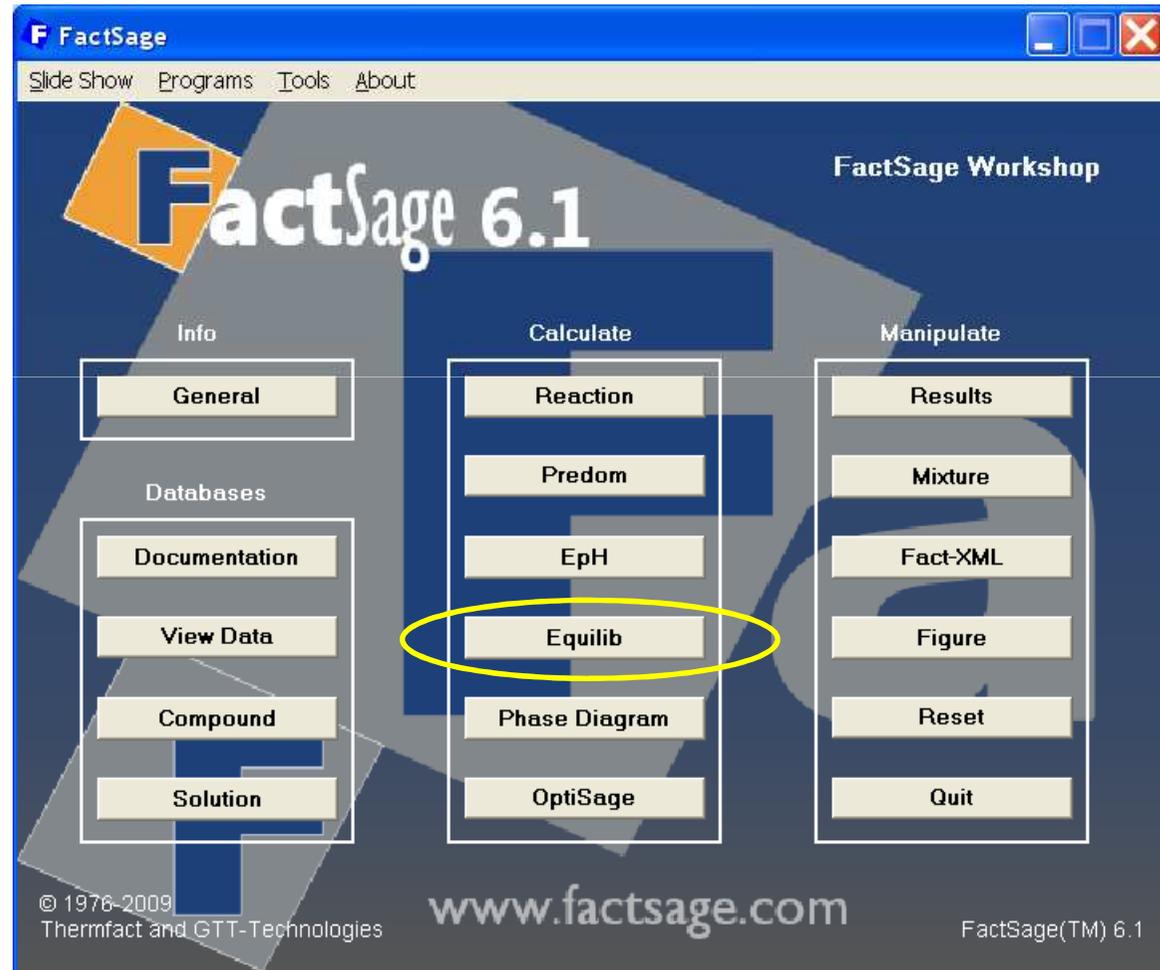


Metal Treatment (Al & Mg)

- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**

5.52% Mg
3.21% Zn
0.21% Mn
Balance Al



Metal Treatment (Al & Mg)

- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**

F Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 4

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
91.06	Al	s			1	
+ 5.52	Mg	s			1	
+ 3.21	Zn	s			1	
+ 0.21	Mn	s			1	

Initial Conditions

Next >>

FactSage 6.2 beta Compound: 2/24 databases Solution: 1/22 databases

Metal Treatment (Al & Mg)

- Example #0: Vapor Pressure of Al-Mg-Zn-Mn

Data Search

Databases - 2/24 compound databases, 1/22 solution databases

<input type="checkbox"/> ELEM	<input type="checkbox"/> FScopt	<input type="checkbox"/> BINS	<input type="checkbox"/> compounds only	Miscellaneous			
<input type="checkbox"/> FACT	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS	<input type="checkbox"/> solutions only		<input type="checkbox"/> EXAM	<input type="checkbox"/> SGSL	<input type="checkbox"/> SGTE*
<input checked="" type="checkbox"/> Fact53	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE	<input type="checkbox"/> no data				
<input type="checkbox"/> FToxid	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	Clear All				
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSupsi	<input type="checkbox"/> SGsold	Select All				
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGnucl	Add/Remove Data				
<input type="checkbox"/> FTHall	Other	<input type="checkbox"/> TDnucl	RefreshDatabases				
<input type="checkbox"/> FTHeig	<input type="checkbox"/> OLIP	<input type="checkbox"/> OLIC					
<input type="checkbox"/> FTpulp	<input type="checkbox"/> OLIG	<input type="checkbox"/> OLIL					
<input checked="" type="checkbox"/> FTlite							

Information -
Click on a box to include (or exclude) a database in the data search. Normally databases are 'coupled' - that is both the compound and solution database (when available) will be selected. To 'uncouple' a databases click-mouse-right-button (note, this is NOT recommended).
If database is stored on your PC but no

Options

Default

Include

- gaseous ions (in aemas)
- aqueous species
- limited data compounds (25C)

Limits

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

Cancel Summary ... OK

Next >>

FactSage 6.2 beta Compound: 2/24 databases Solution: 1/22 databases

FTlite = solid & liquid phases
FACT53 = gaseous species

Metal Treatment (Al & Mg)

- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**

F Menu - Equilib: last system

File Units Parameters Help

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

Reactants (4)

(gram) 91.06 Al + 5.52 Mg + 3.21 Zn + 0.21 Mn

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 0
- suppress duplicates

species: 0

Solution species

*	+	Base-Phase	Full Name
	I	FTlite-Liqu	Liquid
	I	FTlite-FCC	FCC_A1
	I	FTlite-HCP	HCP_A3
	I	FTlite-BCC	BCC_A2
	+	FTlite-CBCC	CBCC_A12
	+	FTlite-CUB1	CUB_A13
	I	FTlite-LC14	Laves_C14
	I	FTlite-LC15	Laves_C15

Legend

- I - immiscible 7
- + - selected 12

Show all selected

species: 144

solutions: 26

include molar volumes

Total Species (max 1500) 144

Total Solutions (max 40) 26

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		720	1	

10 steps Table

Equilibrium

- normal normal + transitions
- transitions only open
- predominant

FactSage 6.2 beta

Metal Treatment (Al & Mg)

- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**

Reactants (4)
(gram) 91.06 Al + 5.52 Mg + 3.21 Zn + 0.21 Mn

Products

Compound species
 gas ideal real 6
 aqueous 0
 pure liquids 0
 pure solids 0
 suppress duplicates
species: 6

Solution species

*	+	Base-Phase	Full Name
	I	FTlite-Liqu	Liquid
	I	FTlite-FCC	FCC_A1
	I	FTlite-HCP	HCP_A3
	I	FTlite-BCC	BCC_A2
	+	FTlite-CBCC	CBCC_A12
	+	FTlite-CUB1	CUB_A13
	I	FTlite-LC14	Laves_C14
	I	FTlite-LC15	Laves_C15

Legend
I - immiscible 7
+ - selected 12
species: 144
solutions: 26

Equilibrium
 normal normal + transitions
 transitions only open
 predominant

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		720	1	

10 steps Table

FactSage 6.2 beta

Metal Treatment (Al & Mg)

- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**

Dbi-Click on "pure solids"

+	Code	Species	Data	Phase	T	V	Activity
	17	Al8Mg5(s)	FACT5	beta		o	
	18	Al29Mg21(s)	FACT5	r-phase		o	
	19	Mn(s)	FACT5	solid_alpha			
	20	Mn(s2)	FACT5	solid_beta			
	21	Mn(s3)	FACT5	solid_gamma			
	22	Mn(s4)	FACT5	solid_delta			
	23	Zn(s)	FACT5	solid			
+	24	Mg(s)	FTlite	hcp_a3		V	
+	25	Mg(s2)	FTlite	hcp_zn			
+	26	Mg(s3)	FTlite	fcc_a1		V	
+	27	Mg(s4)	FTlite	bcc_a2			
+	28	Mg(s5)	FTlite	cbcc_a12			
+	29	Mg(s6)	FTlite	cub_a13			
+	30	Al(s)	FTlite	fcc_a1		V	
+	31	Al(s2)	FTlite	hcp_a3			

Metal Treatment (Al & Mg)

- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**

At this point, I would like to calculate the vapor pressure of this alloy as a function of T.

Independent variable = T

Dependant variable = P

A “**formation target**” on the **gas phase** will be used

Metal Treatment (Al & Mg)

- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**

Menu - Equilib: last system

File Units Parameters Help

T(C) P(atm)

Reactants (4)

- 1 Mg(g)
- clear
- + - select
- standard stable phase
- dormant (metastable) phase
- F - formation target phase**
- P - precipitate target phase
- S - Scheil cooling gas phase
- C - composition target ...
- Ideal Solution
- a Activity
- Help ...

Products

- Compound specie
- gas** ideal
- aqueous
- pure liquids
- * pure solids
- suppress dup
- * - custom selection
- spe

Target

- none -

Estimate T(K): 1000

Mass(g): 0

Final Conditions

<A>		T(C)	P(atm)
		720	1

10 steps Table

1 calculation predominant **Calculate >>**

FactSage 6.2 beta

Selection - Equilib

File Edit Show Sort

Selected: 6/6 **GAS** Page 41 Refresh

+ Code	Species	Data	Phase	T	V	Activity
1	Mg(g)	FACT5	gas			
+	Al(g)	FACT5	gas			
+	Si(g)	FACT5	gas			
+	Fe(g)	FACT5	gas			
+	Mn(g)	FACT5	gas			
+	Zn(g)	FACT5	gas			

Now Selected Select All Select/Clear... Clear OK

Metal Treatment (Al & Mg)

- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**

The screenshot shows the 'Selection - Equilib' dialog box in FactSage 6.2 beta. The dialog box has a menu bar with 'File', 'Edit', 'Show', and 'Sort'. Below the menu bar, there is a 'Selected: 6/6' indicator, a 'GAS' button, a 'Page 41' dropdown, and a 'Refresh' button. The main content is a table with the following columns: '+', 'Code', 'Species', 'Data', 'Phase', 'T', 'V', and 'Activity'. The table contains six rows of data, all of which are highlighted in cyan. A red box highlights the first column of the table, which contains the letter 'F'. Below the table, there is a blue box with the text 'F = "formation target"'. At the bottom of the dialog box, there are buttons for 'Show Selected', 'Select All', 'Select/Clear...', 'Clear', and 'OK'. The background shows the 'Menu - Equilib: last system' window with various options for 'Reactants (4)', 'Products', and 'Final Conditions'.

+	Code	Species	Data	Phase	T	V	Activity
F	1	Mg(g)	FACT5	gas			
F	2	Mg2(g)	FACT5	gas			
F	3	Al(g)	FACT5	gas			
F	4	Al2(g)	FACT5	gas			
F	5	Mn(g)	FACT5	gas			
F	6	Zn(g)	FACT5	gas			

F = "formation target"

Metal Treatment (Al & Mg)

- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**

Reactants (4)
(gram) 91.06 Al + 5.52 Mg + 3.21 Zn + 0.21 Mn

Products

Compound species
 F gas • ideal real 6
 aqueous 0
 pure liquids 0
 + pure solids 42
 suppress duplicates apply
*- custom selection
species: 48

Formation Target
GAS
Estimate P(atm): 1.0
Mass(g): 0

Solution species

*	+	Base-Phase	Full Name
	I	FTlite-Liqu	Liquid
	I	FTlite-FCC	FCC_A1
	I	FTlite-HCP	HCP_A3
	I	FTlite-BCC	BCC_A2
	+	FTlite-CBCC	CBCC_A12
	+	FTlite-CUB1	CUB_A13
	I	FTlite-LC14	Laves_C14
	I	FTlite-LC15	Laves_C15

Legend
I - immiscible 7
+- selected 12
Show all selected
species: 144
solutions: 26
Select

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

Pseudonyms
apply List ...
 include molar volumes
Total Species (max 1500) 192
Total Solutions (max 40) 26
Default

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		350 800 10		

10 steps Table 46 calculations

Equilibrium
 normal normal + transitions
 transitions only open
 predominant
Calculate >>

FactSage 6.2 beta

Metal Treatment (Al & Mg)

- Example #0: Vapor Pressure of Al-Mg-Zn-Mn

F Results - Equilib 350 C, 1.544E-06 atm (page 1/46) FactSage 6.2 beta

Output Edit Show Pages

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

550 C, 4.731E-04 atm	560 C, 5.279E-04 atm	570 C, 5.834E-04 atm	580 C, 6.375E-04 atm	590 C, 6.871E-04 atm
500 C, 2.026E-04 atm	510 C, 2.557E-04 atm	520 C, 3.208E-04 atm	530 C, 3.694E-04 atm	540 C, 4.200E-04 atm
450 C, 5.731E-05 atm	460 C, 7.481E-05 atm	470 C, 9.695E-05 atm	480 C, 1.248E-04 atm	490 C, 1.595E-04 atm
400 C, 1.265E-05 atm	410 C, 1.824E-05 atm	420 C, 2.459E-05 atm	430 C, 3.287E-05 atm	440 C, 4.357E-05 atm
350 C, 1.544E-06 atm	360 C, 2.420E-06 atm	370 C, 3.736E-06 atm	380 C, 5.685E-06 atm	390 C, 8.535E-06 atm

(gram) 91.06 Al + 5.52 Mg + 3.21 Zn + 0.21 Mn =

```

0.00000 mol gas_ideal
(350.00 C, 1.5442E-06 atm, a=1.0000)
( 0.95557 Zn ←
+ 4.4425E-02 Mg
+ 7.0551E-12 Mg2
+ 1.6192E-15 Al
+ 4.3004E-19 Mn
+ 1.1252E-26 Al2
FACT53
FACT53
FACT53
FACT53
FACT53
FACT53)

+ 96.466 gram FCC Al#1
(96.466 gram, 3.5540 mol)
(350.00 C, 1.5442E-06 atm, a=1.0000)
( 93.053 wt.% Al
+ 4.9963 wt.% Mg
+ 2.1562E-02 wt.% Mn
+ 1.9296 wt.% Zn
FTlite
FTlite
FTlite
FTlite)

System component Mole fraction Mass fraction
Zn 8.0096E-03 1.9296E-02
Mn 1.0653E-04 2.1562E-04
Al 0.93609 0.93053
Mg 5.5796E-02 4.9963E-02

+ 2.7868 gram AlMgZn Tau
    
```

Metal Treatment (Al & Mg)

- Example #0: Vapor Pressure of Al-Mg-Zn-Mn

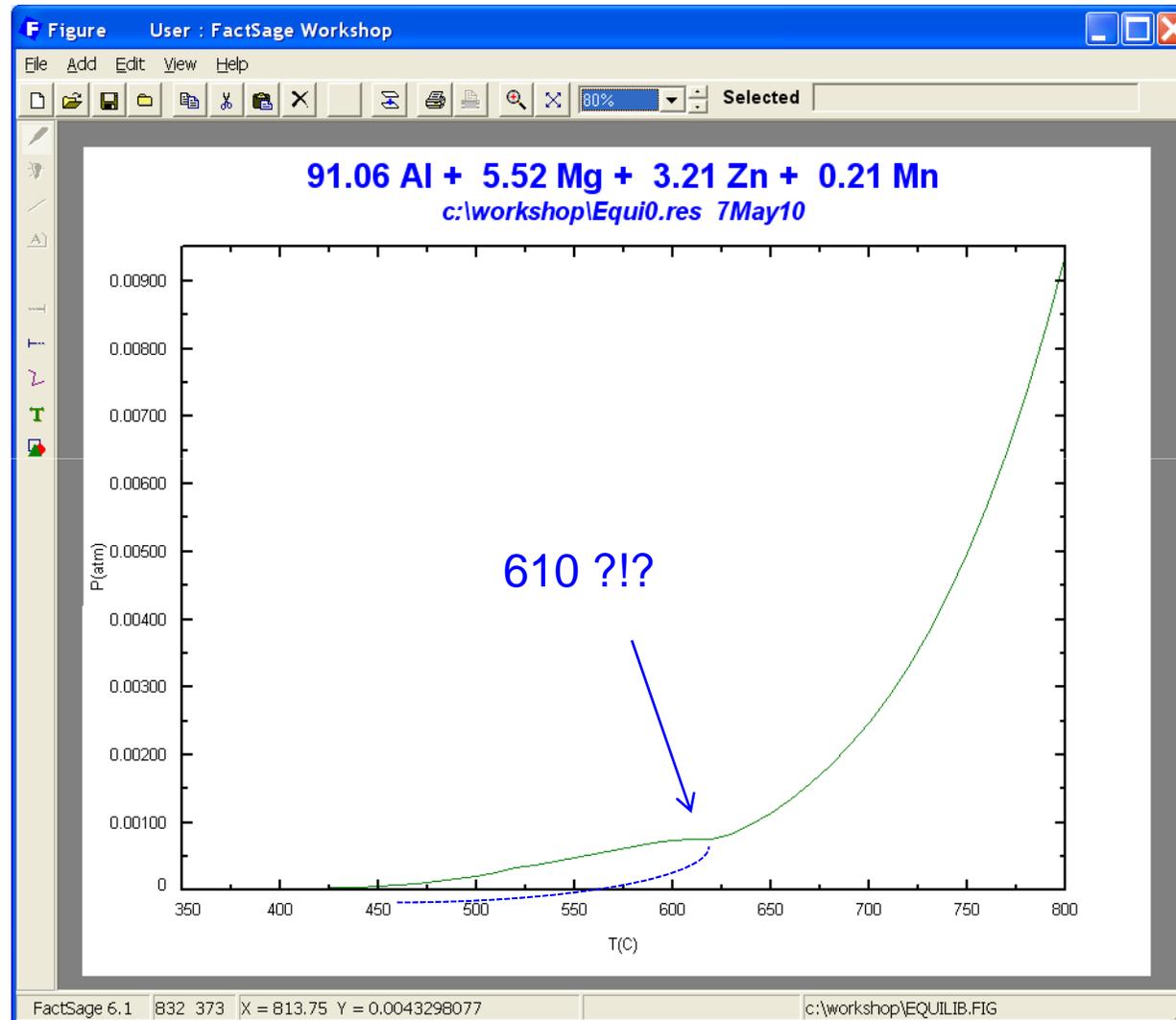
The screenshot displays the FactSage 6.2 beta interface. The main window is titled "Results - Equilib 350 C, 1.544E-06 atm (page 1/46) FactSage 6.2 beta". A menu is open with "Plot" selected, and a sub-menu shows "Plot Results ...". A dialog box titled "Results Processor: c:\workshop\Equi0.res" is active, showing a composition of "91.06 Al + 5.52 Mg + 3.21 Zn + 0.21 Mn". A table of properties is visible:

	T(C)	P(atm)	Energy(J)	Mass(g)	Vol(litre)
activity	0	1.			
mole	0	3.6549			
mole fract	0	1			

Below the table, a list of components is shown with their activities and mole fractions. A dialog box titled "Axes: P(atm) vs T(C)" is open, allowing configuration of the plot axes. The Y-axis is set to "P(atm)" and the X-axis is set to "T(C)". The Y-axis settings are: maximum 0.0095, minimum 0, tick every 0.0005. The X-axis settings are: maximum 800, minimum 350, tick every 25. The dialog box also includes options for "reactants", "file name", and "Figure".

