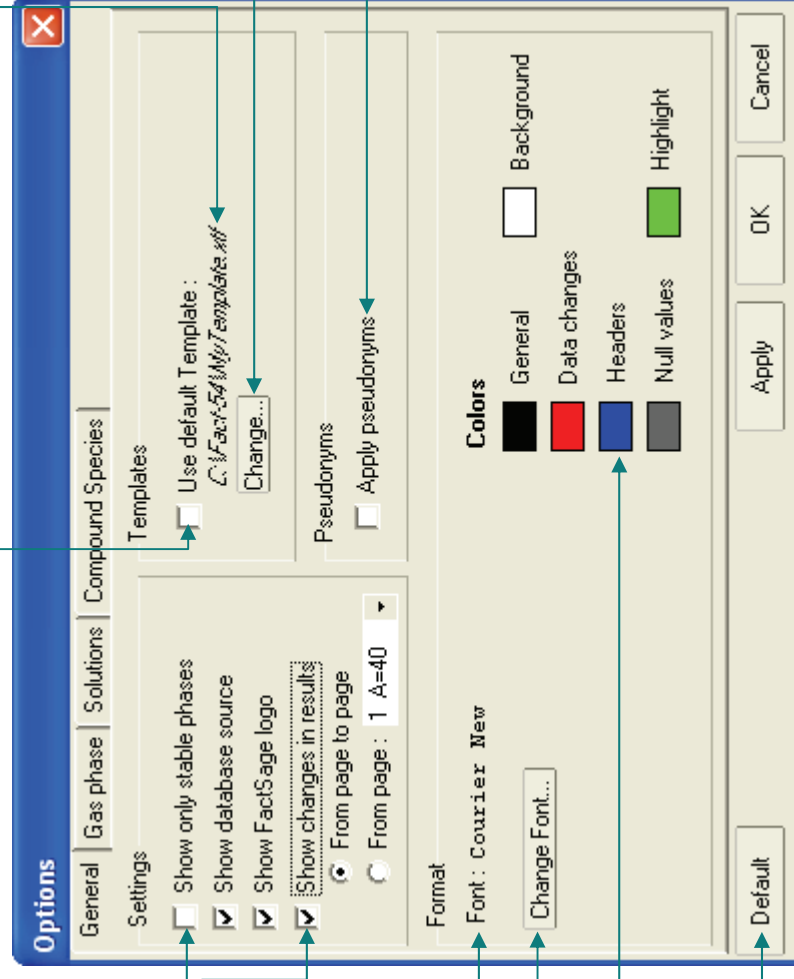
Select « **Show changes in results** »

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
- Show database source
- Show FactSage logo
- Show changes in results
 - From page to page
 - From page: 1 A=40

Page 3 - A=42

(gram) <A> FeO + 475-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

	litre		vol.%	SO2
0.00000		0.55184		
+ 0.000000		+ 0.27788E-02	vol.%	SO
		+ 0.11641E-02	vol.%	Cu
		+ 0.19718E-03	vol.%	S2
		+ 0.29536E-04	vol.%	Zn
		+ 0.29436E-04	vol.%	CuS
		+ 0.19830E-04	vol.%	SSO
		+ 0.16911E-04	vol.%	Pb
		+ 0.74683E-05	vol.%	S
		+ 0.49087E-05	vol.%	PbS
		+ 0.18510E-05	vol.%	S03
		+ 0.17249E-05	vol.%	PbO
		+ 0.10000E-05	vol.%	O2
		(1250.00 C, 1.0000 atm, Gas, a= 0.55609E-02)		

	gram	wt.%	Cu
+ 108.80		98.090	
+ 0.69200E-01		+ 1.8504	wt.% S
		+ 0.41578E-01	wt.% Fe
		+ 0.17353E-01	wt.% O
		+ 0.39872E-03	wt.% Pb
		(1250.00 C, 1.0000 atm, Cu-liq_or_speiss)	

	gram	wt.%	FeO
+ 96.636		56.384	
- 0.44490E-01		+ 34.149	wt.% SiO2
		+ 6.0949	wt.% Fe2O3
		+ 3.3008	wt.% Cu2O
		+ 0.66015E-01	wt.% FeS
		+ 0.35129E-02	wt.% Cu2S
		+ 0.12455E-02	wt.% ZnO
		+ 0.51880E-03	wt.% PbO
		(1250.00 C, 1.0000 atm, Slag-liq#1)	