Metal Treatment (Al & Mg)

- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**



Metal Treatment (Al & Mg)

- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**

F Results - Equilib 350 C, 1.544E-06 atm (page 1/46) FactSage 6.2 beta

Output Edit Show Pages

Save or Print

Plot Plot Results

Equilib Results file Repeat Plot

Stream File 460 C, 7.48

Format 110 C, 1.824E-06

Fact-XML 10 C, 2.420E-06

Fact-Optimal 5.52 Mg

Refresh ...

gas_idea

(350.00 c, 1.544E-06)

(0.95557

+ 4.4425E-02

+ 7.0551E-12

+ 1.6192E-15

+ 4.3004E-19

+ 1.1252E-26

+ 96.466 gram FCC_Al#1

(96.466 gram, 3.5540 mol)

(350.00 c, 1.544E-06)

(93.053 wt. %

+ 4.9963 wt. %

+ 2.1562E-02 wt. %

+ 1.9296 wt. %

System component

Zn

Mn

Al

Mg

+ 2.7868 gram AlMgZn Tau

F Plot: P(atm) vs T(C)

File Help

91.06 Al + 5.52 Mg + 3.21 Zn + 0.21 Mn

activity	0	1.
mole	0	3.6549

F Axes: weight % vs T(C)

Y-variable X-variable Swap Axes

Y-axis: weight %

X-axis: T(C)

maximum: 50

minimum: 0

tick every: 2

maximum: 800

minimum: 350

tick every: 25

Cancel Refresh OK

Plot >>

FactSage 6.1 c:\workshop\Equi0.res 7May10 46 sets

Metal Treatment (Al & Mg)

- Example #0: Vapor Pressure of Al-Mg-Zn-Mn

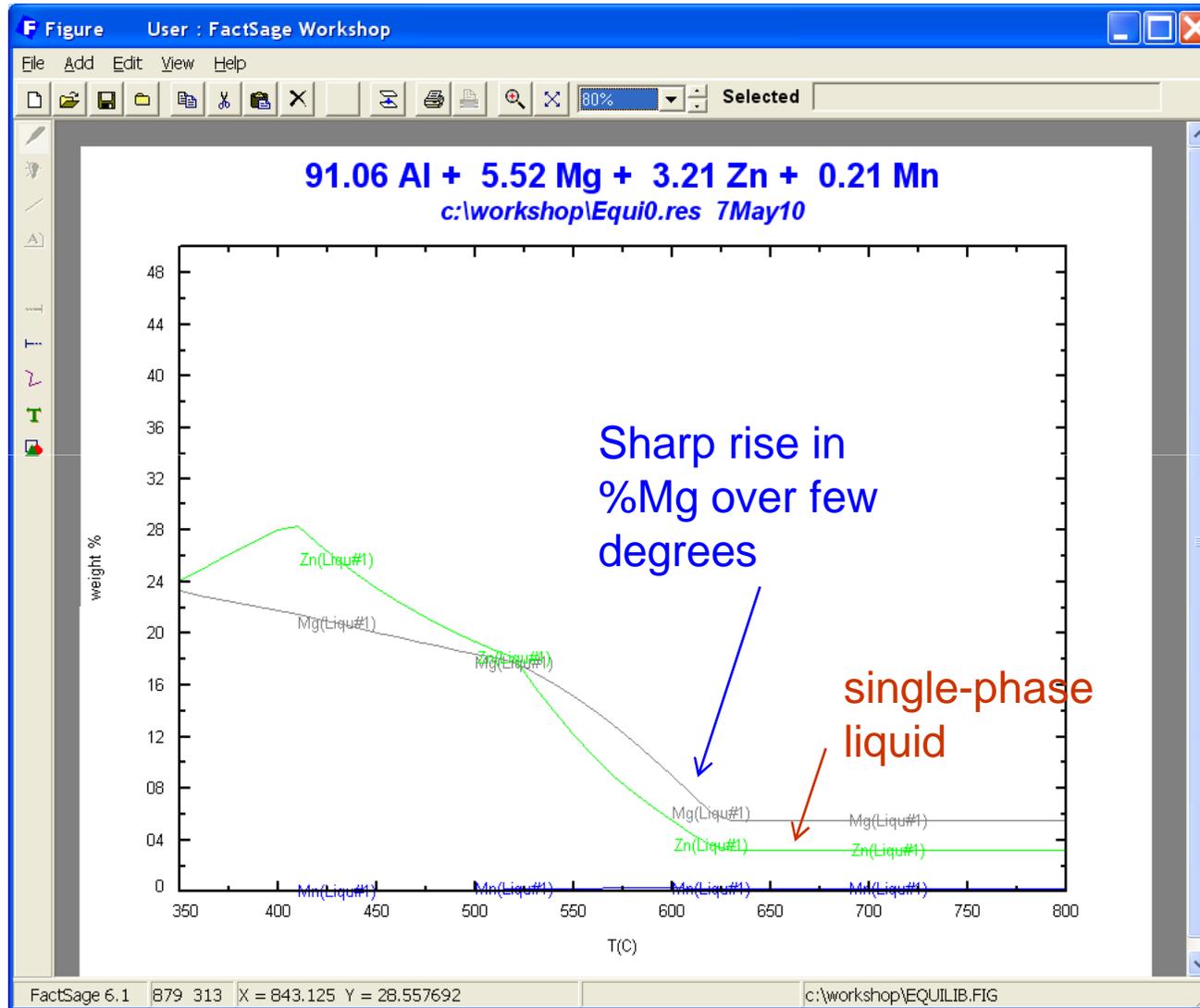
Species Selection - EQUILIB Results: weight % vs T(C)

#	Species	Mole (min)	Mole (max)	Fract. (min)	Fract. (max)	Act. (min)	Act. (max)	
Gas Phase								
1	Mg(g)	0	0	4.4033E-02	0.2131	6.8601E-08	1.9982E-03	
2	Mg2(g)	0	0	7.0551E-12	2.5896E-07	1.0894E-17	2.4282E-09	
3	Al(g)	0	0	1.6192E-15	6.4152E-08	2.5004E-21	6.0153E-10	
4	Al2(g)	0	0	1.1252E-26	9.3366E-14	1.7375E-32	8.7547E-16	
5	Mn(g)	0	0	4.3004E-19	9.0289E-11	6.6407E-25	8.4661E-13	
6	Zn(g)	0	0	0.786899	0.955967	1.4756E-06	7.3785E-03	
FTlite- Liqu								
7	Al(Liqu#1)	0	3.3749	0.584864	0.923384	0.466486	0.924435	
+	8	Mg(Liqu#1)	0	0.227114	6.2139E-02	0.291655	3.8326E-02	0.114068
+	9	Mn(Liqu#1)	0	3.8225E-03	3.6279E-05	1.2836E-03	2.6696E-09	2.4638E-06
+	10	Zn(Liqu#1)	0	4.9090E-02	1.3431E-02	0.136261	2.3939E-02	0.11342
FTlite- FCC#								
11	Al(FCC#1)	0	3.3749	0.584864	0.923384	0.466486	0.924435	
12	Mg(FCC#1)	0	0	6.2139E-02	0.291655	3.8326E-02	0.114068	
13	Mn(FCC#1)	0	0	3.6279E-05	1.2836E-03	2.6696E-09	2.4638E-06	
14	Zn(FCC#1)	0	0	1.3431E-02	0.136261	2.3939E-02	0.11342	

Mass: mole, gram, source
 Order: integer #, mass (max), fraction (max), activity (max)
 Select Top: 15, 3 species selected
 Buttons: Clear, Refresh, OK

Metal Treatment (Al & Mg)

- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**



- **Examples**

- 1) Solubility of hydrogen (H_2) in liquid alloys

- a) Mg alloys : AZ91 @ fixed $P(H_2)$

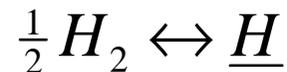
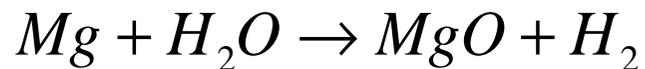
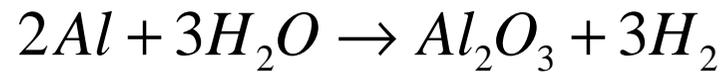
- b) Degassing AZ91 with Ar

- 2) Comparison of 2 salt fluxes for alkali removal

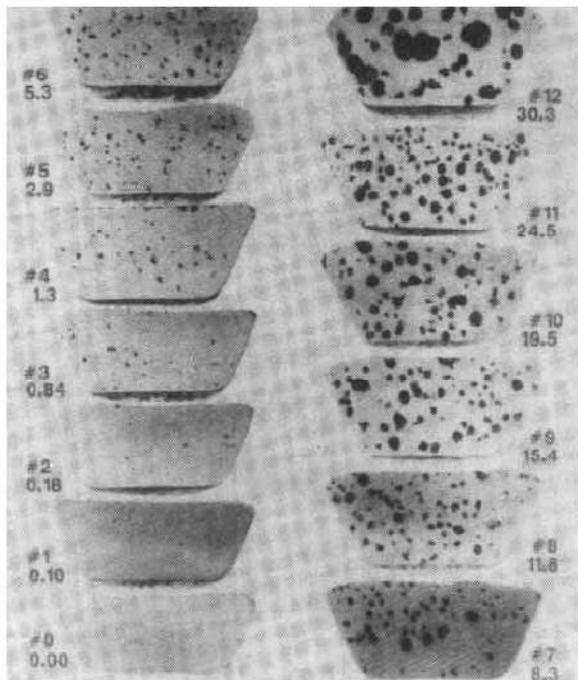
- a) Al-5%Mg with (40 ppm Na and 20 ppm Ca) treated with 2 fluxes based on NaCl-KCl-MnCl₂

- Examples
 - 1) Solubility of hydrogen (H_2) in liquid alloys
 - a) **Mg alloys : AZ91 @ fixed $P(H_2)$**

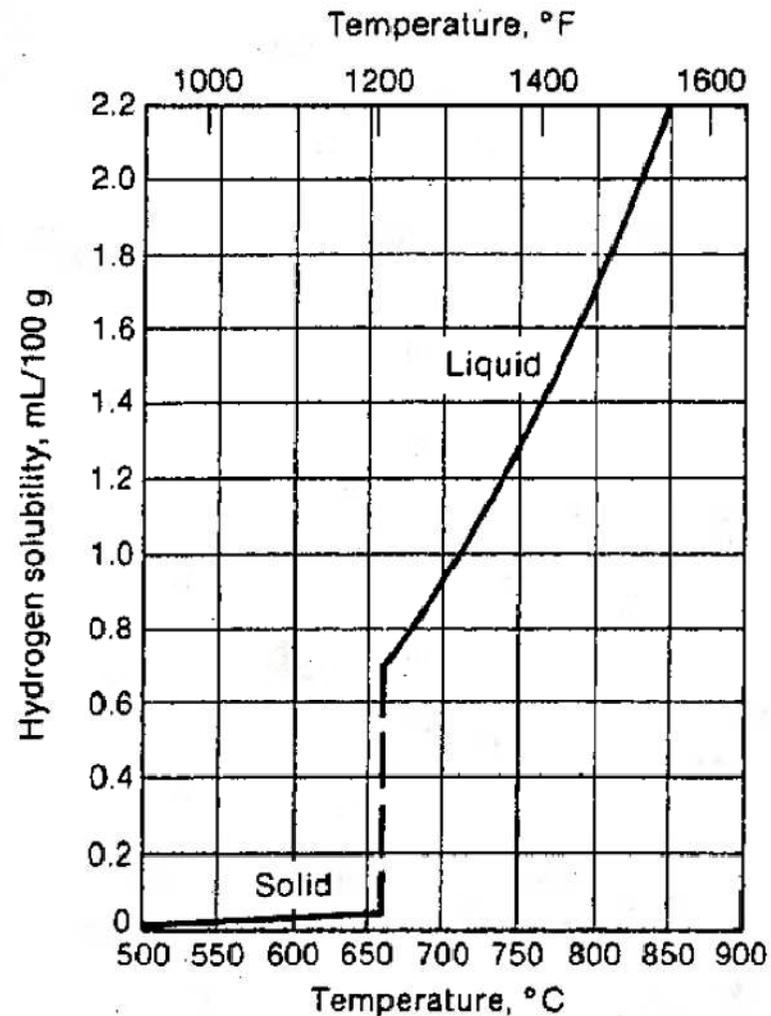
Solubility of H₂ in Liquid Alloys



$$\frac{1}{2} H_2 \leftrightarrow \underline{H} \quad S \propto P_{H_2}^{\frac{1}{2}}$$



Porosity in Al alloys as a function of the H₂-solubility in mL/100 g



Metal Treatment (Al & Mg)

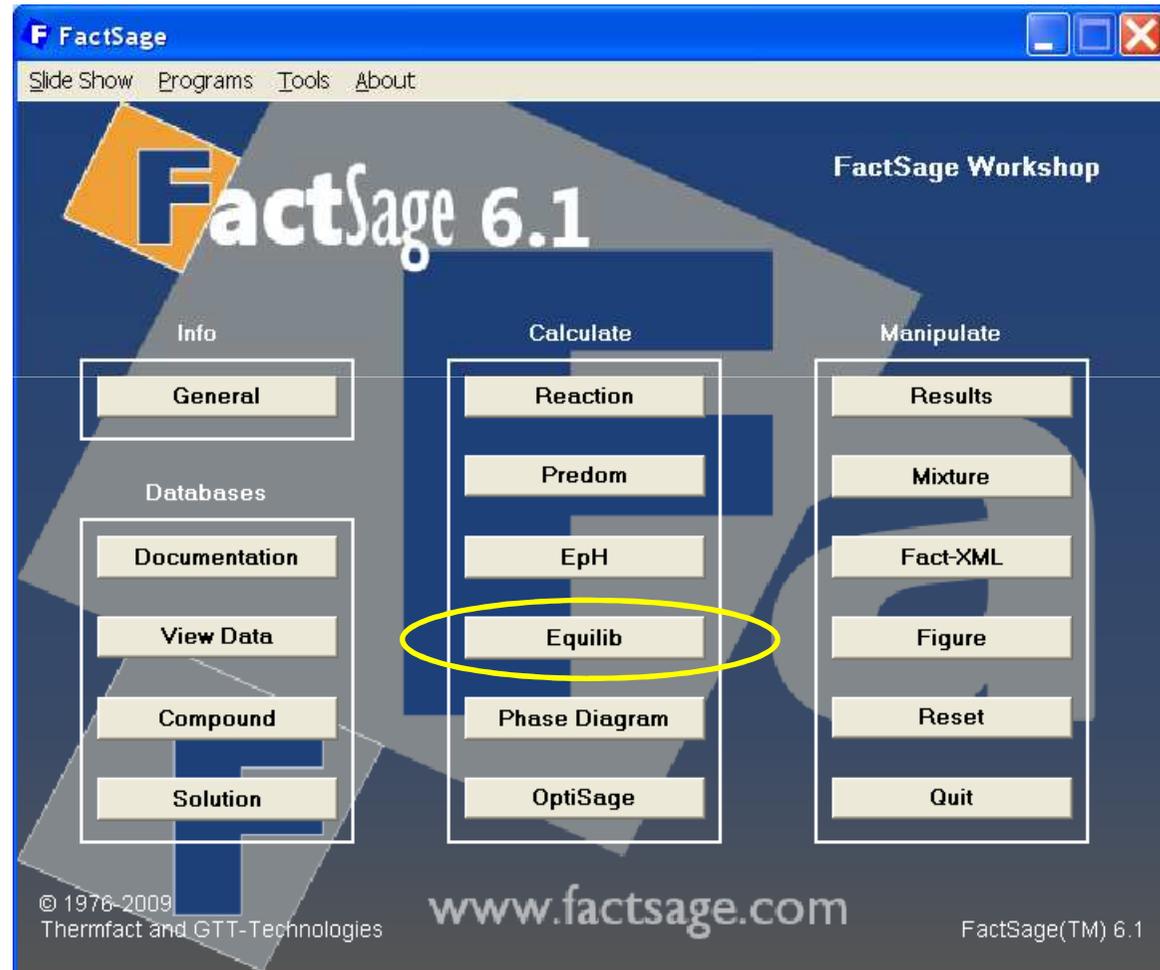
- **Example #1: Solubility of hydrogen (H₂) in liquid alloys**
 - a) Mg alloys : AZ91 @ fixed $P(\text{H}_2)$

9% Al

1% Zn

Bal. Mg

700°C



Metal Treatment (Al & Mg)

- Example #1a: Solubility of hydrogen (H₂) in liquid AZ91

F Reactants - Equilib

File Edit Table Units **Data Search** Help

Mass(mol) Specie

1

F Data Search

Databases - 2/24 compound databases, 1/22 solution databases

Fact **FactSage™** **SGTE**

ELEM FScopp BINS compounds only
 FACT FSlead SGPS solutions only
 Fact53 FSlite SGTE no data
 FToxid FSstel SGnobl EXAM SGSL SGTE*
 FTsalt FSupsi SGsold
 FTmisc FSnobl SGnucl
 FThall
 FThehg **Other** TDnucl
 FTouln OLIP OLIC
 FTlite OLIG OLIL

Information -
Click on a box to include (or exclude) a database in the data search. Normally databases are 'coupled' - that is both the compound and solution database (when available) will be selected. To 'uncouple' a databases click-mouse-right-button (note, this is NOT recommended).
If database is stored on your PC but not listed here then you must 'add the database to the list' - click on 'Add/Remove ...'.

Options

Default

Include

gaseous ions (in plasmas)
 aqueous species
 limited data compounds (25C)

Limits

Organic species CxHy... X(max) =
Minimum solution components: 1 2 cpts

Cancel Summary ... OK

Next >>

FactSage 6.2 beta Compound: 2/24 databases Solution: 1/22 databases

Metal Treatment (Al & Mg)

- **Example #1a: Solubility of hydrogen (H₂) in liquid AZ91**

The screenshot displays the FactSage 6.2 beta interface. The main window is titled "Reactants - Equilib" and has a menu bar with "File", "Edit", "Table", "Units", "Data Search", and "Help". The "Units" menu item is highlighted with a red box. Below the menu bar, there are icons for file operations and a status bar showing "T(C) P(atm) Energy(J) Mass(mol) Vol(litre)".

The "Units" dialog box is open, showing the following options:

- Temperature:** Kelvin, K; Celsius, °C; Fahrenheit, °F
- Pressure:** bar; atm; psi; Pa; GPa
- Energy:** J; cal; Btu; kwh
- Mass:** mol; g; lb
- Volume:** litre; ft³. A note below states: "Volume units are set by pressure units."

Below the unit selection, the "Universal gas constant" is listed:

```
Universal gas constant:  
R = 8.314510 J/mol-K  
  = 8.314510/4.184 cal/mol-K  
  = 22.4141/273.15 l-atm/mol-K
```

Buttons for "Cancel", "SI", "Eng", and "OK" are at the bottom of the dialog. In the main window, the "Initial Conditions" checkbox is also highlighted with a red box. A "Next >>" button is located at the bottom of the main window.

The status bar at the bottom of the main window shows: "FactSage 6.2 beta Compound: 2/24 databases Solution: 1/22 databases".

Metal Treatment (Al & Mg)

- **Example #1a: Solubility of hydrogen (H₂) in liquid AZ91**

Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 4

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
90	Mg	s			1	
+ 9	Al	s			1	
+ 1	Zn	s			1	
+ 0	H2	g			1	

Initial Conditions

Next >>

FactSage 6.2 beta Compound: 2/24 databases Solution: 1/22 databases

Metal Treatment (Al & Mg)

- **Example #1a: Solubility of hydrogen (H₂) in liquid AZ91**

Menu - Equilib: last system

File Units Parameters Help

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

Reactants (4)

(gram) 90 Mg + 9 Al + Zn + 0 H2

Products

Compound species

- gas ideal real 9
- aqueous 0
- pure liquids 0
- pure solids 38
- suppress duplicates apply

species: 47

Solution species

*	+	Base-Phase	Full Name
		FTlite-Liqu	Liquid
		FTlite-FCC	FCC_A1
		FTlite-HCP	HCP_A3
		FTlite-BCC	BCC_A2
		FTlite-LC14	Laves_C14
		FTlite-LC15	Laves_C15
		FTlite-LC36A	ALaves_C36
		FTlite-LC36B	BLaves_C36

Legend

Show all selected

species: 0
solutions: 0

Select

Custom Solutions

- 0 fixed activities
- 0 ideal solutions
- 0 activity coefficients

Details...

Pseudonyms

apply List...

include molar volumes

Total Species (max 1500) 47
Total Solutions (max 40) 0

Default

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1000	1	

10 steps Table 1 calculation

Equilibrium

- normal normal + transitions
- transitions only open
- predominant

Calculate >>

FactSage 6.2 beta

Metal Treatment (Al & Mg)

- **Example #1a: Solubility of hydrogen (H₂) in liquid AZ91**

Menu - Equilib: last system

File Units Parameters Help

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

Reactants (4)

(gram) 90 Mg + 9 Al + Zn +

Products

Compound species

- gas ideal real 9
- aqueous 0
- pure liquids 0
- pure solids 38
- suppress duplicates apply

species: 47

Target

- none -

Estimate T(K): 1000

Mass(g): 0

Solution species

*	+	Base-Phase	Full
		FTlite-Liqu	Li
		FTlite-FCC	FC
		FTlite-HCP	HC
		FTlite-BCC	BC
		FTlite-LC14	Lave
		FTlite-LC15	Lave
		FTlite-LC36A	ALav
		FTlite-LC36B	BLav

Legend

- Show all

species: solutions:

Enter the compound database priority list (most important first) fro

FTlite FACT53

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1000	1	

10 steps Table 1 calculation

Equilibrium

- normal normal + transitions
- transitions only open
- predominant

Calculate >>

FactSage 6.2 beta

Metal Treatment (Al & Mg)

- **Example #1a: Solubility of hydrogen (H₂) in liquid AZ91**

The screenshot shows the FactSage 6.2 beta interface. The main window is titled 'Menu - Equilib: last system'. The 'Reactants (4)' section contains '2 H2(g)'. The 'Products' section is empty. The 'Final Conditions' section shows 'T(C)' set to 1000 and 'P(atm)' set to 1. The 'Equilibrium' section has 'normal' selected. The 'Selection - Equilib' dialog box is open, showing a table of species and their phases. The table has columns for '+', 'Code', 'Species', 'Data', 'Phase', 'T', 'V', and 'Activity'. The row for 'H2(g)' is highlighted in red. A dropdown menu is open over the 'Activity' column, showing 'activity' and 'log10(activity)' options.

+	Code	Species	Data	Phase	T	V	Activity
+	1	H(g)	FACT5	gas			
+	2	H2(g)	FACT5	gas			
+	3	Mg(g)	FACT5	gas			
+	4	Mg2(g)	FACT5	gas			
+	5	MgH(g)	FACT5	gas			
+	6	Al(g)	FACT5	gas			
+	7	Al2(g)	FACT5	gas			
+	8	AlH(g)	FACT5	gas			
+	9	Zn(g)	FACT5	gas			

Metal Treatment (Al & Mg)

- **Example #1a: Solubility of hydrogen (H₂) in liquid AZ91**

The screenshot shows the FactSage software interface. The main window is titled "F Selection - Equilib". It has a menu bar with "File", "Edit", "Show", and "Sort". Below the menu bar, it says "Selected: 9/9" and "GAS" (highlighted in a blue box). To the right, it says "Sorted by Code".

+ Code	Species	Data	Phase	T	V	Activity
+ 1	H(g)	FACT5	gas			
+ 2	H2(g)	FACT5	gas			
+ 3	Mg(g)	FACT5	gas			
+ 4	Mg2(g)	FACT5	gas			
+ 5	MgH(g)	FACT5	gas			
+ 6	Al(g)	FACT5	gas			
+ 7	Al2(g)	FACT5	gas			
+ 8	AlH(g)	FACT5	gas			
+ 9	Zn(g)	FACT5	gas			

To the left of the main window, there is a list of species: "2 H2(g)", "- clear", "✓ + - select", "✓ - standard stable phase", "! - dormant (metastable) phase", "F - formation target phase", "P - precipitate target phase", "S - Scheil cooling gas phase", "C - composition target ...", "Ideal Solution", "a Activity", and "Help ...". The "a Activity" option is selected, and a sub-menu is open showing "activity" and "log10(activity)".

Below the main window, there is a "Fixed Partial Pressure" dialog box. It contains the text: "Enter the value of log10(p) (or for a range of values enter 'first last step') for 2 H2(g). Press [Cancel] if the partial pressure is no longer fixed." The input field contains the text "-5 -0.5 0.1".

$-5 < \log_{10} P(\text{H}_2) < -0.5$ by step of 0.1

Metal Treatment (Al & Mg)

- **Example #1a: Solubility of hydrogen (H₂) in liquid AZ91**

F Menu - Equilib: last system

File Units Parameters Help

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

Reactants (4)

(gram) 90 Mg + 9 Al + Zn + 0 H2

Products

Compound species

- gas ideal real 9
- aqueous 0
- pure liquids 0
- * pure solids 33
- suppress duplicates apply
- * - custom selection species: 42

Solution species

*	+	Base-Phase	Full Name
	I	FTlite-Liqu	Liquid
	I	FTlite-FCC	FCC_A1
	I	FTlite-HCP	HCP_A3
	I	FTlite-BCC	
	I	FTlite-LC14	
	I	FTlite-LC15	
	I	FTlite-LC36A	ALaves_C36
	I	FTlite-LC36B	BLaves_C36

Custom Solutions

- 1 fixed activities
- 0 ideal solutions
- 0 activity coefficients

Details ...

Summary ...

Edit 2: H2(g): Log10(a) = -5 -0.5 0.1 ...

Legend

- I - immiscible 7
- + - selected 8

species: 106

solutions: 22

select

include molar volumes

Total Species (max 1500) 148

Total Solutions (max 40) 22

Default

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		700	1	

10 steps Table

46 calculations

Equilibrium

- normal normal + transitions
- transitions only open
- predominant

Calculate >>

FactSage 6.2 beta

Metal Treatment (Al & Mg)

- Example #1a: Solubility of hydrogen (H₂) in liquid AZ91

Results - Equilib a=1.00E-05 (page 1/46) FactSage 6.2 beta

Output Edit Show Pages

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

a=0.0006 | a=0.0008 | a=0.001 | a=0.0013 | a=0.0016 | a=0.002 | a=0.0025 |
a=7.94E-05 | a=1.00E-04 | a=0.0001 | a=0.0002 | a=0.0002 | a=0.0003 | a=0.0004 | a=0.0005 |
a=1.00E-05 | a=1.26E-05 | a=1.58E-05 | a=2.00E-05 | a=2.51E-05 | a=3.16E-05 | a=3.98E-05 | a=5.01E-05 | a=6.31E-05 |

(gram) 90 Mg + 9 Al + Zn + 0 H2 =
+ 1.1586E-05 H2

0.00000 mol gas_ideal
(700.00 C, 1 atm, a=8.6845E-03)
(8.5864E-03 Mg FACT53
+ 8.7910E-05 Zn FACT53
+ 1.0000E-05 H2 FACT53
+ 1.1779E-07 MgH FACT53
+ 5.7019E-08 Mg2 FACT53
+ 3.4127E-12 H FACT53
+ 9.7874E-13 Al FACT53
+ 8.8516E-14 AlH FACT53
+ 1.6869E-20 Al2 FACT53)

+ 100.00 gram Liquid#1
(100.00 gram, 4.0518 mol)
(700.00 C, 1 atm, a=1.0000)
(9.0000 wt.% Al FTlite
+ 1.1586E-05 wt.% H FTlite
+ 90.000 wt.% Mg FTlite
+ 1.0000 wt.% Zn FTlite)

System component	Mole fraction	Mass fraction
Zn	3.7743E-03	1.0000E-02
Al	8.2324E-02	9.0000E-02
Mg	0.91390	0.90000
H	2.8370E-06	1.1586E-07

Metal Treatment (Al & Mg)

- **Example #1a: Solubility of hydrogen (H₂) in liquid AZ91**

Results - Equilib a=1.00E-05 (page 1/46) FactSage 6.2 beta

Output Edit Show Pages

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

a=0.0006 | a=0.0008 | a=0.001 | a=0.0013 | a=0.0016 | a=0.002 | a=0.0025 |
a=7.94E-05 | a=1.00E-04 | a=0.0001 | a=0.0002 | a=0.0002 | a=0.0003 | a=0.0003 | a=0.0004 | a=0.0005 |
a=1.00E-05 | a=1.26E-05 | a=1.58E-05 | a=2.00E-05 | a=2.51E-05 | a=3.16E-05 | a=3.98E-05 | a=5.01E-05 | a=6.31E-05 |

(gram) 90 Mg + 9 Al + Zn + 0 H2 =

+ 1.1586E-05 H2

0.00000 mol gas_ideal
(700.00 C, 1 atm, a=8.6845E-03)
(8.5864E-03 Mg FACT53
+ 8.7910E-05 Zn FACT53
+ 1.0000E-05 H2 FACT53
+ 1.1779E-07 MgH FACT53
+ 5.7019E-08 Mg2 FACT53
+ 3.4127E-12 H FACT53
+ 9.7874E-13 Al FACT53
+ 8.8516E-14 AlH FACT53
+ 1.6869E-20 Al2 FACT53)

+ 100.00 gram Liquid#1
(100.00 gram, 4.0518 mol)
(700.00 C, 1 atm, a=1.0000)
(9.0000 wt.% Al FTlite
+ 1.1586E-05 wt.% H FTlite
+ 90.000 wt.% Mg FTlite
+ 1.0000 wt.% Zn FTlite)

System component	Mole fraction	Mass fraction
Zn	3.7743E-03	1.0000E-02
Al	8.2324E-02	9.0000E-02
Mg	0.91390	0.90000
H	2.8370E-06	1.1586E-07

Metal Treatment (Al & Mg)

- Example #1a: Solubility of hydrogen (H₂) in liquid AZ91

Results - Equilib a=1.00E-05 (page 1/46) FactSage 6.2 beta

Output Edit Show Pages

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

a=0.0006 | a=0.0008 | a=0.001 | a=0.0013 | a=0.0016 | a=0.002 | a=0.0025 |
a=7.94E-05 | a=1.00E-04 | a=0.0001 | a=0.0002 | a=0.0002 | a=0.0003 | a=0.0004 | a=0.0005 |
a=1.00E-05 | a=1.26E-05 | a=1.58E-05 | a=2.00E-05 | a=2.51E-05 | a=3.16E-05 | a=3.98E-05 | a=5.01E-05 | a=6.31E-05 |

```
(gram) 90 Mg + 9 Al + Zn + 0 H2 =
+ 1.1586E-05 H2

0.00000 mol gas_ideal
(700.00 C, 1 atm, a=8.6845E-03)
( 8.5864E-03 Mg FACT53
+ 8.7910E-05 Zn FACT53
+ 1.0000E-05 H2 FACT53
+ 1.1779E-07 MgH FACT53
+ 5.7019E-08 Mg2 FACT53
+ 3.4127E-12 H FACT53
+ 9.7874E-13 Al FACT53
+ 8.8516E-14 AlH FACT53
+ 1.6869E-20 Al2 FACT53)

+ 100.00 gram Liquid#1
(100.00 gram, 4.0518 mol)
(700.00 C, 1 atm, a=1.0000)
( 9.0000 wt.% Al FTlite
+ 1.1586E-05 wt.% H FTlite
+ 90.0000 wt.% Mg FTlite
+ 1.0000 wt.% Zn FTlite)

System component Mole fraction Mass fraction
Zn 3.7743E-03 1.0000E-02
Al 8.2324E-02 9.0000E-02
Mg 0.91390 0.90000
H 2.8370E-06 1.1586E-07
```

Metal Treatment (Al & Mg)

• Example #1a: Solubility of hydrogen (H₂) in liquid AZ91

The screenshot shows the FactSage 6.2 beta interface. The main window displays the chemical reaction $90 \text{ Mg} + 9 \text{ Al} + \text{Zn} + 0 \text{ H}_2$ and a list of components with their mole fractions. The 'Results Processor' window is open, showing the 'Axes' dialog box. The Y-axis is set to 'mole' and the X-axis is set to 'log10(activity)'. The 'Graph' section is also visible, showing options for labels and display.

System component	Mole fraction
Zn	3.7743E-03
Al	8.2324E-02
Mg	0.91390
H	2.8370E-06

Metal Treatment (Al & Mg)

• Example #1a: Solubility of hydrogen (H₂) in liquid AZ91

Plot: weight % vs log10(activity)

90 Mg + 9 Al + Zn + 0 H₂

Y-axis: weight %
maximum: 0.004
minimum: 0
tick every: 0.0002

X-axis: log10(activity)
maximum: 0
minimum: -6
tick every: 0.5

Graph

Labels: size: 9 no: 4

Display: color full screen
 reactants Viewer
 file name Figure

Plot >>

6May10 46 sets

Output Edit Show Pages

Save or Print

Plot Plot Results ...

Equilib Results file Repeat Plot - ...

Stream File

Format a=1.58E-05 a=2.00E-05 a=2.5

Fact-XML Al + Zn + 0 H₂ =

Fact-Optimal

Refresh ... gas_ideal

System component	Mole frac
Zn	3.7743E-06
Al	8.2324E-06
Mg	0.91390
H	2.8370E-06

Metal Treatment (Al & Mg)

- Example #1a: Solubility of hydrogen (H₂) in liquid AZ91

Species Selection - EQUILIB Results: weight % vs log10(activity)

#	Species	Mole (min)	Mole (max)	Fract. (min)	Fract. (max)	Act. (min)	Act. (max)
Gas Phase							
1	H(g)	0	0	3.9296E-10	5.7871E-09	3.4127E-12	6.0687E-10
2	H2(g)	0	0	1.1515E-03	0.973255	1.0000E-05	0.316228
3	Mg(g)	0	0	2.6409E-02	0.988706	8.5808E-03	8.5864E-03
4	Mg2(g)	0	0	1.7526E-07	6.5656E-06	5.6945E-08	5.7019E-08
5	MgH(g)	0	0	1.3563E-05	1.9973E-04	1.1779E-07	2.0933E-05
6	Al(g)	0	0	3.0154E-12	1.1270E-10	9.7874E-13	9.7977E-13
7	Al2(g)	0	0	5.2026E-20	1.9424E-18	1.6869E-20	1.6904E-20
8	AlH(g)	0	0	1.0192E-11	1.5013E-10	8.8516E-14	1.5757E-11
9	Zn(g)	0	0	2.7087E-04	1.0123E-02	8.7910E-05	8.8011E-05
FTlite- Liqu							
10	Al(Liqu#1)	0.333561	0.333561	8.2283E-02	8.2324E-02	5.5451E-02	5.5509E-02
+	H(Liqu#1)	1.1495E-05	2.0396E-03	2.8370E-06	5.0312E-04	4.2900E-09	7.6288E-07
12	Mg(Liqu#1)	3.7029	3.7029	0.913442	0.913899	0.909946	0.910535
13	Zn(Liqu#1)	1.5293E-02	1.5293E-02	3.7724E-03	3.7743E-03	1.0976E-03	1.0989E-03
FTlite- Liqu							
14	Al(Liqu#2)	0	0	8.2283E-02	8.2324E-02	5.5451E-02	5.5509E-02
15	H(Liqu#2)	0	0	2.8370E-06	5.0312E-04	4.2900E-09	7.6288E-07
16	Mg(Liqu#2)	0	0	0.913442	0.913899	0.909946	0.910535

Species Selection Dialog:

- Y-axis: weight %
- X-axis: log10(activity)
- Species: 0 selected
- Mass: mole (selected)
- Order: integer # (selected)
- Select Top: 15
- 1 species selected

Species Selection Table:

Y-axis	X-axis	Species
weight %	log10(activity)	H2(g)

Metal Treatment (Al & Mg)

- Example #1a: Solubility of hydrogen (H₂) in liquid AZ91

Species Selection - EQUILIB Results: weight % vs log10(activity)

#	Species	Mole (min)	Mole (max)	Fract. (min)	Fract. (max)	Act. (min)	Act. (max)	
Gas Phase								
1	H(g)	0	0	3.9296E-10	5.7871E-09	3.4127E-12	6.0687E-10	
2	H2(g)	0	0	1.1515E-03	0.973255	1.0000E-05	0.316228	
3	Mg(g)	0	0	2.6409E-02	0.988706	8.5808E-03	8.5864E-03	
4	Mg2(g)	0	0	1.7526E-07	6.5656E-06	5.6945E-08	5.7019E-08	
5	MgH(g)	0	0	1.3563E-05	1.9973E-04	1.1779E-07	2.0933E-05	
6	Al(g)	0	0	3.0154E-12	1.1270E-10	9.7874E-13	9.7977E-13	
7	Al2(g)	0	0	5.2026E-20	1.9424E-18	1.6869E-20	1.6904E-20	
8	AlH(g)	0	0	1.0192E-11	1.5013E-10	8.8516E-14	1.5757E-11	
9	Zn(g)	0	0	2.7087E-04	1.0123E-02	8.7910E-05	8.8011E-05	
FTlite- Liqu								
10	Al(Liqu#1)	0.333561	0.333561	8.2283E-02	8.2324E-02	5.5451E-02	5.5509E-02	
+	11	H(Liqu#1)	1.1495E-05	2.0396E-03	2.8370E-06	5.0312E-04	4.2900E-09	7.6288E-07
	12	Mg(Liqu#1)	3.7029	3.7029	0.913442	0.913899	0.909946	0.910535
	13	Zn(Liqu#1)	1.5293E-02	1.5293E-02	3.7724E-03	3.7743E-03	1.0976E-03	1.0989E-03
FTlite- Liqu								
	14	Al(Liqu#2)	0	0	8.2283E-02	8.2324E-02	5.5451E-02	5.5509E-02
	15	H(Liqu#2)	0	0	2.8370E-06	5.0312E-04	4.2900E-09	7.6288E-07
	16	Mg(Liqu#2)	0	0	0.913442	0.913899	0.909946	0.910535

Plot: weight % vs log10(activity)

90 Mg + 9 Al + Zn + 0 H2

Y-axis: weight %
X-axis: activity

Y: weight %
X: log10(activity)

Mass: mole, gram, source
Order: integer #, mass (max), fraction (max), activity (max)

Select Top: 15, 1 species selected

Buttons: Clear, Repeat, Refresh, OK

FactSage 6.1 | c:\workshop\Equi0.res | 6May10 | 46 sets

Metal Treatment (Al & Mg)

- Example #1a: Solubility of hydrogen (H₂) in liquid AZ91

F Plot: weight % vs log10(activity)

File Help

90 Mg + 9 Al + Zn + 0 H2

X-axis	activity	0	1.
	mole	0	4.0538
	mole fract.	0	0.991706
	gram	0	100.
Y-axis	weight %	0	99.11
	Alpha	-9.	0
	T(C)	700.	700.
	P(atm)	1.	1.
	Cp(J)	138.2	138.24
	G(J)	-1.9302E+05	-1.9285E+05
	Vol(litre)	0	0
	H(J)	1.1101E+05	1.1109E+05
	V(litre)	0	0
	S(J)	312.24	312.49
	- page -	1.	46.

Axes
weight % vs log10(activity)
Axes

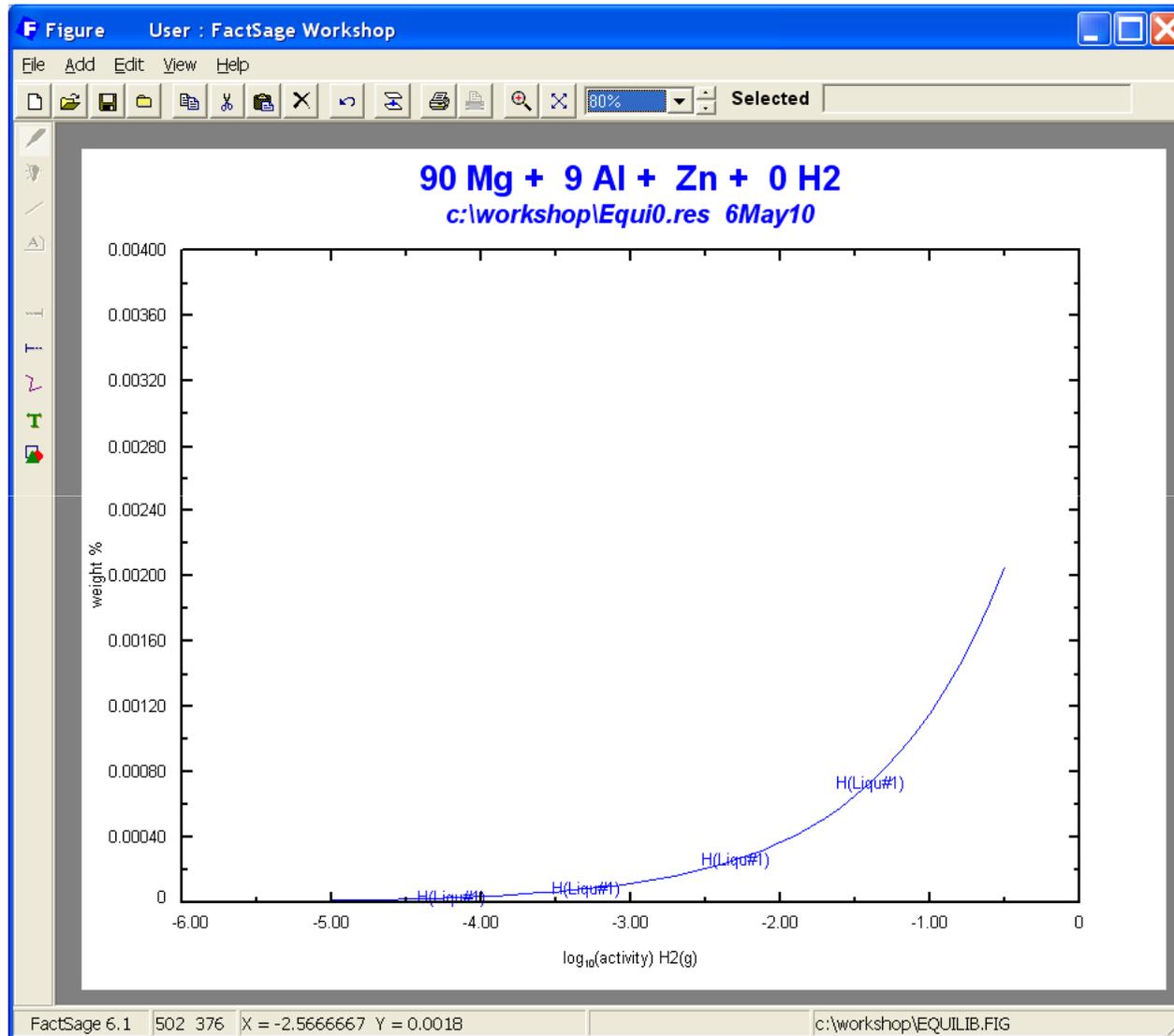
Species
1 selected
Select
Repeat

Graph
Labels: size: 9 no: 4
 chemical
 integer #
 none
Display:
 color
 full screen
 reactants
 viewer
 file name
 Figure
Plot >>

FactSage 6.1 | c:\workshop\Equi0.res | 6May10 | 46 sets

Metal Treatment (Al & Mg)

- **Example #1a: Solubility of hydrogen (H₂) in liquid AZ91**



Metal Treatment (Al & Mg)

- **Example #1a: Solubility of hydrogen (H₂) in liquid AZ91**

The screenshot shows the FactSage 6.2 beta interface. The title bar reads "F Results - Equilib a=1.00E-05 (page 1/46) FactSage 6.2 beta". A red box highlights the "Show Pages" menu, which is open and shows options: "Go to" (selected), "<< Previous Pages", "Next Pages >>", "Go to page ...", "Delete page 'a=0.3162' ...", "Delete all 'Abort' pages ...", and "Swap pages ...". The "Go to" sub-menu is also open, showing "Pages 1 - 25 [a=1.00E-05 - a=0.0025]" and "Pages 26 - 46 [a=0.0032 - a=0.3162]".