- 0.38610E-03	FACT53	- 0.16800E-02	FTmisc
- 0.19440E-05	FACT53	- 0.32530E-02	FTmisc
+ 0.90000E-06	FACT53	+ 0.15803E-02	FTmisc
- 0.27600E-08	FACT53	- 0.14200E-04	FTmisc
+ 0.18180E-05	FACT53	+ 0.12126E-04	FTmisc
- 0.20370E-07	FACT53		
- 0.27750E-07	FACT53		
+ 0.52750E-06	FACT53		
- 0.52250E-08	FACT53		
+ 0.14982E-06	FACT53		
- 0.12940E-08	FACT53		
- 0.53813E-07	FACT53		
+ 0.00000	FACT53		
		+ 0.63733	FToxid
		- 1.0186	FToxid
		+ 0.43998	FToxid
		- 0.63134E-01	FToxid
		+ 0.43343E-02	FToxid
		+ 0.12962E-03	FToxid
		- 0.20570E-05	FToxid
		- 0.18066E-04	FToxid

Colors

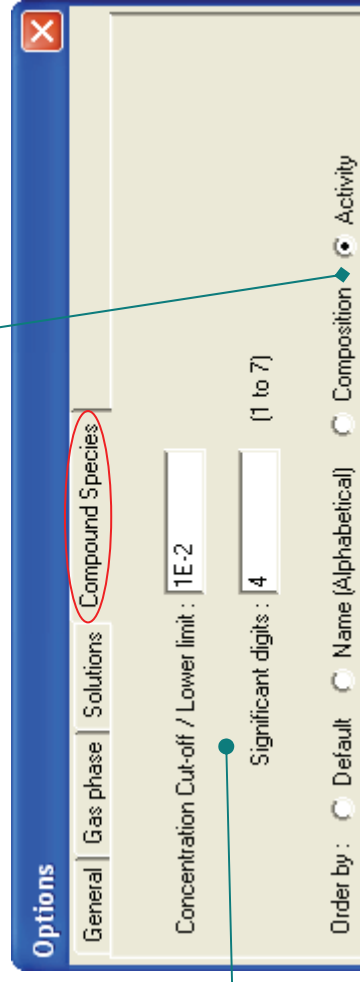
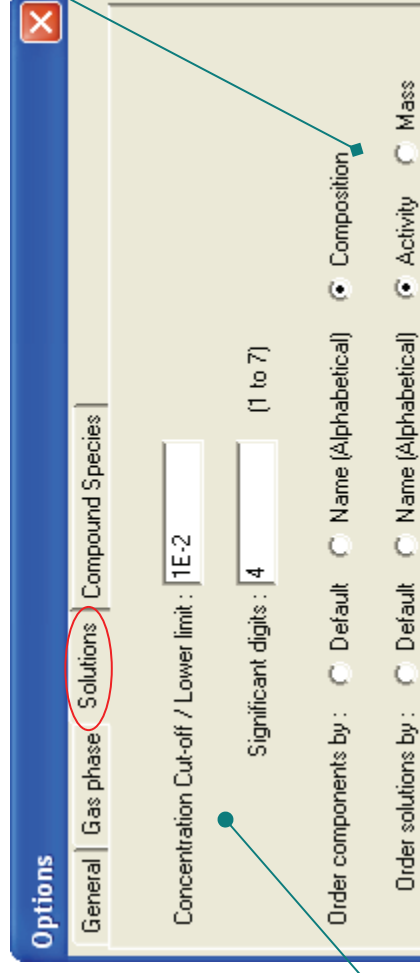
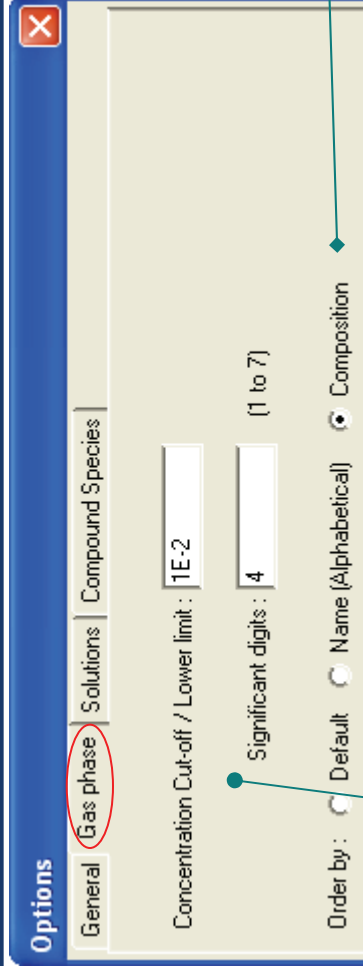
- General
- Data changes
- Headers
- Null values
- Background
- Highlight