The main output window displays the following text:

```
(gram) 90
+ 1.1586E-05
0.00000 mol gas_ideal
(700.00 C, 1 atm, a=8.6845E-03)
( 8.5864E-03 Mg FACT53
+ 8.7910E-05 Zn FACT53
+ 1.0000E-05 H2 FACT53
+ 1.1779E-07 MgH FACT53
+ 5.7019E-08 Mg2 FACT53
+ 3.4127E-12 H FACT53
+ 9.7874E-13 Al FACT53
+ 8.8516E-14 AlH FACT53
+ 1.6869E-20 Al2 FACT53)
+ 100.00 gram Liquid#1
(100.00 gram, 4.0518 mol)
(700.00 C, 1 atm, a=1.0000)
( 9.0000 wt.% Al FTlite
+ 1.1586E-05 wt.% H FTlite
+ 90.000 wt.% Mg FTlite
+ 1.0000 wt.% Zn FTlite)
System component Mole fraction Mass fraction
Zn 3.7743E-03 1.0000E-02
Al 8.2324E-02 9.0000E-02
Mg 0.91390 0.90000
H 2.8370E-06 1.1586E-07
```

Metal Treatment (Al & Mg)

- Example #1a: Solubility of hydrogen (H₂) in liquid AZ91

Results - Equilib a=0.01 (page 31/46) FactSage 6.2 beta

Output Edit Show Pages

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

a=0.1995 | a=0.2512 | a=0.3162 |
a=0.0251 | a=0.0316 | a=0.0398 | a=0.0501 | a=0.0631 | a=0.0794 | a=0.1 | a=0.1259 | a=0.1585 |
a=0.0032 | a=0.004 | a=0.005 | a=0.0063 | a=0.0079 | - a=0.01 - | a=0.0126 | a=0.0158 | a=0.02 |

```
(gram) 90 Mg + 9 Al + Zn + 0 H2 =
+ 3.6624E-04 H2
0.00000 mol gas_ideal
(700.00 C, 1 atm, a=1.8677E-02)
( 1.0000E-02 H2 FACT53
+ 8.5854E-03 Mg FACT53
+ 8.7928E-05 Zn FACT53
+ 3.7245E-06 MgH FACT53
+ 5.7006E-08 Mg2 FACT53
+ 1.0792E-10 H FACT53
+ 2.7996E-12 AlH FACT53
+ 9.7892E-13 Al FACT53
+ 1.6875E-20 Al2 FACT53)
+ 100.00 gram Liquid#1
(100.00 gram, 4.0522 mol)
(700.00 C, 1 atm, a=1.0000)
( 9.0000 wt.% Al FTlite
+ 3.6624E-04 wt.% H FTlite
+ 90.0000 wt.% Mg FTlite
+ 1.0000 wt.% Zn FTlite)

System component Mole fraction Mass fraction
Zn 3.7740E-03 1.0000E-02
Al 8.2317E-02 9.0000E-02
Mg 0.91382 0.90000
H 8.9670E-05 3.6624E-06
```

Metal Treatment (Al & Mg)

- **Example #1a: Solubility of hydrogen (H₂) in liquid AZ91**

The screenshot shows the FactSage 6.2 beta interface. The 'Stream File' menu is open, with 'Save stream file' and 'Save solutions' highlighted. The 'Save solutions' submenu is also open, showing a list of solution types, with 'FTlite-Liqu#1 gas' selected. The main window displays the following data:

Component	Mole fraction	Mass fraction
Zn	3.7740E-03	1.0000E-02
Al	8.2317E-02	9.0000E-02
Mg	0.91382	0.90000
H	8.9670E-05	3.6624E-06

Metal Treatment (Al & Mg)

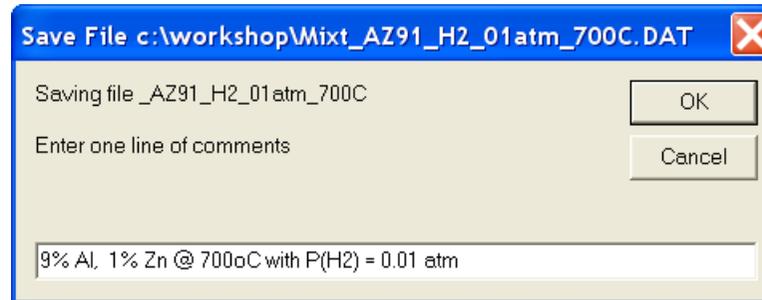
- **Example #1a: Solubility of hydrogen (H₂) in liquid AZ91**

The screenshot shows the FactSage 6.2 beta interface. The main window displays the 'Results - Equilib a=0.01' page. The 'Stream File' menu is open, and the 'Save solutions' option is selected, opening a sub-menu where 'FTlite-Liqu#1 gas' is highlighted. A 'Save File' dialog box is open in the foreground, showing the file path 'c:\workshop\Mixt_AZ91_H2_01atm_700C.DAT'. The dialog box contains the text 'Saving file _AZ91_H2_01atm_700C' and a text input field with the comment '9% Al, 1% Zn @ 700oC with P(H2) = 0.01 atm'. The background window shows a table of system components and their mole and mass fractions.

System component	Mole fraction	Mass fraction
Zn	3.7740E-03	1.0000E-02
Al	8.2317E-02	9.0000E-02
Mg	0.91382	0.90000
H	8.9670E-05	3.6624E-06

Metal Treatment (Al & Mg)

- **Example #1a: Solubility of hydrogen (H₂) in liquid AZ91**



The liquid AZ91 saturated with H at $P(\text{H}_2) = 0.01 \text{ atm}$ & 700°C is now stored in the **stream file**

C:\workshop\Mixt_AZ91_H2_01atm_700C.dat

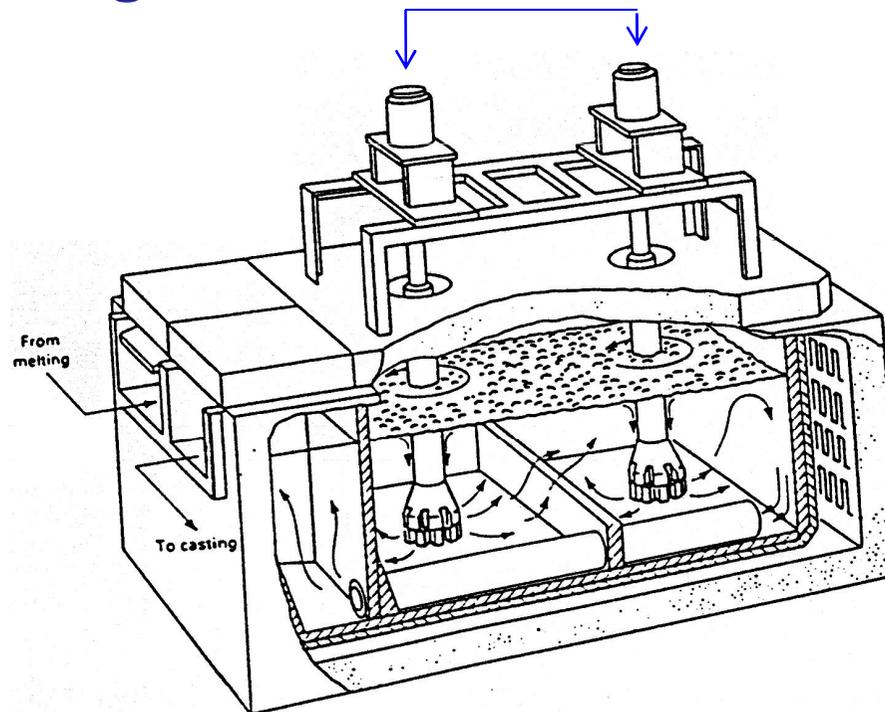
A **stream file** can be automatically retrieved as an input for the next calculation where Ar will be injected to remove soluble H

- Examples

- 1) Solubility of hydrogen (H_2) in liquid alloys

- b) Degassing AZ91 with Ar**

In-line Degassing Unit
for Al-Treatment



Metal Treatment (Al & Mg)

- **Example #1b: Degassing AZ91 with Ar**

The screenshot shows the 'Reactants - Equilib' window in FactSage 6.2 beta. The 'File' menu is open, with 'New' highlighted. The main window displays a table with the following data:

	Species	Phase	T(C)	P(total)**	Stream#	Data
	Mg	s			1	
+ 9	Al	s			1	
+ 1	Zn	s			1	
+ 0	H2	g			1	

At the bottom of the window, there is a 'Next >>' button and a status bar showing 'FactSage 6.2 beta', 'Compound: 2/24 databases', and 'Solution: 1/22 databases'. A checkbox for 'Initial Conditions' is also present.

Metal Treatment (Al & Mg)

- **Example #1b: Degassing AZ91 with Ar**

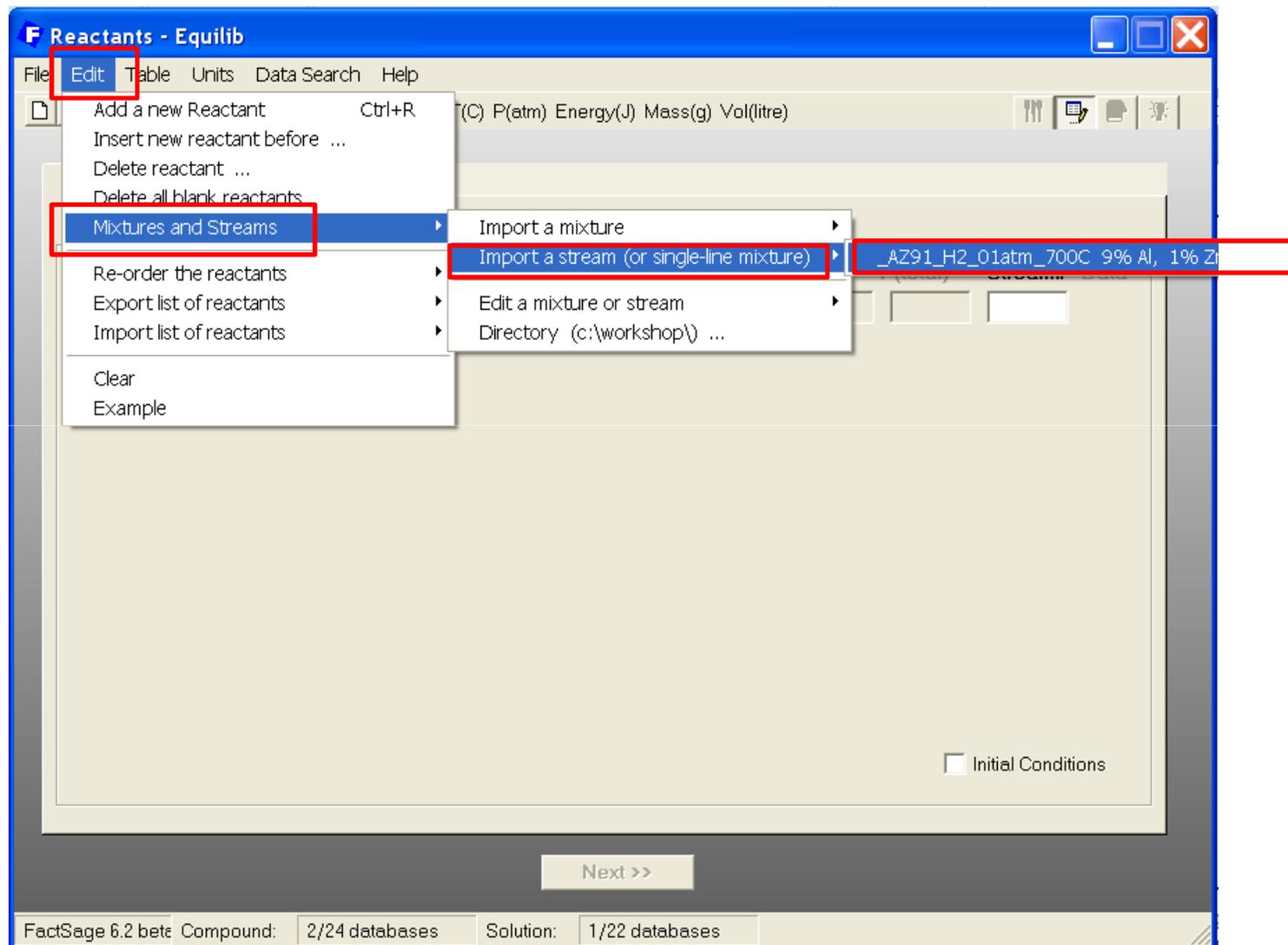
The screenshot shows the 'Reactants - Equilib' window in FactSage. The 'File' menu is open, and the 'New' option is highlighted. A 'New Reaction' dialog box is displayed, asking for confirmation to clear the current system. The 'Yes' button is circled in yellow. The main window contains a table of reactants:

	Species	Phase	T(C)	P(total)**	Stream#	Data
	Mg	s			1	
	Al	s			1	
+ 1	Zn	s			1	
+ 0	H2	g			1	

At the bottom of the window, there is a 'Next >>' button and a status bar showing 'FactSage 6.2 beta', 'Compound: 2/24 databases', and 'Solution: 1/22 databases'.

Metal Treatment (Al & Mg)

- **Example #1b: Degassing AZ91 with Ar**



Metal Treatment (Al & Mg)

- **Example #1b: Degassing AZ91 with Ar**

1-2

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100%	[_AZ91_H2_01atm]				1	
+ 1						

Initial Conditions

Next >>

FactSage 6.2 beta Compound: 2/24 databases Solution: 1/22 databases

Metal Treatment (Al & Mg)

- **Example #1b: Degassing AZ91 with Ar**

The screenshot shows the 'Reactants - Equilib' window in FactSage 6.2 beta. The interface includes a menu bar (File, Edit, Table, Units, Data Search, Help) and a toolbar. The main area contains a table for defining reactants. A red box highlights the input for two reactants:

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
1.0E+06	[_AZ91_H2_01atm]				1	
<1783.393A>	Ar	g			2	

Below the table is a 'Next >>' button. At the bottom, the status bar shows 'FactSage 6.2 beta', 'Compound: 2/24 databases', and 'Solution: 1/22 databases'.

**1.0E+06 g = 1.0 ton of AZ91D
equilibrated with $P(H_2) = 0.01 \text{ atm}$ @ 700°C**

<1783.393A> g Ar = 1 m³ Ar @ STP

The screenshot shows a Microsoft Excel spreadsheet with the following data:

	A	B	C	D	E
1	1 g	Ar			
2	39.948 g/mol	Ar			
3	0.025033 mol	Ar			
4	22.4 L/mol	Ar		"@ 273.15; 1 atm"	
5	0.560729 L	Ar			
6	1000 L	Ar			
7	1783.393 g	Ar			

Metal Treatment (Al & Mg)

- **Example #1b: Degassing AZ91 with Ar**

The screenshot shows the FactSage Equilib software interface. The window title is "F Menu - Equilib:". The menu bar includes "File", "Units", "Parameters", and "Help". The main area is divided into several sections:

- Reactants (2):** A text box contains "(gram) 1.0E+06 [_AZ91_H2_01atm_700C] + <1783.393A> Ar".
- Products:** A list of compound species is shown on the left, including "gas", "aqueous", "pure liquids", "pure solids", and "suppress duplicates". A "Solution species" table is in the center, and a "Legend" is at the bottom left of this section.
- Final Conditions:** A table at the bottom left shows conditions for two calculations. The first calculation is highlighted with a red box, showing T(C) = 700 and P(atm) = 1.
- Equilibrium:** Radio buttons for "normal", "normal + transitions", "transitions only", and "predominant" are on the right, along with a "Calculate >>" button.

* +	Base-Phase	Full Name
	I	FTlite-Liqu
	I	FTlite-FCC
	I	FTlite-HCP
	I	FTlite-BCC
	I	FTlite-LC14
	I	FTlite-LC15
	I	FTlite-LC36A
		FTlite-LC36B

T(C)	P(atm)	Product H(J)
700	1	

Metal Treatment (Al & Mg)

- **Example #1b: Degassing AZ91 with Ar**

The screenshot shows the FactSage Equilib software interface. The window title is "F Menu - Equilib:". The menu bar includes "File", "Units", "Parameters", and "Help". The main area is divided into several sections:

- Reactants (2):** A text box contains "(gram) 1.0E+06 [_AZ91_H2_01atm_700C] + <1783.393A> Ar".
- Products:** A list of compound species is shown on the left, including "gas" (ideal/real), "aqueous", "pure liquids", "pure solids", and "suppress duplicates". A "species: 48" label is present.
- Solution species:** A table lists various phases and their full names:

*	+	Base-Phase	Full Name
	I	FTlite-Liqu	Liquid
	I	FTlite-FCC	FCC_A1
	I	FTlite-HCP	HCP_A3
	I	FTlite-BCC	
	I	FTlite-LC14	
	I	FTlite-LC15	
	I	FTlite-LC36A	
		FTlite-LC36B	
- Target:** "Estimate T(K): 1000" and "Mass(g): 0".
- Legend:** "I - immiscible 7", "+ - selected 8".
- Final Conditions:** A table with columns for "<A>", "", "T(C)", "P(atm)", and "Product H(J)". The first row has "1" in the "<A>" column and "700" in the "T(C)" column. The second row has "50" in the "<A>" column and "steps" in the "" column.
- Equilibrium:** Radio buttons for "normal", "normal + transitions", "transitions only", and "predominant". The "open" radio button is selected and highlighted with a red box.
- Buttons:** "Calculate >>" and "Details ...".

At the bottom left, the text "FactSage 6.2 beta" is visible.

"open"

<A> = 1 (corresponds to 1 m³) Ar is injected every step

After each step the gas phase is removed

50 steps will be performed

Metal Treatment (Al & Mg)

- Example #1b: Degassing AZ91 with Ar

Output Edit Show Pages

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

Step 25

Step 13 | Step 14 | Step 15 | Step 16 | Step 17 | Step 18 | Step 19 | Step 20 | Step 21 | Step 22 | Step 23 | Step 24

Step 1 | Step 2 | Step 3 | Step 4 | Step 5 | Step 6 | Step 7 | Step 8 | Step 9 | Step 10 | Step 11 | Step 12

(gram) 1.0E+06 [_AZ91_H2_01atm_700C] + <1783.393A> ArTotal <A> = 1.0000

45.345 mol gas_ideal

(1793.6 gram, 45.345 mol, 3621.0 litre, 4.9534E-04 g/ml)

(700.00 C, 1 atm, a=1.0000)

{ 0.98446 Ar FACT53

+ 8.5856E-03 Mg FACT53

+ 6.8652E-03 H2 FACT53

+ 8.7923E-05 Zn FACT53

+ 3.0860E-06 MgH FACT53

+ 5.7008E-08 Mg2 FACT53

+ 8.9418E-11 H FACT53

+ 2.3196E-12 AlH FACT53

+ 9.7890E-13 Al FACT53

+ 1.6874E-20 Al2 FACT53)

+ 9.9999E+05 gram Liquid#1

(9.9999E+05 gram, 40320. mol)

(700.00 C, 1 atm, a=1.0000)

{ 9.0001 wt.% Al FTLite

+ 9.7599E-06 wt.% Ar FTLite

+ 3.0348E-04 wt.% H FTLite

+ 90.000 wt.% Mg FTLite

+ 0.99998 wt.% Zn FTLite)

System component	Mole fraction	Mass fraction
Zn	3.7740E-03	9.9998E-03
Ar	6.0293E-08	9.7599E-08
Al	8.2319E-02	9.0001E-02
Mg	0.91383	0.90000

Metal Treatment (Al & Mg)

- **Example #1b: Degassing AZ91 with Ar**

Results Processor: c:\workshop\Equi0.res

1.0E+06 [_AZ91_H2_01atm_700C] + <1783.393A> Ar

activity	0	1.
mole	0	4.0520E+04
mole fract.	0	0.991706
gram	0	9.9999E+05
weight %	0	99.461
Alpha	0	0
T(C)	700.	700.
P(atm)	1.	1.
Cp(J)	1.2124E+06	1.3840E+06
G(J)	-1.9360E+09	-1.6965E+09
Vol(litre)	0	0
H(J)	9.7314E+08	1.1109E+09
V(litre)	3592.2	3616.6
S(J)	2.7433E+06	3.1309E+06
- page -	1.	50.