Incremental changes from page 2 A=41

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

The screenshot shows the 'Graph - Setup' dialog box. It is divided into several sections:

- Variables:** A list of variables 'a', 'b', and 'c' with a 'clear' button.
- Figure Settings:** Includes 'Font size: 12', '# labels per line: 5', a 'line colors...' button, and a 'Full Screen' checkbox.
- Graph Axes Preview:** A small graph showing 'Activity' on the y-axis (ranging from 0 to 1) and 'Page #' on the x-axis (ranging from 1 to 19).
- Y-Axis:** A panel for the y-axis with 'Activity' selected as the variable. It includes a 'Formula:' field, 'MIN: 0', 'MAX: 1', 'STEP: 0.01', and 'Label every: 0.1'.
- X-Axis:** A panel for the x-axis with 'Page #' selected as the variable. It includes a 'Formula:' field, 'MIN: 1', 'MAX: 19', 'STEP: 0.18', and 'Label every: 1.8'.
- Species/phases:** A table with columns for Species, Phase, DB, Activity, MIN, and MAX. The table contains data for species O, O2, O3, Si, Si2, and Si3, all in the 'Gas' phase.
- Bottom Panel:** Includes a 'Clear' button, a 'Copy points' button, a 'Draw >>' button with a graph icon, and a 'Cancel' button.

Variables frame

Figure Settings frame

Y-axis frame

X-axis frame

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

Command frame

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**.

Y-Axis

Activity ▾

Formula: Y

+ variable

MIN 0 MAX 1 STEP 0.01 Label every 0.1

Selection of the axis scale

Set as variable button

Formula text box

Axis settings

Activity

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

Sp Cgint Cppar G Gint Gint (xs) Gpar Gpar (xs) H Hint Hint (xs) Hpar Hpar (xs) S Sint Sint (xs) Spar Spar (xs) Y Vint

Species/phases:

Species	Phase	DB	Activity	MIN	MAX	Pseudonym
0	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	2.866E-11	7.836E-11	

Species panel

Click to select the species or the phases

Species/phases:

Species	Phase	DB	Sint (xs)	MIN	MAX	Pseudonym
0	Gas		-2.868E-01	-2.868E-01	-2.868E-01	
Cu <liq...< li=""></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	

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 $\text{Fe}^{2+}/\text{Fe}^{3+}$ ratio in the slag vs Alpha <A>. The ratio is:

$$\frac{\text{Fe}^{2+}}{\text{Fe}^{3+}} = \frac{X_{\text{FeO}} + X_{\text{FeS}}}{2 X_{\text{Fe}_2\text{O}_3}}$$

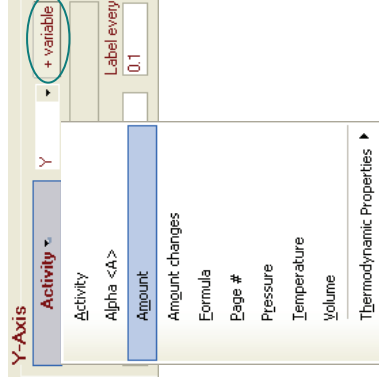
where X_c is the mole fraction of the compound c in the slag.

In order to use the Formula feature, we must select the variables: X_{FeO} , X_{FeS} and $X_{\text{Fe}_2\text{O}_3}$ 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.