Output

```

+ 9.9999E+05 gram Liquid#1
(9.9999E+05 gram, 40520. mol)
(700.00 C, 1 atm, a=1.0000)
( 9.0001 wt.% Al
+ 9.7599E-06 wt.% Ar
+ 3.0348E-04 wt.% H
+ 90.000 wt.% Mg
+ 0.99998 wt.% Zn

System component      Mole fr
Zn                    3.774
Ar                    6.029
Al                    8.231
Mcr                   0.913
    
```

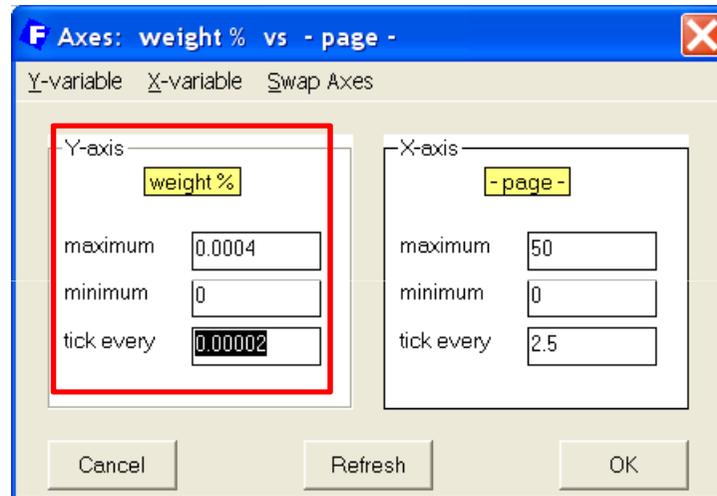
Metal Treatment (Al & Mg)

- Example #1b: Degassing AZ91 with Ar

The screenshot shows the FactSage 6.1 Results Processor interface. The main window title is "Results Processor: c:\workshop\Equi0.res". The main window contains a table with columns for activity, mole fraction, and weight percent. A dialog box titled "F Axes: weight % vs - page -" is open, showing the configuration for the graph axes. The Y-axis is labeled "weight %" and has a maximum of 0.004, a minimum of 0, and a tick every 0.0002. The X-axis is labeled "- page -" and has a maximum of 50, a minimum of 0, and a tick every 2.5. The "Graph" section shows "Display" options: color (checked), full screen (checked), reactants (checked), file name (checked), and Figure (selected). The "Plot >>" button is visible. The status bar at the bottom shows "FactSage 6.1", "Equi0.res", "6May10", and "50 sets".

Metal Treatment (Al & Mg)

- **Example #1b: Degassing AZ91 with Ar**



Metal Treatment (Al & Mg)

- Example #1b: Degassing AZ91 with Ar

Species Selection - EQUILIB Results: weight % vs - page -

#	Species	Phase	Mole (min)	Mole (max)	Fract. (min)	Fract. (max)	Act. (min)	Act. (max)
Gas								
1	H(g)		1.2078E-10	4.0547E-09	2.6820E-12	8.9418E-11	2.6820E-12	8.9418E-11
2	H2(g)		2.7814E-04	0.311304	6.1763E-06	6.8652E-03	6.1763E-06	6.8652E-03
3	Mg(g)		0.386681	0.389316	8.5856E-03	8.5865E-03	8.5856E-03	8.5865E-03
4	Mg2(g)		2.5678E-06	2.5850E-06	5.7008E-08	5.7020E-08	5.7008E-08	5.7020E-08
5	MgH(g)		4.1689E-06	1.3994E-04	9.2573E-08	3.0860E-06	9.2573E-08	3.0860E-06
6	Al(g)		4.4077E-11	4.4388E-11	9.7875E-13	9.7890E-13	9.7875E-13	9.7890E-13
7	Al2(g)		7.5966E-19	7.6515E-19	1.6869E-20	1.6874E-20	1.6869E-20	1.6874E-20
8	AlH(g)		3.1328E-12	1.0518E-10	6.9565E-14	2.3196E-12	6.9565E-14	2.3196E-12
9	Ar(g)		44.64	44.643	0.984458	0.991319	0.984458	0.991319
10	Zn(g)		3.9531E-03	3.9869E-03	8.7781E-05	8.7923E-05	8.7781E-05	8.7923E-05
FTlite- Liqu								
11	Al(Liqu#1)		2922.	3335.6	8.2319E-02	8.2326E-02	5.5451E-02	5.5460E-02
12	Ar(Liqu#1)		2.1556E-03	2.4431E-03	6.0293E-08	6.0731E-08	6.2732E-08	6.3169E-08
+	13	H(Liqu#1)	7.9136E-02	3.0108	2.2296E-06	7.4304E-05	3.3715E-09	1.1240E-07
	14	Mg(Liqu#1)	3.2438E+04	3.7029E+04	0.913833	0.913903	0.91045	0.910541
	15	Zn(Liqu#1)	133.77	152.92	3.7688E-03	3.7740E-03	1.0960E-03	1.0978E-03
ETlite- Liqu								
	16	Al(Liqu#2)	0	0	8.2319E-02	8.2326E-02	5.5451E-02	5.5460E-02

Species: 0 selected

Mass: mole, gram, source

Order: integer #, mass (max), fraction (max), activity (max)

Select Top: 15, 1 species selected

Buttons: Clear, Refresh, OK

Click on the "+" column to add or remove species.

FactSage 6.1 | c:\workshop\Equi0.res | 6May10 | 50 sets

Metal Treatment (Al & Mg)

- Example #1b: Degassing AZ91 with Ar

The screenshot shows the FactSage software interface for plotting. The window title is "Plot: weight % vs - page -". The main area contains a table of thermodynamic data for the system "1.0E+06 [_AZ91_H2_01atm_700C] + <1783.393A> Ar". The Y-axis is set to "weight %" and the X-axis is set to "- page -". The "Display" options are set to "full screen", "color", "reactants", and "file name". The "Plot >>" button is highlighted with a yellow circle.

	activity	0	1.
	mole	0	4.0520E+04
	mole fract.	0	0.991706
	gram	0	9.9999E+05
Y-axis	weight %	0	99.461
	Alpha	0	0
	T(O)	700.	700.
	P(atm)	1.	1.
	Cp(J)	1.2124E+06	1.3840E+06
	G(J)	-1.9360E+09	-1.6965E+09
	Vol(litre)	0	0
	H(J)	9.7314E+08	1.1109E+09
	V(litre)	3592.2	3616.6
	S(J)	2.7433E+06	3.1309E+06
X-axis	- page -	1.	50.

Axes
weight %
vs
- page -
Axes

Species
1 selected
Select
Repeat

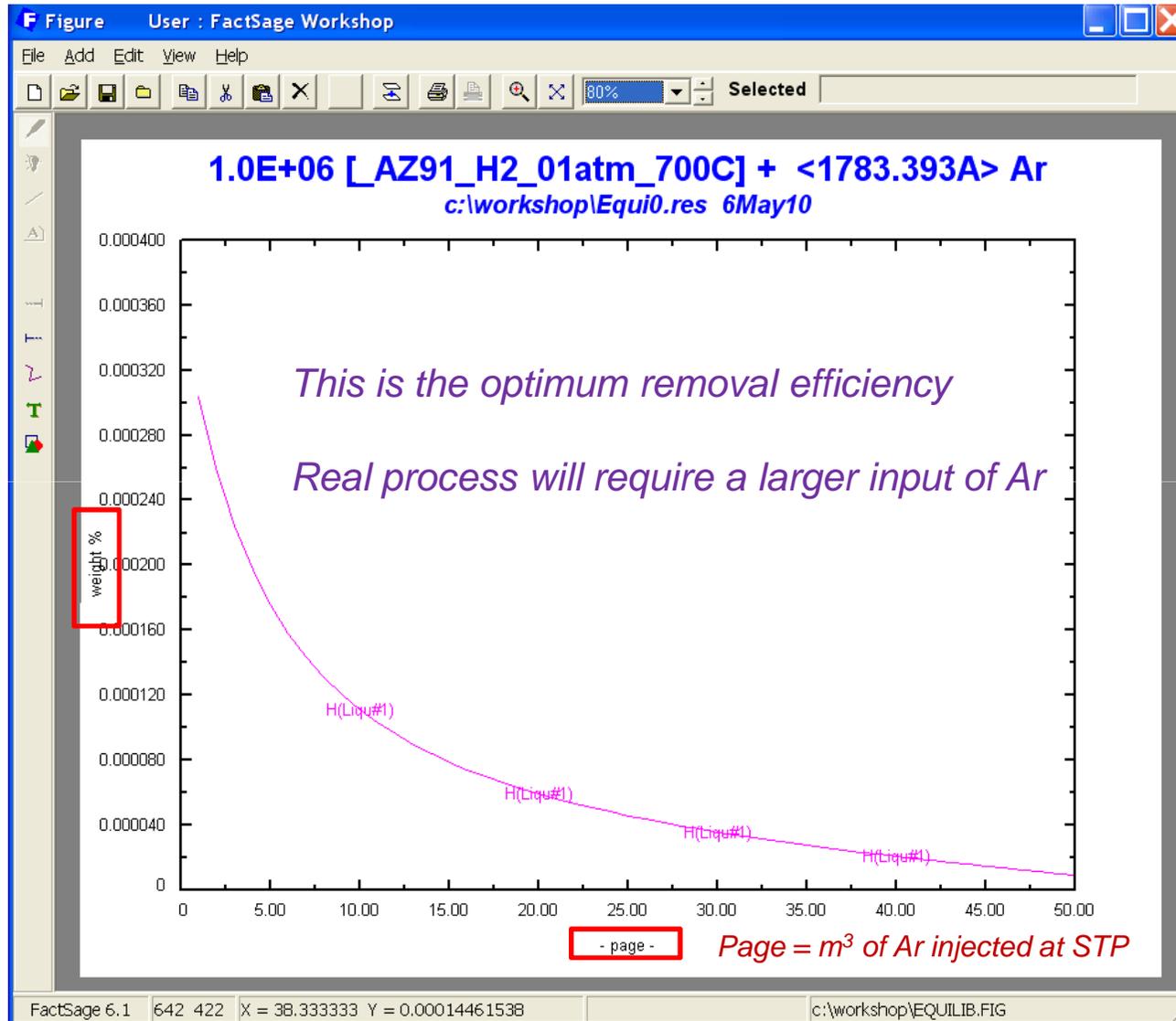
Graph
Labels
size: 9 no: 4
 chemical
 integer #
 none

Display
 color
 reactants
 file name
 full screen
 Viewer
 Figure
Plot >>

FactSage 6.1 c:\workshop\Equi0.res 6May10 50 sets

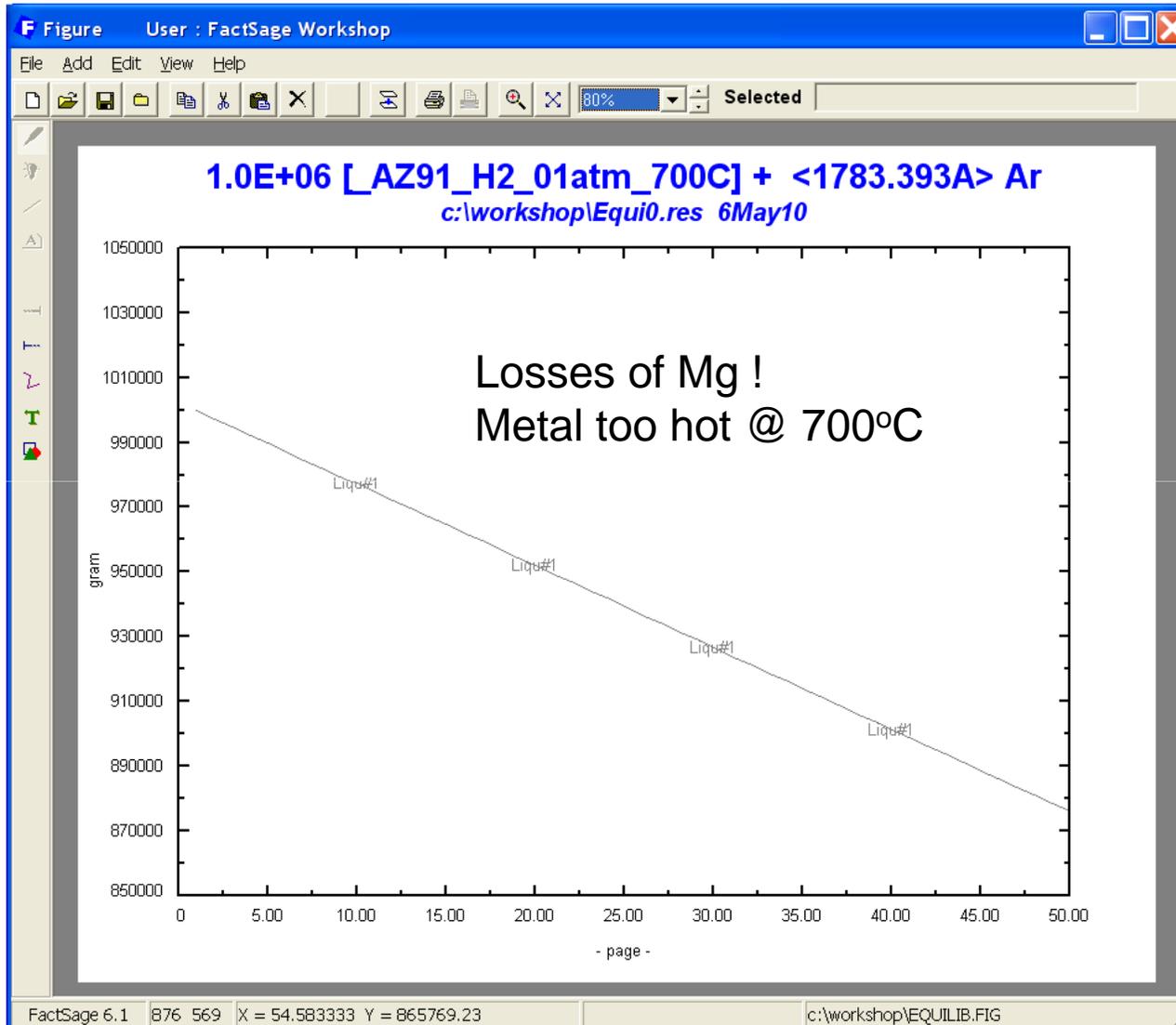
Metal Treatment (Al & Mg)

- **Example #1b: Degassing AZ91 with Ar**



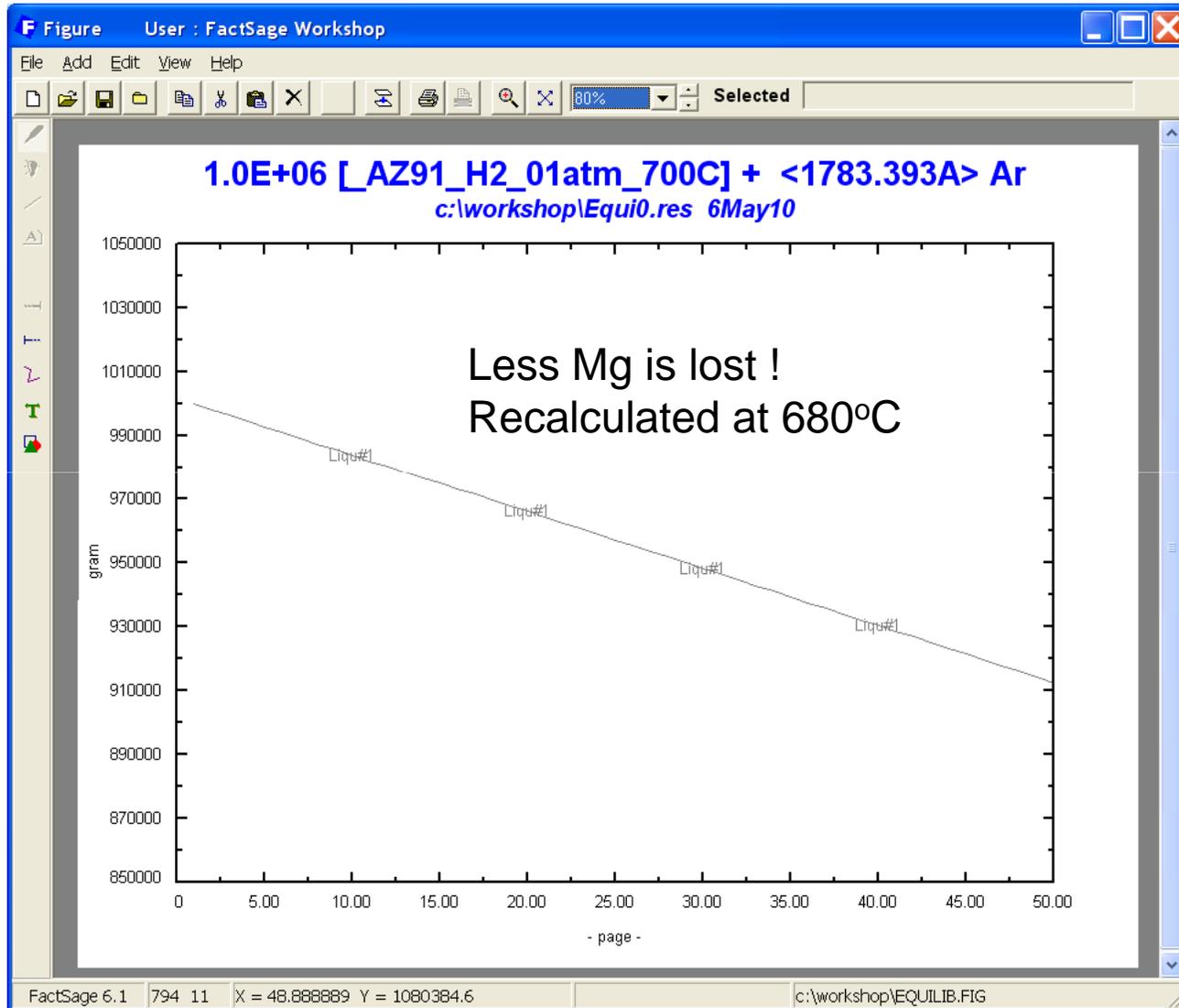
Metal Treatment (Al & Mg)

- **Example #1b: Degassing AZ91 with Ar**



Metal Treatment (Al & Mg)

- **Example #1b: Degassing AZ91 with Ar**



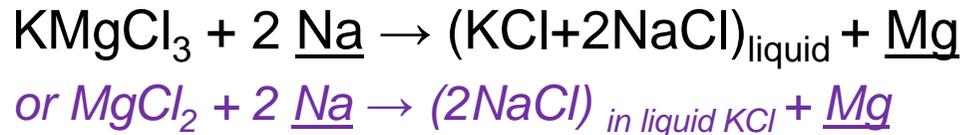
- Examples

- 1) Comparison of 2 salt fluxes for alkali removal

- a) Al-5%Mg with (40 ppm Na and 20 ppm Ca) treated with 2 fluxes based on NaCl-KCl-MnCl₂

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

KMgCl₃ is used to remove Na & Ca from **liquid Al alloys**



For kinetic purposes, the removal efficiency is better if the flux is melting faster (i.e. lower T_{eutectic} , lower T_{liquidus} , lower ΔH_{fus})

Can we **replace KMgCl₃ by a NaCl-KCl-MnCl₂ mixture** that will potentially melt faster but will keep its ability to remove Na and Ca ?
What would be a good composition ?



- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Strategy:

- 1) **Liquidus projection → NaCl-KCl-MnCl₂ :**
GOAL : identify 1 or 2 low melting compositions
PHASE DIAGRAM

- 2) **H_T-H_{25C} for the mixture(s) → enthalpy requirement for melting**
GOAL : identify the lowest melting enthalpy
EQUILIB

- 3) **Same for KMgCl_{3(s)}**
GOAL : compare the mixture(s) with the reference flux
EQUILIB

- 4) **Alkali removal from a Al-5%Mg alloy with the fluxes**
GOAL: check if the capability to remove Na and Ca is similar

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Strategy :

1) **Liquidus projection** → **NaCl-KCl-MnCl₂** :

GOAL : identify 1 or 2 low melting compositions

PHASE DIAGRAM

2) $H_T - H_{25C}$ for the mixture(s) → enthalpy requirement for melting

GOAL : identify the lowest melting enthalpy

EQUILIB

3) Same for **KMgCl_{3(s)}**

GOAL : compare the mixture(s) with the reference flux

EQUILIB

4) Calculate the alkali removal from a **Al-5%Mg** alloy with the fluxes

GOAL: check if the capability to remove Na and Ca is similar

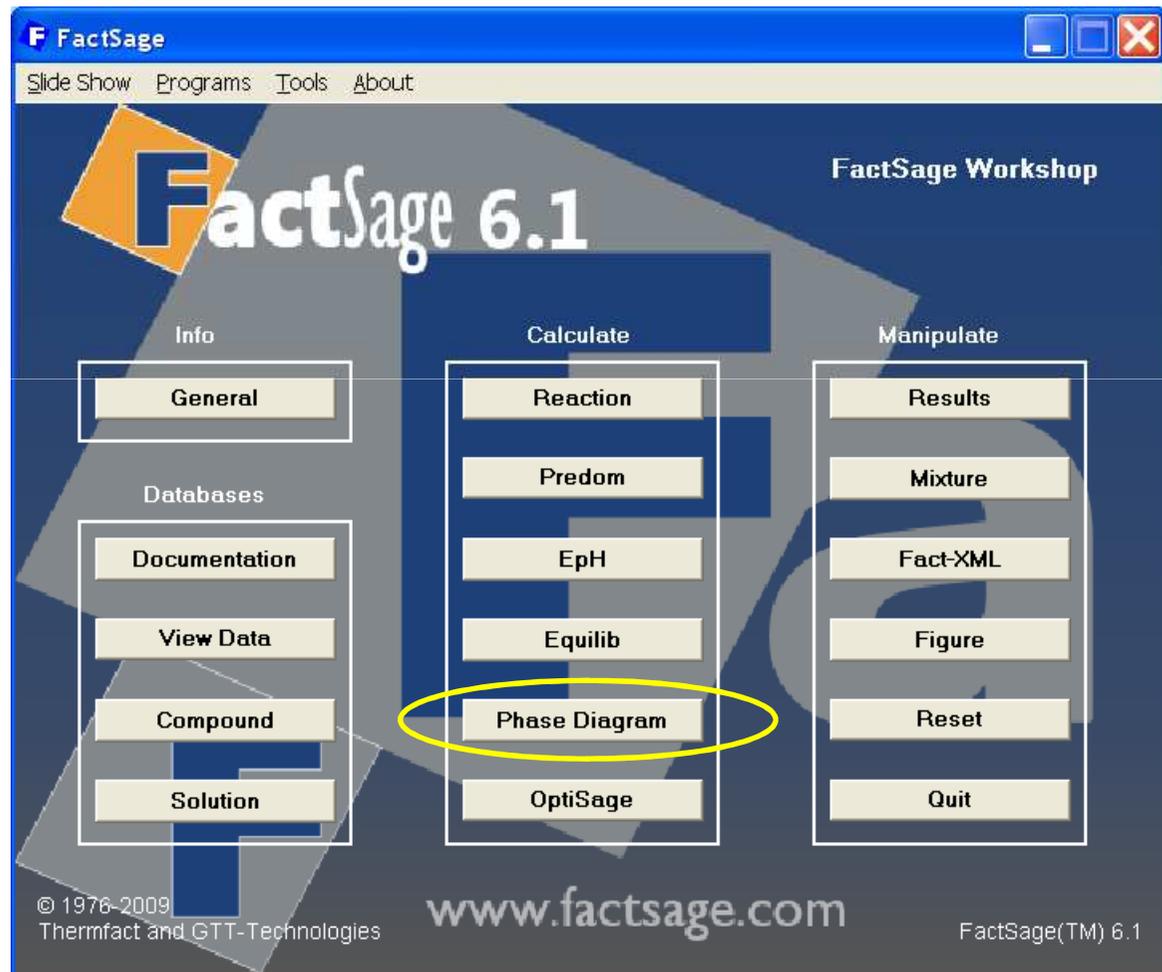
Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Liquidus Projection

- NaCl
- KCl
- MnCl₂

FTsalt



Metal Treatment (Al & Mg)

- Example #2: Comparison of 2 salt fluxes for alkali removal

Data Search

Databases - 1/24 compound databases, 1/22 solution databases

<input type="checkbox"/> ELEM	<input type="checkbox"/> FScopp	<input type="checkbox"/> BINS	<input type="checkbox"/> EXAM
<input type="checkbox"/> FACT	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS	<input type="checkbox"/> SGSL
<input type="checkbox"/> Fact53	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE	<input type="checkbox"/> SGTE*
<input type="checkbox"/> FToxid	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	
<input checked="" type="checkbox"/> FTsalt	<input type="checkbox"/> FSupsi	<input type="checkbox"/> SGsold	
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGnucl	
<input type="checkbox"/> FThall			
<input type="checkbox"/> FThelg	Other	<input type="checkbox"/> TDnucl	
<input type="checkbox"/> FTpulp	<input type="checkbox"/> OLIP	<input type="checkbox"/> OLIC	
<input type="checkbox"/> FTlite	<input type="checkbox"/> OLIG	<input type="checkbox"/> OLIL	

Information

Compound: c:\workshop\FACTDATA\FTsalt53base.cdb
- FTsalt - FACT salt compounds (2009)

Solution: c:\workshop\FACTDATA\FTsalt53soln.sda
- FTsalt - FACT salt solutions (2009)

Options

Include

- gaseous ions (in aemas)
- aqueous species
- limited data compounds (25C)

Limits

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

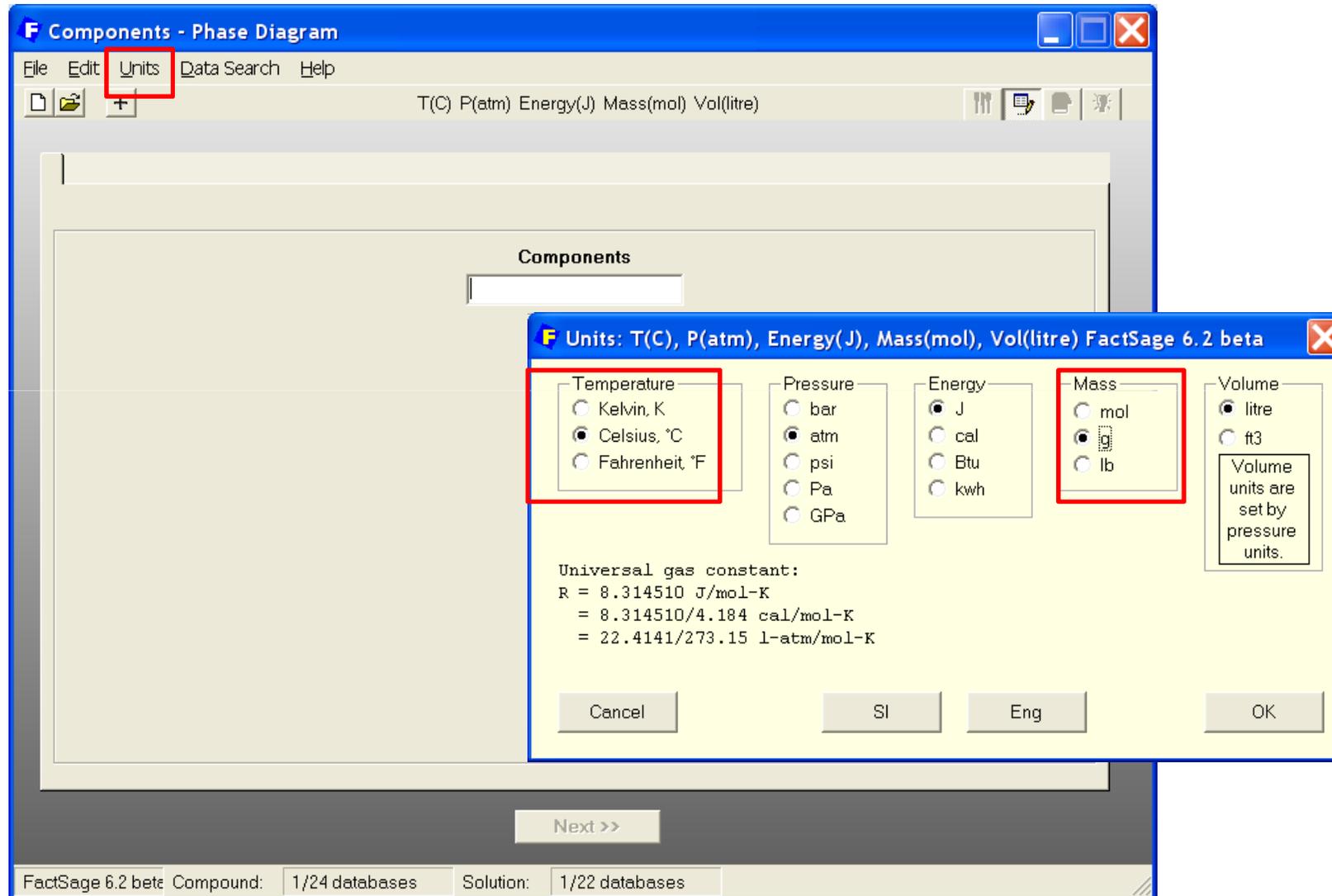
Buttons: Cancel, Summary..., OK

Next >>

FactSage 6.2 beta Compound: 1/24 databases Solution: 1/22 databases

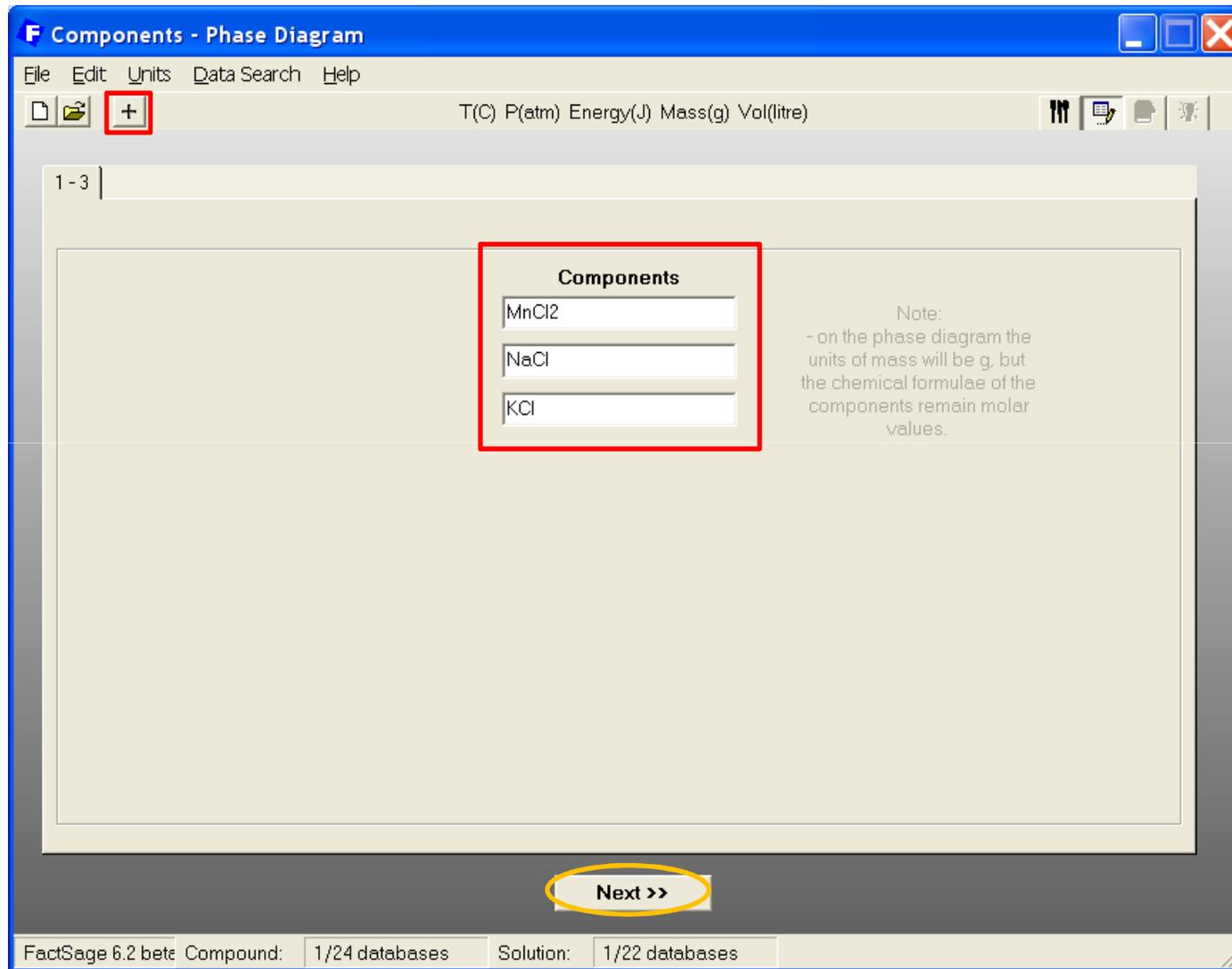
Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

F Menu - Phase Diagram: last system

File Units Parameters Variables Help

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

Components (3)

(gram) MnCl2 + NaCl + KCl

Products

Compound species
gas ideal real 0
aqueous 0
pure liquids 0
* + pure solids 7
 suppress duplicates apply
*- custom selection
species: 7

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

Solution species

		Base-Phase	Full Name
*	+	FTsalt-ACL_B	BAIkCl-ss_rocksalt
		FTsalt-AMX4A	AAIk2MX4
		FTsalt-PRVKA	AAMX3-Perovskite
	+	FTsalt-SALTB	BSalt-liquid

Legend
| - immiscible 3
+ - selected 1

Show all selected
species: 17
solutions: 7 **Select**

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

Pseudonyms
apply **List ...**

include molar volumes
Total Species (max 1500) 24
Total Solutions (max 40) 7
Default

Variables

T(C)	NaCl/(MnCl2+Na)	MnCl2/(MnCl2+N)		
Projection	0 1	0 1		

A = NaCl, B = KCl, C = MnCl2

Phase Diagram

A
B C
Projection

univariants
 isotherms
Calculate >>

FactSage 6.2 beta

Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Menu - Phase Diagram: last system

File Units Parameters Variables Help

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

Components (3)

(gram) MnCl2 + NaCl + KCl

Products

Solution FTsalt-SALTB

- clear
- ✓ - all species
- * - custom select species
- m - merge dilute solution from ▶
- ✓ + - single phase
- I - possible 2-phase immiscibility
- J - possible 3-phase immiscibility
- ✓ - standard stable phase
- I - dormant (metastable) phase
- ✓ **O - Only plot this single phase**

Help ...

Solution species

*	+	Base-Phase	Full Name
	I	FTsalt-ACL_B	BAIkCl-ss_rocksalt
	I	FTsalt-AMX4A	AAIk2MX4
	I	FTsalt-PRVKA	AAMX3-Perovskite
	O	FTsalt-SALTB	BSalt-liquid

Legend
I - immiscible 3

✓ Show all selected

species: 17
solutions: 7 **Select**

Custom Solutions

- 0 fixed activities
- 0 ideal solutions
- 0 activity coefficients

Details ...

Pseudonyms

apply **List ...**

include molar volumes

Total Species (max 1500) 24
Total Solutions (max 40) 7

Default

Variables

T(C)	NaCl/(MnCl2+Na)	MnCl2/(MnCl2+N)		
Projection	0 1	0 1		

A = NaCl, B = KCl, C = MnCl2

Phase Diagram

A
B C
Projection

- univariants
- isotherms

Calculate >>

FactSage 6.2 beta

Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

F Menu - Phase Diagram: last system

File Units Parameters **Variables** Help

Components (3)

(gram)

Products

Compound species

gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	0
aqueous			0
pure liquids			0
pure solids	<input checked="" type="radio"/>		7

suppress duplicates apply

* - custom selection

species: 7

Target

- none -

Estimate T(K): 1000

Mass(g): 0

Variables

Variable	NaCl/(MnCl2+Na)	MnCl2/(MnCl2+N)
T(C)		
Projection	0 1	0 1

A = NaCl, B = KCl, C = MnCl2

FactSage 6.2 beta

F Variables: MnCl2-NaCl-KCl composition #1. vs composition #1.

Variables

Y compositions 2

X log10(a) 0

Y steps: 10

X steps: 10

Next >>

T and P

Temperature

T(C) P(atm) constant

projection

Max: - calculated

Min: - calculated

T(inc): 20

define min and max isotherms

isothermal sections every 20 C

Pressure

log P 1

Compositions (mass)

#1. 1 MnCl2 + 0 NaCl + 0 KCl = A-Corner

1 MnCl2 + 1 NaCl + 1 KCl = 1 (max)

0 (min)

#2. 0 MnCl2 + 1 NaCl + 0 KCl = C-Corner

1 MnCl2 + 1 NaCl + 1 KCl = 1 (max)

0 (min)

#3. 0 MnCl2 + 0 NaCl + 1 KCl = B-Corner

1 MnCl2 + 1 NaCl + 1 KCl = 1 (max)

0 (min)

Cancel OK

Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Parameters - Phase Diagram

Phase Diagram

Display

full screen: color: title: sub-title:

Labels & Lines

8 label size 5 - 20 bold italic underline label underline label

2 line width 1 - 20 (0.1 - 2.0 mms) line color line style

Show

status: tie-lines: warning: labels:

Compound Source

show (s) never always only multiple data chemical numerical

Default

Iso-T Section

Colors

color T scale phase

Labels

T value T units phase

Enthalpy line

color style

Polythermal Projection

list T(min) and T(max) list intersection phases list intersection compositions and temperatures label phase surfaces label intersection # or temperature # or temperature color label intersection points intersection point color

Dimensions

Description	Used	Max
Reactant components:	3	24
Species retrieved from databanks:	37	no limit
Magnetic species retrieved from databanks:	0	no limit
Species selected for products:	24	1500
Components (elements + electron phases):	4	48
Number of Gibbs energy/Cp equations for a constituent:		20
Total number of Gibbs energy/Cp equations:		4400

Target Limits

	min.	max.
T(K):	1	10000
P(bar):	1.0E-35	1.0E+08
V(l):	1.0E-08	1.0E+35
Alpha:	1.0e-5	1.0

Default

Default settings for new systems

Temperature Pressure Energy Mass suppress duplicates include molar weights

not set not set not set not set

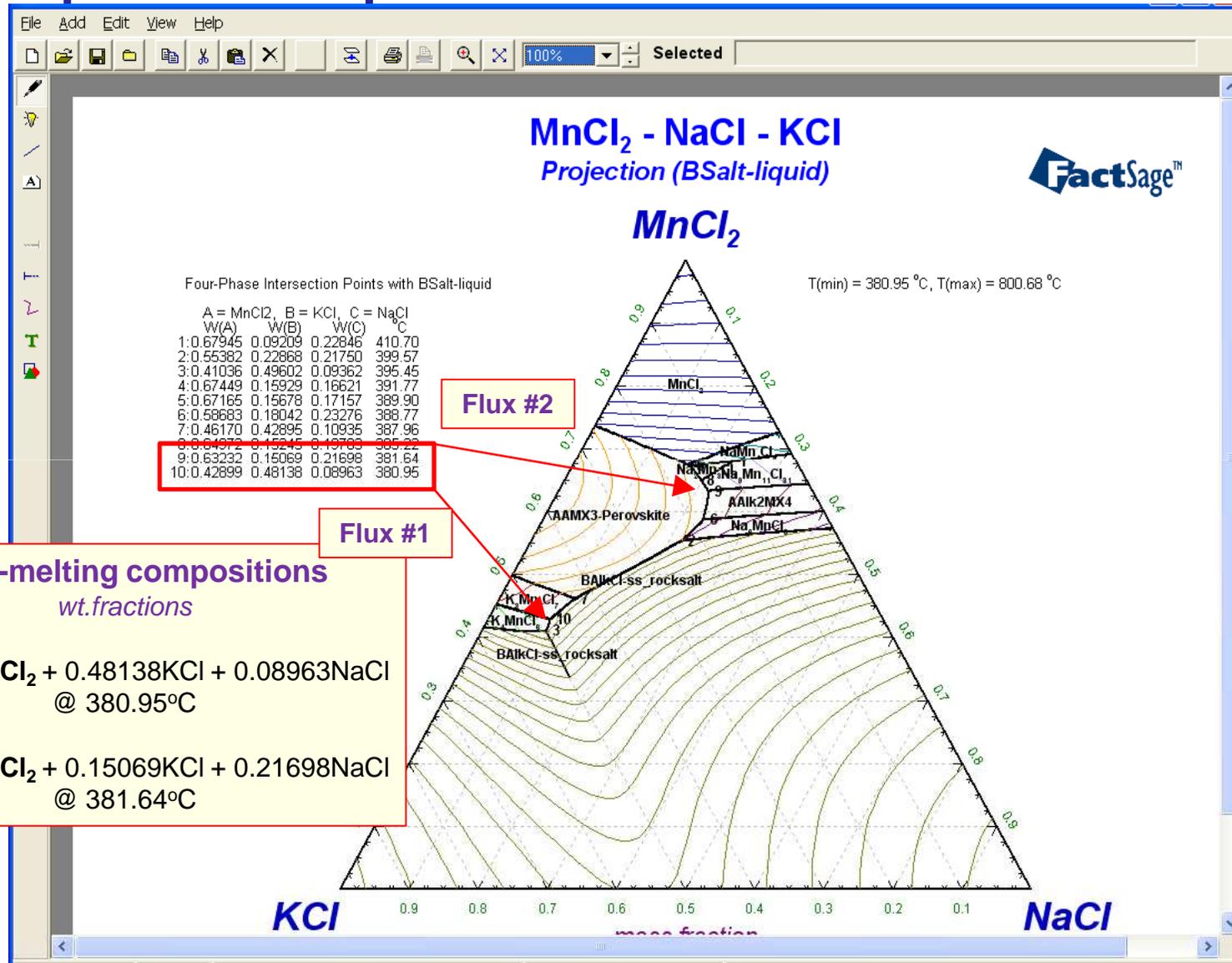
Stop Window

yes refresh: 2 sec

Help OK

Metal Treatment (Al & Mg)

• Example #2: Comparison of 2 salt fluxes for alkali removal



- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Strategy :

- 1) Liquidus projection \rightarrow NaCl-KCl-MnCl₂ :
GOAL : identify 1 or 2 low melting compositions
PHASE DIAGRAM
- 2) $H_T - H_{25C}$ for the mixture(s) \rightarrow enthalpy requirement for melting
GOAL : identify the lowest melting enthalpy
EQUILIB
- 3) Same for KMgCl_{3(s)}
GOAL : compare the mixture(s) with the reference flux
EQUILIB
- 4) Calculate the alkali removal from a Al-5%Mg alloy with the fluxes
GOAL: check if the capability to remove Na and Ca is similar

Metal Treatment (Al & Mg)

- Example #2: Comparison of 2 salt fluxes for alkali removal

F Reactants - Equilib

File Edit Table Units **Data Search** Help

Mass(g) S

F Data Search

Databases - 1/24 compound databases, 1/22 solution databases

<input type="checkbox"/> Fact	<input type="checkbox"/> FactSage™	<input type="checkbox"/> SGTE	<input type="checkbox"/> compounds only	<input type="checkbox"/> Miscellaneous
<input type="checkbox"/> ELEM	<input type="checkbox"/> FScopp	<input type="checkbox"/> BINS	<input type="checkbox"/> solutions only	<input type="checkbox"/> EXAM
<input type="checkbox"/> FACT	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS	<input type="checkbox"/> no data	<input type="checkbox"/> SGSL
<input type="checkbox"/> Fact53	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE		<input type="checkbox"/> SGTE*
<input type="checkbox"/> FToxid	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	Clear All	
<input checked="" type="checkbox"/> FTsalt	<input type="checkbox"/> FSupsi	<input type="checkbox"/> SGsold	Select All	
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGnucl	Add/Remove Data	
<input type="checkbox"/> FTHall	Other	<input type="checkbox"/> TDnucl	RefreshDatabases	
<input type="checkbox"/> FTHelg	<input type="checkbox"/> OLIP	<input type="checkbox"/> OLIC		
<input type="checkbox"/> FTpulp	<input type="checkbox"/> OLIG	<input type="checkbox"/> OLIL		
<input type="checkbox"/> FTlite				

Information -

Compound: c:\workshop\FACTDATA\FTsalt53base.cdb
- FTsalt - FACT salt compounds (2009)

Solution: c:\workshop\FACTDATA\FTsalt53soln.sda
- FTsalt - FACT salt solutions (2009)

Options

Default

Include

- gaseous ions (in aemas)
- aqueous species
- limited data compounds (25C)

Limits

Organic species CxHy... X(max) =

Minimum solution components: 1 2 cpts

Cancel Summary ... OK

Next >>

FactSage 6.2 beta Compound: 2/24 databases Solution: 1/22 databases

Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
0.42899	MnCl2	s			1	
0.48318	KCl	s			1	
0.08963	NaCl	s			1	

Next >>

FactSage 6.2 beta Compound: 1/24 databases Solution: 1/22 databases

2 low-melting compositions

wt.fractions

**0.42899 MnCl₂ + 0.48138KCl + 0.08963NaCl
@ 380.95°C**

**0.63232 MnCl₂ + 0.15069KCl + 0.21698NaCl
@ 381.64°C**

Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
<0.42899A>	MnCl2	s			1	
+ <0.48318A>	KCl	s			1	
+ <0.08963A>	NaCl	s			1	

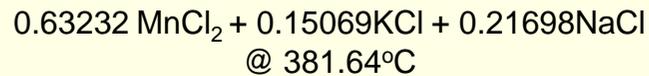
<A> is added

Initial Conditions

Next >>

FactSage 6.2 beta Compound: 1/24 databases Solution: 1/22 databases

2 low-melting compositions
wt.fractions



Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

F Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 6

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
<0.42899A>	MnCl ₂	s			1	
+ <0.48318A>	KCl	s			1	
+ <0.08963A>	NaCl	s			1	
+ <0.63232B>	MnCl ₂	s			1	
+ <0.15069B>	KCl	s			1	
+ <0.21698B>	NaCl	s			1	

** is added**

<A>=1 =0 1st flux (1 g)

<A>=0 =1 2nd flux (1 g)

Initial Conditions

Next >>

nd: 1/24 databases Solution: 1/22 databases

2 low-melting compositions

wt.fractions

0.42899 MnCl₂ + 0.48138KCl + 0.08963NaCl
@ 380.95°C

0.63232 MnCl₂ + 0.15069KCl + 0.21698NaCl
@ 381.64°C

Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 7

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
<0.42899A>	MnCl2	s			1	
+ <0.48318A>	KCl	s			1	
+ <0.08963A>	NaCl	s			1	
+ <0.63232B>	MnCl2	s			1	
+ <0.15069B>	KCl	s			1	
+ <0.21698B>	NaCl	s			1	
+ 0	KMgCl3					

Initial Conditions

Next >>

FactSage 6.2 beta Compound: 1/24 databases Solution: 1/22 databases

The reference flux (KMgCl_3) is also entered with 0 grams

This amount can be changed later on...

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Strategy :

2) $H_T - H_{25C}$ for the mixture(s) → enthalpy requirement for melting

GOAL : identify the lowest melting enthalpy

EQUILIB

In order to calculate $H_T - H_{25C}$ (a ΔH in fact), the final equilibrium state contributes to H_T , but the initial state (reactants) contribute to H_{25C} .

The “*Initial conditions*” option must now be activated

Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 7

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
<0.42899A>	MnCl2	solid scacchite	25	1.0	1	
+ <0.48318A>	KCl	solid sylvite (nacl_roc	25	1.0	1	
+ <0.08963A>	NaCl	solid halite (rock salt_	25	1.0	1	
+ <0.63232B>	MnCl2	solid scacchite	25	1.0	1	
+ <0.15069B>	KCl	solid sylvite (nacl_roc	25	1.0	1	
+ <0.21698B>	NaCl	solid halite (rock salt_	25	1.0	1	
+ 0	KMgCl3	solid perovskite	25	1.0	1	

** P(total) is the hydrostatic pressure above the phase.
For a gaseous stream this is the sum of the partial pressures of the species in that stream.

Initial Conditions

Next >>

FactSage 6.2 beta Compound: 1/24 databases Solution: 1/22 databases

Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Reactants (7)

(gram) <0.42899A> MnCl2 + <0.48318A> KCl + <0.08963A> NaCl + <0.63232B> MnCl2 + <0.15069B>

(25C,s,#1) (25C,s,#1) (25C,s,#1) (25C,s,#1) (25C,s,#1)

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 17**

suppress duplicates

species: 17

Solution species

*	+	Base-Phase	Full Name
	J	FTsalt-ACL_B	BAIkCl-ss_rocksalt
	J	FTsalt-AMX4A	AAIk2MX4
	J	FTsalt-PRVKA	AAMX3-Perovskite
	I	FTsalt-R-3m	MCl2_SOLID
	I	FTsalt-SALTB	BSalt-liquid

Legend

- I - immiscible 2
- J - 3-immiscible 3

Show all selected

species: 48
solutions: 13

Final Conditions

<A>		T(C)	P(atm)	Delta.H(J)
0.5	1	1000	1	

10 steps Table

Equilibrium

- normal normal + transitions
- transitions only open
- predominant

FactSage 6.2 beta

Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Menu - Equilib: last system

File Units Parameters Help

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

Reactants (7)

(gram) <0.42899A> MnCl2 + <0.48318A> KCl + <0.08963A> NaCl + <0.63232B> MnCl2 + <0.15069B>

(25C,s,#1) (25C,s,#1) (25C,s,#1) (25C,s,#1) (25C,s,#

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

pure solids 17

suppress duplicates apply

species: 17

Solution species

*	+	Base-Phase	Full Name
	J	FTsalt-ACL_B	BAIkCl-ss_rocksalt
	J	FTsalt-AMX4A	AAIk2MX4
	J	FTsalt-PRVKA	AAMX3-Perovskite
	I	FTsalt-R-3m	MCl2_SOLID
	I	FTsalt-SALTB	BSalt-liquid

Custom Solutions

0 fixed activities

0 ideal solutions

0 activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 1500) 65

Total Solutions (max 40) 13

Default

Transitions - temperature

Number of transitions: All

Legend

I - immiscible 2

J - 3-immiscible 3

Show all selected

species: 48

solutions: 13

Select

Final Conditions

<A>		T(C)	P(atm)	Delta H(J)
1	0	25750.5	1	

146+ calculations

Equilibrium

normal

normal + transitions

transitions only

open

predominant

Calculate >>

<A>=1 =0 1st flux

FactSage 6.2 beta

Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

F Results - Equilib 60 C (page 8/152) FactSage 6.2 beta

Output Edit Show Pages

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

135 C | 140 C | 145 C |
80 C | 85 C | 90 C | 95 C | 100 C | 105 C | 110 C | 115 C | 120 C | 125 C | 130 C |
25 C | 30 C | 35 C | 40 C | 45 C | 50 C | 55 C | **- 60 C -** | 65 C | 70 C | 75 C |

(gram) <0.42899A> MnCl₂ + <0.48318A> KCl + <0.08963A> NaCl + <0.63232 (0)> ...
(25,1,s,#1) (25,1,s,#1) (25,1,s,#1) (25,1,s,#1)
(gram) <0.15069 (0)> KCl + <0.21698 (0)> NaCl + 0 KMgCl₃ =
(25,1,s,#1) (25,1,s,#1) (25,1,s,#1)

0.47798 gram AAMX3-Perovskite#1
(0.47798 gram, 2.3852E-03 mol)
(60.00 C, 1 atm, a=1.0000)
(100.00 wt.% KMnCl₃
+ 1.0016E-16 wt.% NaMnCl₃)

Mole fraction of sublattice constituents:

Na	1.0892E-18	Stoichiometry = 1.0000
K	1.0000	

Mn	1.0000	Stoichiometry = 1.0000
----	--------	------------------------

Cl	1.0000	Stoichiometry = 3.0000
----	--------	------------------------

System component	Mole fraction	Mass fraction
Mn	0.20000	0.27415
K	0.20000	0.19511
Cl	0.60000	0.53074
Na	2.1784E-19	1.2496E-19

+ 8.9713E-02 gram BAlkCl-ss_rocksalt#1
(8.9713E-02 gram, 1.5348E-03 mol)
(60.00 C, 1 atm, a=1.0000)
(00 007 wt.% NaCl)

Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

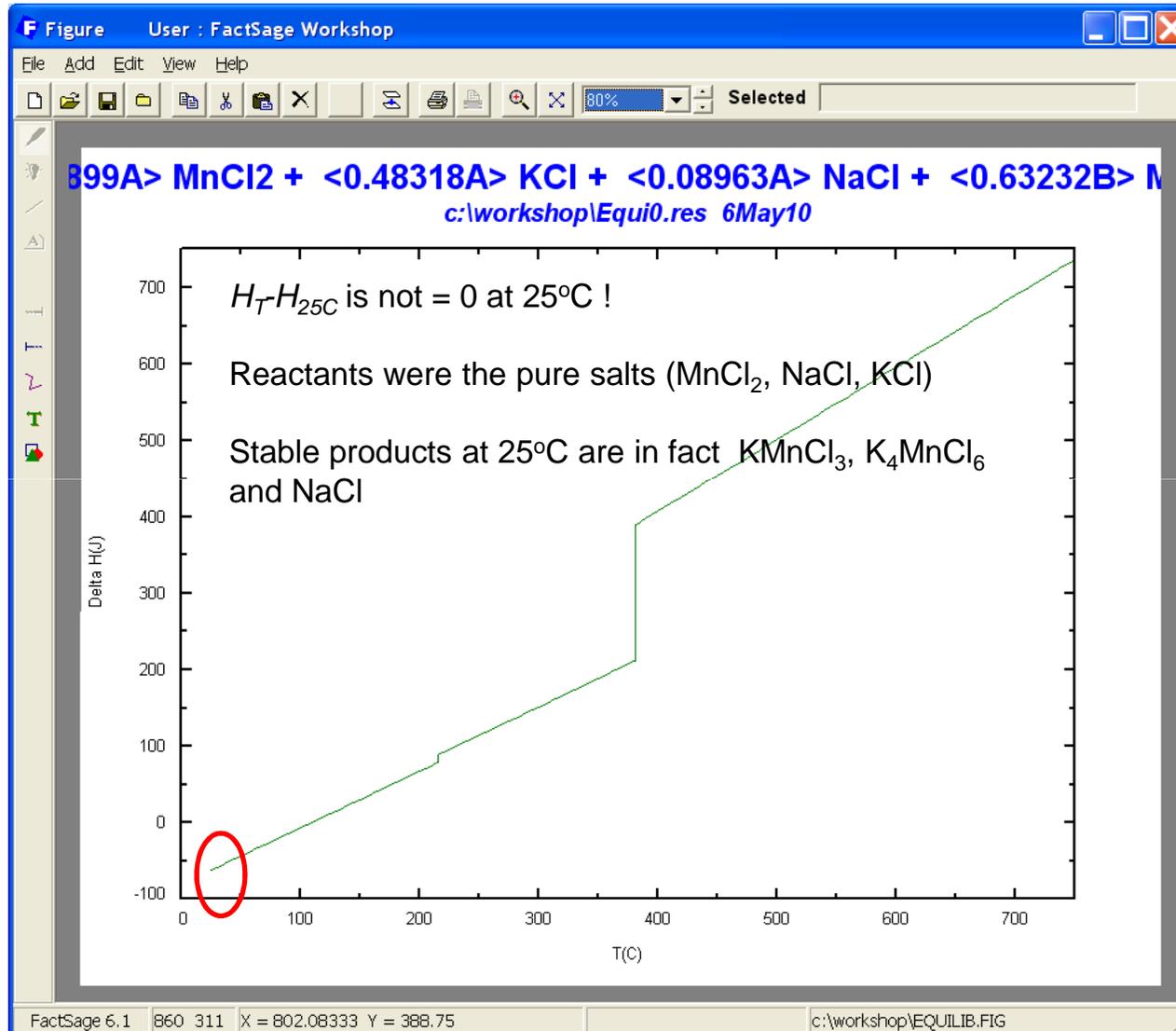
The screenshot shows the FactSage 6.2 beta interface. The main window displays the 'Results - Equilib 60 C (page 8/152)' with a table of thermodynamic data. A 'Plot: Delta H(J) vs T(C)' dialog box is open, allowing the user to configure the plot. The 'Y-axis' is set to 'Delta H(J)' and the 'X-axis' is set to 'T(C)'. The 'Y-axis' settings are: maximum 750, minimum -100, tick every 50. The 'X-axis' settings are: maximum 750, minimum 0, tick every 50. The 'Plot' button is highlighted.

Species	Activity	Mole	Weight
MnCl2	0	0.42899A	1.4822E-02
KCl	1	0.48318A	1.4822E-02
NaCl	1	0.08963A	1.4822E-02

System component	Mole fraction	Mass
Mn	0.20000	0.20000
K	0.20000	0.20000
Cl	0.60000	0.60000
Na	2.1784E-19	1.1784E-19

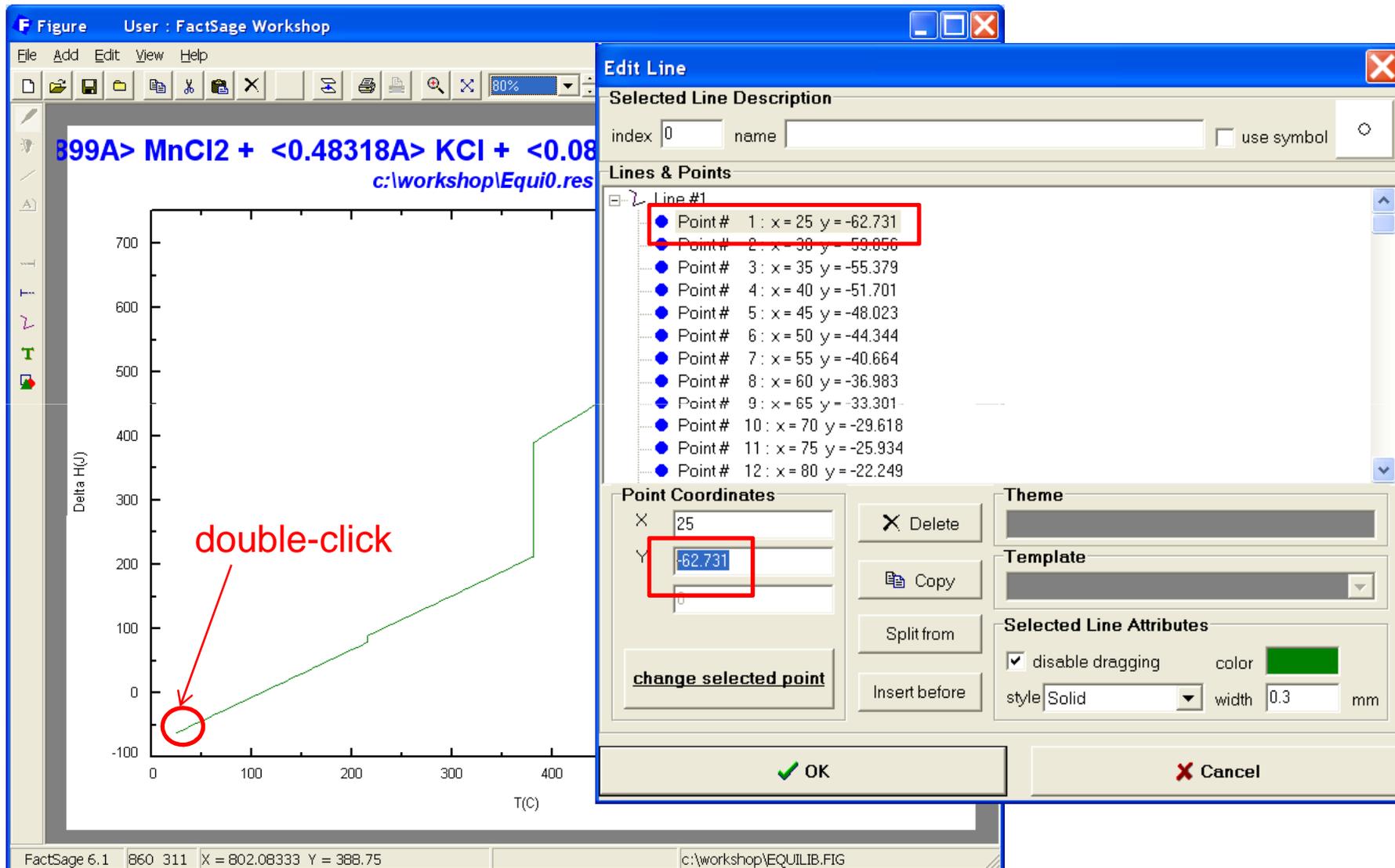
Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