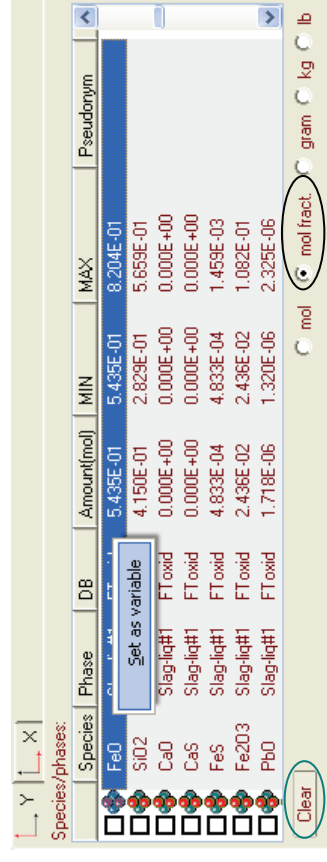
Note: In this case, the selection of Amount displays the Species list in the axis panel and so we also have to select the species and their units (here the **mol fract.** radio button is selected) to use in our formula. After step 2, we can select the variables by one of two methods:

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:

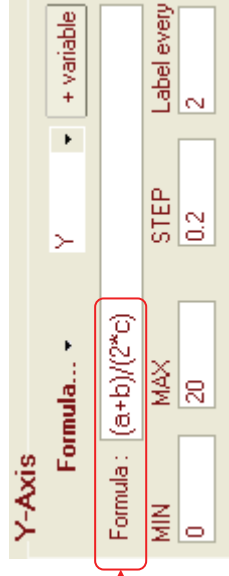


Use this button to **clear** the current variables selection

We can now translate the equation:



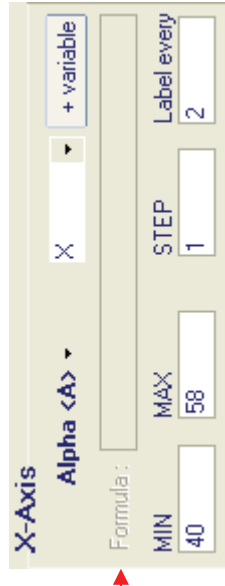
Into this formula:



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

Graph - Setup

Variables
a : Activity (FeO - Slag-liq#1)
b : Activity (FeS - Slag-liq#1)
c : Activity (Fe2O3 - Slag-liq#1)

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

Y-Axis
Formula : $(a+b)/(2^*c)$
MIN 0 MAX 20 STEP 0.2 Label every 2

X-Axis
Alpha <A>
Formula : X
MIN 40 MAX 58 STEP 1 Label every 2

Species/phases :
Species Phase DB Amount(mol) MIN MAX P-pseudonym
Clear

Copy points Draw >> Cancel

Opens the **Line Colors** dialog box

Line colors

Favorite colors :

Color	Style
1	Solid
2	Solid

Use random colors and solid lines

Save Cancel

Uncheck to allow the manual selection of colors

Use random colors and solid lines

Add...

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

Color

Basic colors:

Custom colors:

Hue: 160 Red: 10
Sat: 0 Green: 10
Lum: 0 Blue: 10

ColorSolid

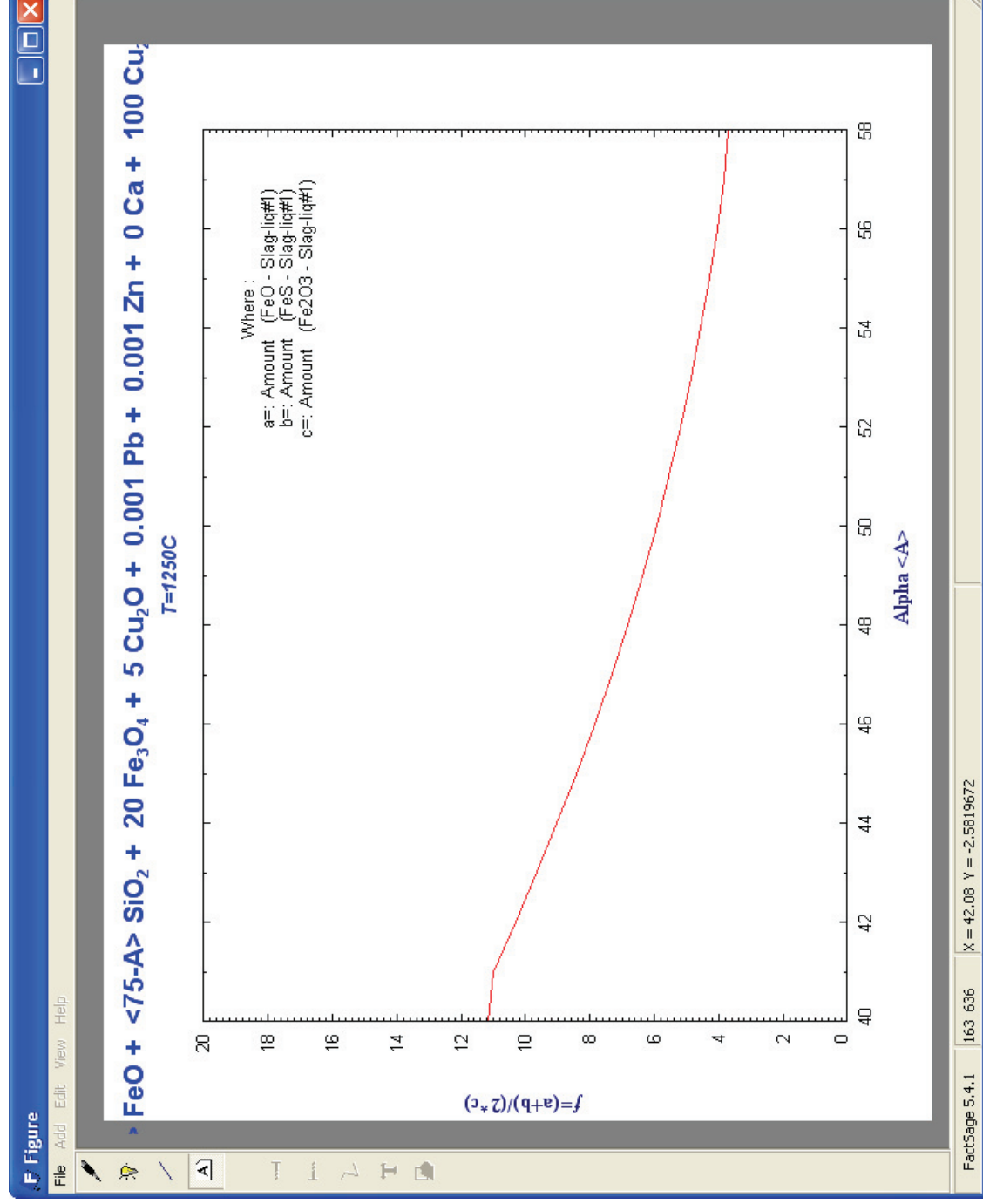
Define Custom Colors >>>

OK Cancel

Add to Custom Colors

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 **Fe₂O₃** 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

The screenshot shows the FactSage software interface. The main window displays a graph titled "F Figure" with the reaction: $\text{FeO} + <75\text{-A}> \text{SiO}_2 + 20 \text{Fe}_3\text{O}_4 + 5 \text{Cu}_2\text{O} + 0.001 \text{Pb} + 0.001 \text{Zn} + 0 \text{Ca} + 100 \text{Cu}$ at $T=1250\text{C}$. The graph plots Amount(mol) on the Y-axis (ranging from 0 to 1) against Alpha <A> on the X-axis (ranging from 40 to 58). Three lines are shown: FeO-Slag(liq#1) in red, Fe₂O₃-Slag(liq#1) in blue, and FeS-Slag(liq#1) in black. The FeO-Slag(liq#1) line is the highest, followed by Fe₂O₃-Slag(liq#1), and FeS-Slag(liq#1) is the lowest.

The "Graph - Setup" dialog box is open, showing the following settings:

- Variables:** a, b, c (clear)
- Figure Settings:** Font size: 12, # labels per line: 5, line colors... Full Screen
- Y-Axis:** Amount (mol), Formula: Y, MIN: 0, MAX: 1, STEP: 0.02, Label every: 0.1, Label every: 2
- X-Axis:** Alpha <A>, Formula: X, MIN: 40, MAX: 58, STEP: 1, Label every: 2
- Species/phases:** EA (to...), FeO, SiO2, CaO, CaS, FeS, Fe2O3. The species are listed with their phases (Matte, Slag-liq#1, FT oxid) and their amounts (MIN, MAX).
- Units:** mol, mol fract, gram, kg, lb
- Buttons:** Clear, Copy points, Draw >>, Cancel

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