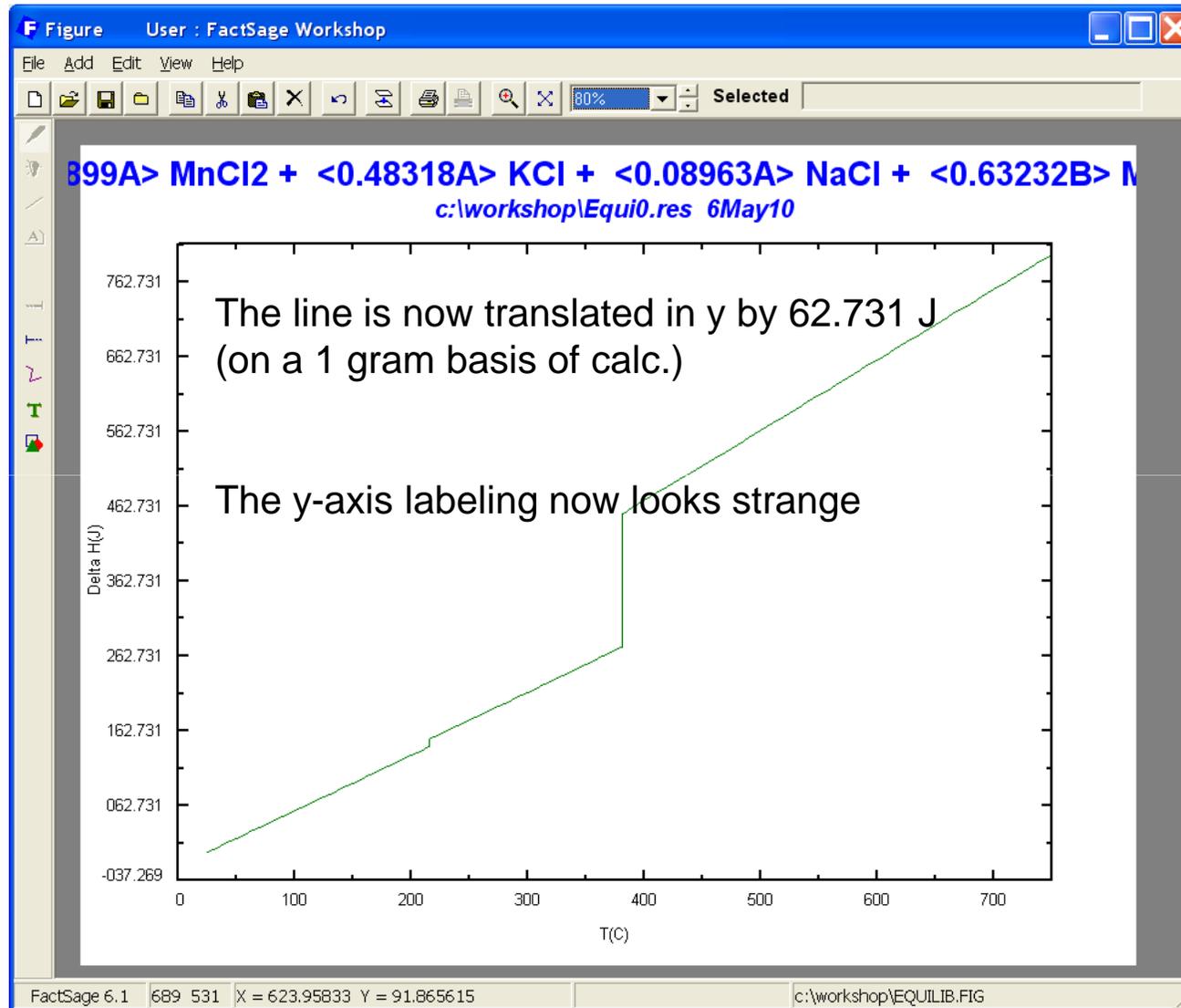
The screenshot shows the FactSage Workshop interface with the 'Change Scale' dialog box open. The dialog box is titled 'Change Scale' and contains the following sections:

- Axis operations are performed first (X then Y) in the order set by the user**
 - X-Axis Operations:** Order 1, 2, 3; scale type X; multiplication factor 1; translation (dX) 0.
 - Y-Axis Operations:** Order 1, 2, 3; scale type Y; multiplication factor 1; translation (dY) 62.731.
- X/Y operations are performed after Axis operations**
 - none
 - flip (1/Y)
 - swap axis
 - flip (1/X)
 - rotate around (X=Y)
- Gibbs Triangle Operations**
 - No Swap
 - A-B Swap
 - A-C Swap
 - B-C Swap
 - A-Axis multiplier: 1.0
 - B-Axis multiplier: 1.0
 - C-Axis multiplier: 1.0

The 'OK' button is highlighted with a green checkmark, and the 'Cancel' button is highlighted with a red X. The background plot shows Delta H(J) on the y-axis (0 to 400) and composition on the x-axis (18A > KCI, c:\workshop).

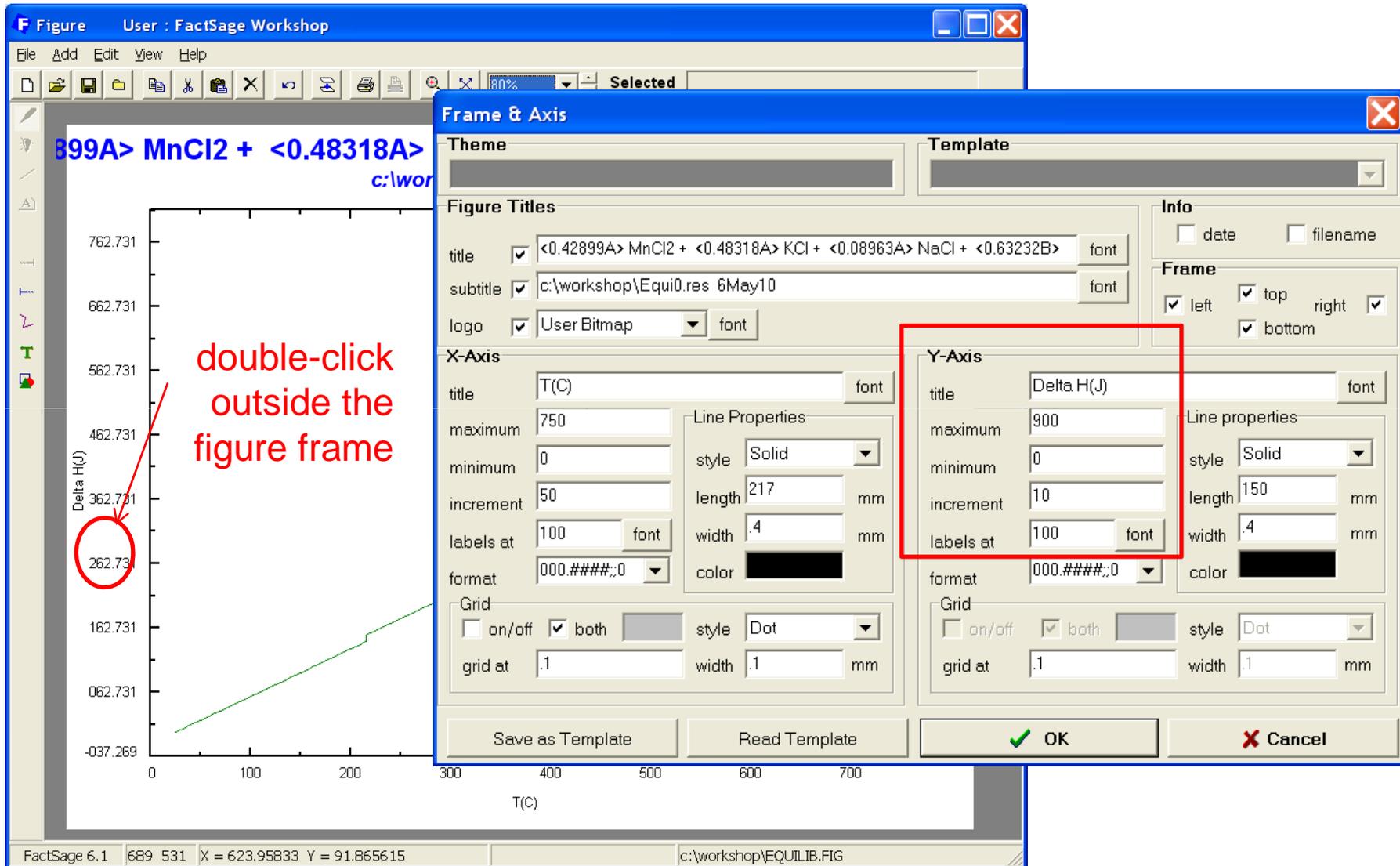
Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



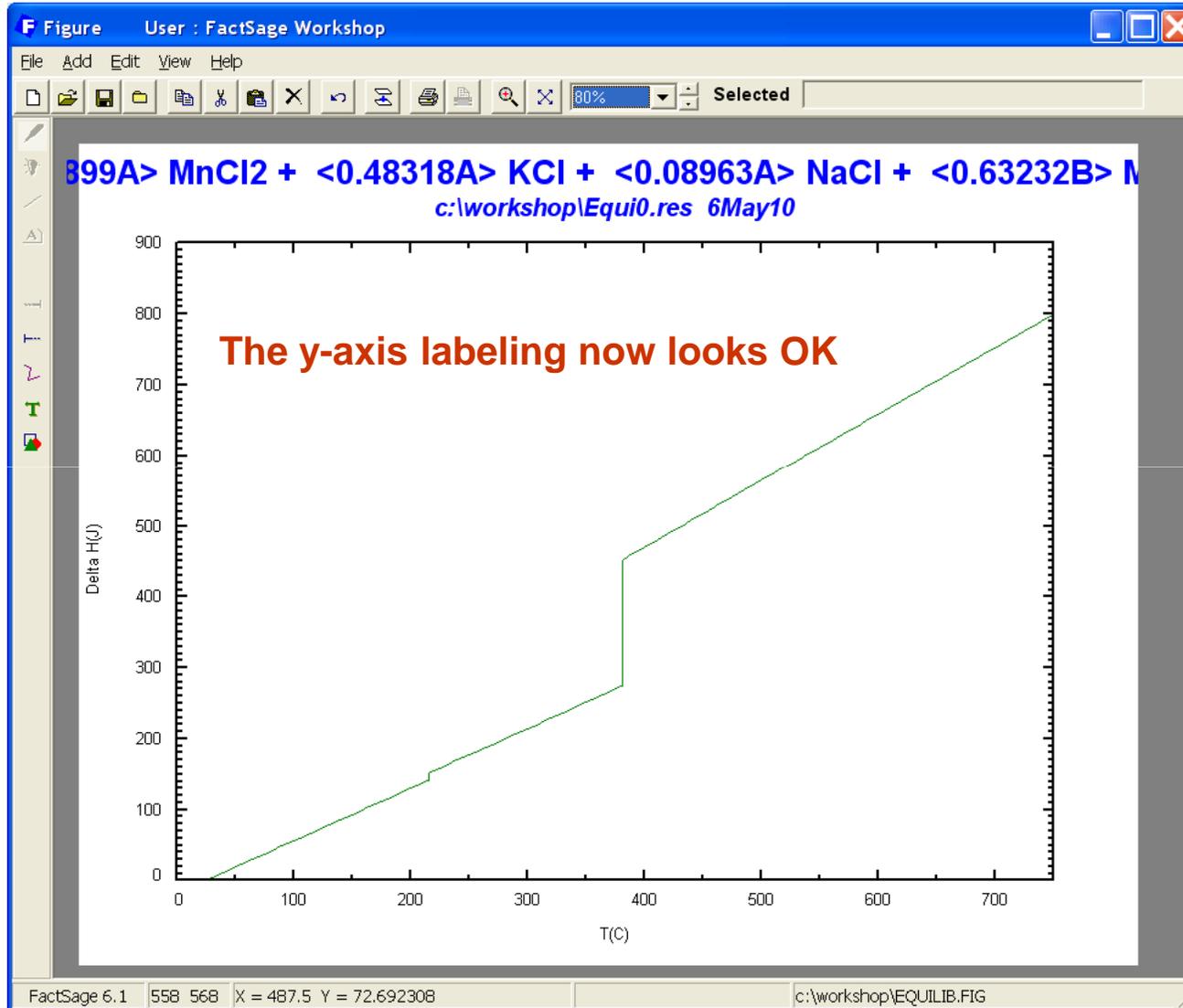
Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



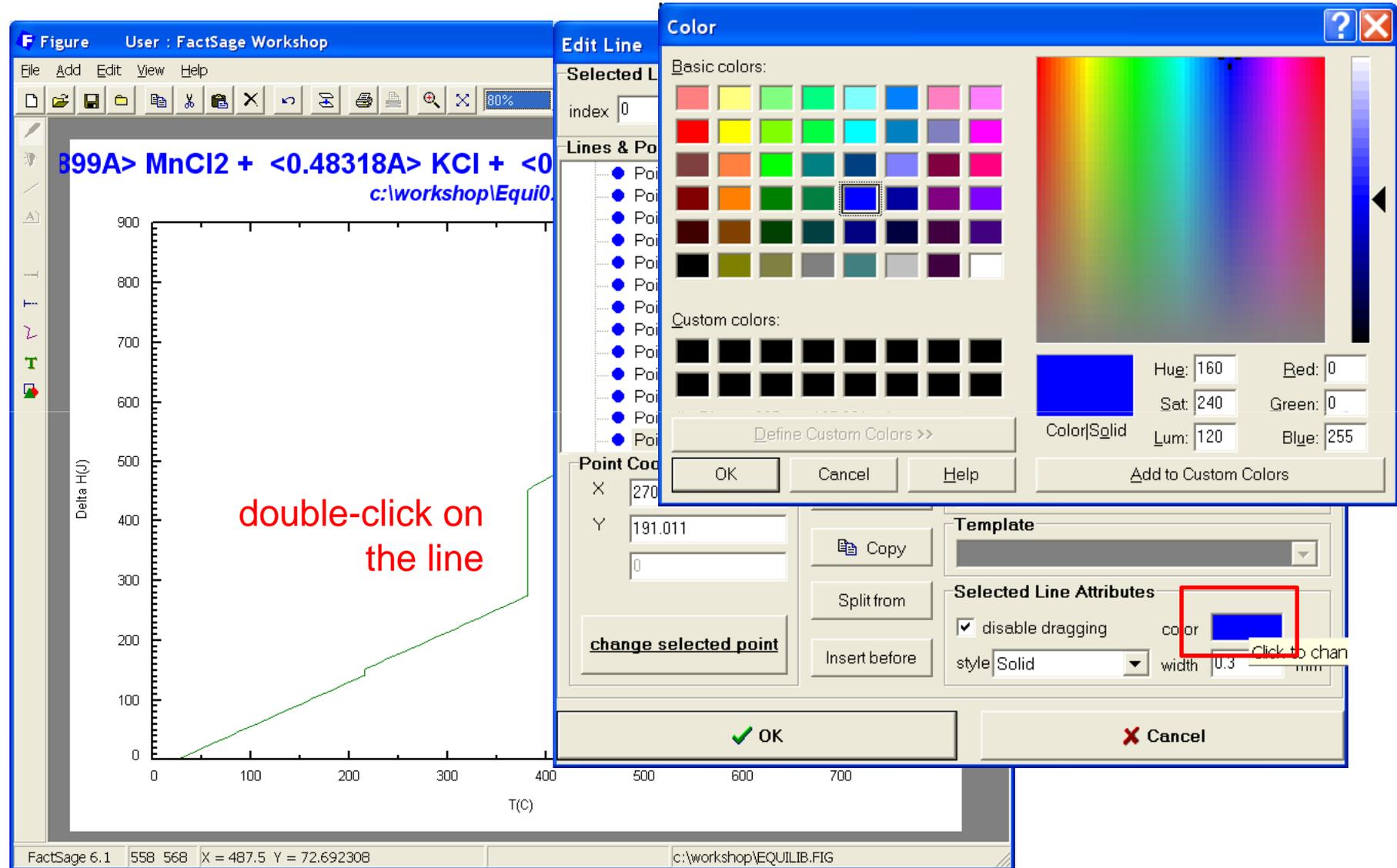
Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

The screenshot shows the FactSage Workshop interface. The 'File' menu is open, and 'Save as...' is selected. The 'Save File' dialog box is displayed, showing the file name 'Flux1.FIG' and 'Save as type' 'FACT figures (*.fig)'. A red box highlights the file name field. A blue arrow points from the text 'Save the file to later compare with flux #2' to the file name field.

Save the file to later compare with flux #2

Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Menu - Equilib: last system

File Units Parameters Help

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

Reactants (7)

(gram) <0.42899A> MnCl2 + <0.48318A> KCl + <0.08963A> NaCl + <0.63232B> MnCl2 + <0.15069B>

(25C,s,#1) (25C,s,#1) (25C,s,#1) (25C,s,#1) (25C,s,#1)

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

pure solids 17

suppress duplicates apply

species: 17

Solution species

*	+	Base-Phase	Full Name
	J	FTsalt-ACL_B	BAIKCl-ss_rocksalt
	J	FTsalt-AMX4A	AAlk2MX4
	J	FTsalt-PRVKA	AAMX3-Perovskite
	I	FTsalt-R-3m	MCl2_SOLID
	I	FTsalt-SALTB	BSalt-liquid

Legend

I - immiscible 2

J - 3-immiscible 3

Show all selected

species: 48

solutions: 13

Custom Solutions

0 fixed activities

0 ideal solutions

0 activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 1500) 65

Total Solutions (max 40) 13

Default

Final Conditions

<A>		T(C)	P(atm)	Delta H(J)
0	1	25 750 5	1	

Equilibrium

normal normal + transitions

transitions only open

predominant

Calculate >>

146+ calculations

FactSage 6.2 beta

<A>=0 =1 2nd flux

Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

F Results - Equilib Abort (page 1/152) FactSage 6.2 beta

Output Edit Show Pages

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

130 C | 135 C | 140 C |
75 C | 80 C | 85 C | 90 C | 95 C | 100 C | 105 C | 110 C | 115 C | 120 C | 125 C |
Abort | 25 C | 30 C | 35 C | 40 C | 45 C | 50 C | 55 C | 60 C | 65 C | 70 C |

(gram) <0.42899A> MnCl2 + <0.48318A> KCl + <0.08963A> NaCl + <0.63232 (1)> ...
(25,1,s,#1) (25,1,s,#1) (25,1,s,#1) (25,1,s,#1)
(gram) <0.15069 (1)> KCl + <0.21698 (1)> NaCl + 0 KMgCl3 =
(25,1,s,#1) (25,1,s,#1) (25,1,s,#1)

P = 1.00000E+00 atm

Target calculation aborted, no
275.00 to 280.00 C

~~~~~

P = 1.00000E+00 atm

STREAM CONSTITUENTS  
MnCl2\_scacchite(s) AMOU  
KCl\_sylvite\_(nacl\_roc(s) AMOU  
NaCl\_halite\_(rock\_sal(s) AMOU

STREAM CONSTITUENTS TEMPERATURE/C PRESSURE/atm STREAM  
MnCl2\_scacchite(s) 25.00 1.0000E+00 1  
KCl\_sylvite\_(nacl\_roc(s) 25.00 1.0000E+00 1  
NaCl\_halite\_(rock\_sal(s) 25.00 1.0000E+00 1  
MnCl2\_scacchite(s) 25.00 1.0000E+00 1  
KCl\_sylvite\_(nacl\_roc(s) 25.00 1.0000E+00 1  
NaCl\_halite\_(rock\_sal(s) 25.00 1.0000E+00 1  
KMgCl3\_perovskite(s) 25.00 1.0000E+00 1

One calculation aborted when calculating a transition. This sometimes happens.

The TAB will bear the name "Abort"

In order to obtain a nice  $H_T-H_{25C}$  curve, that abort TAB must be deleted

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

The screenshot shows the FactSage 6.2 beta interface. The title bar reads "F Results - Equilib\_Abort (page 1/152) FactSage 6.2 beta". The "Output" menu is open, and the "Show Pages" option is selected. A sub-menu is displayed with the following options: "Go to", "<< Previous Pages", "Next Pages >>", "Go to page ...", "Delete page 'Abort' ...", "Delete all 'Abort' pages ...", and "Swap pages ...". The "Delete all 'Abort' pages ..." option is highlighted with a blue selection bar. The main output window displays the following text:

```
(gram) <0 (25,1,s,#1) > KCl + <0.08963A> NaCl + <0.63232 (1)> ...
(gram) <0 (25,1,s,#1) > NaCl + 0 KMgCl3 =
(25,1,s,#1) (25,1,s,#1) (25,1,s,#1)

P = 1.00000E+00 atm

Target calculation aborted, no solution found within the interval
275.00 to 280.00 c

~~~~~

P = 1.00000E+00 atm

STREAM CONSTITUENTS
MnCl2_scacchite(s) AMOUNT/mol = 5.0247E-03
KCl_sylvite_(nacl_roc(s) AMOUNT/mol = 2.0213E-03
NaCl_halite_(rock_sal(s) AMOUNT/mol = 3.7127E-03

STREAM CONSTITUENTS TEMPERATURE/C PRESSURE/atm STREAM
MnCl2_scacchite(s) 25.00 1.0000E+00 1
KCl_sylvite_(nacl_roc(s) 25.00 1.0000E+00 1
NaCl_halite_(rock_sal(s) 25.00 1.0000E+00 1
MnCl2_scacchite(s) 25.00 1.0000E+00 1
KCl_sylvite_(nacl_roc(s) 25.00 1.0000E+00 1
NaCl_halite_(rock_sal(s) 25.00 1.0000E+00 1
KMgCl3_naravchite(s) 25.00 1.0000E+00 1
```

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

The screenshot shows the FactSage 6.2 beta interface. The 'Plot' menu is open, with 'Repeat Plot - Delta H(J) vs T(C) ...' selected. The main window displays the following data:

```
MnCl2 + <0.48318A> KCl + <0.08963A> NaCl + <0.63232 (1)> ...
1,s,#1) (25,1,s,#1) (25,1,s,#1)
) > KCl + <0.21698 (1)> NaCl + 0 KMgCl3 =
1,s,#1) (25,1,s,#1)

0.18888 gram AAMX3-Perovskite#1
(0.40506 gram, 2.0213E-03 mol)
(25.00 C, 1 atm, a=1.0000)
(100.00 wt.% KMnCl3
+ 1.6485E-16 wt.% NaMnCl3)

Mole fraction of sublattice constituents:
Na 1.7926E-18 Stoichiometry = 1.0000
K 1.0000

Mn 1.0000 Stoichiometry = 1.0000

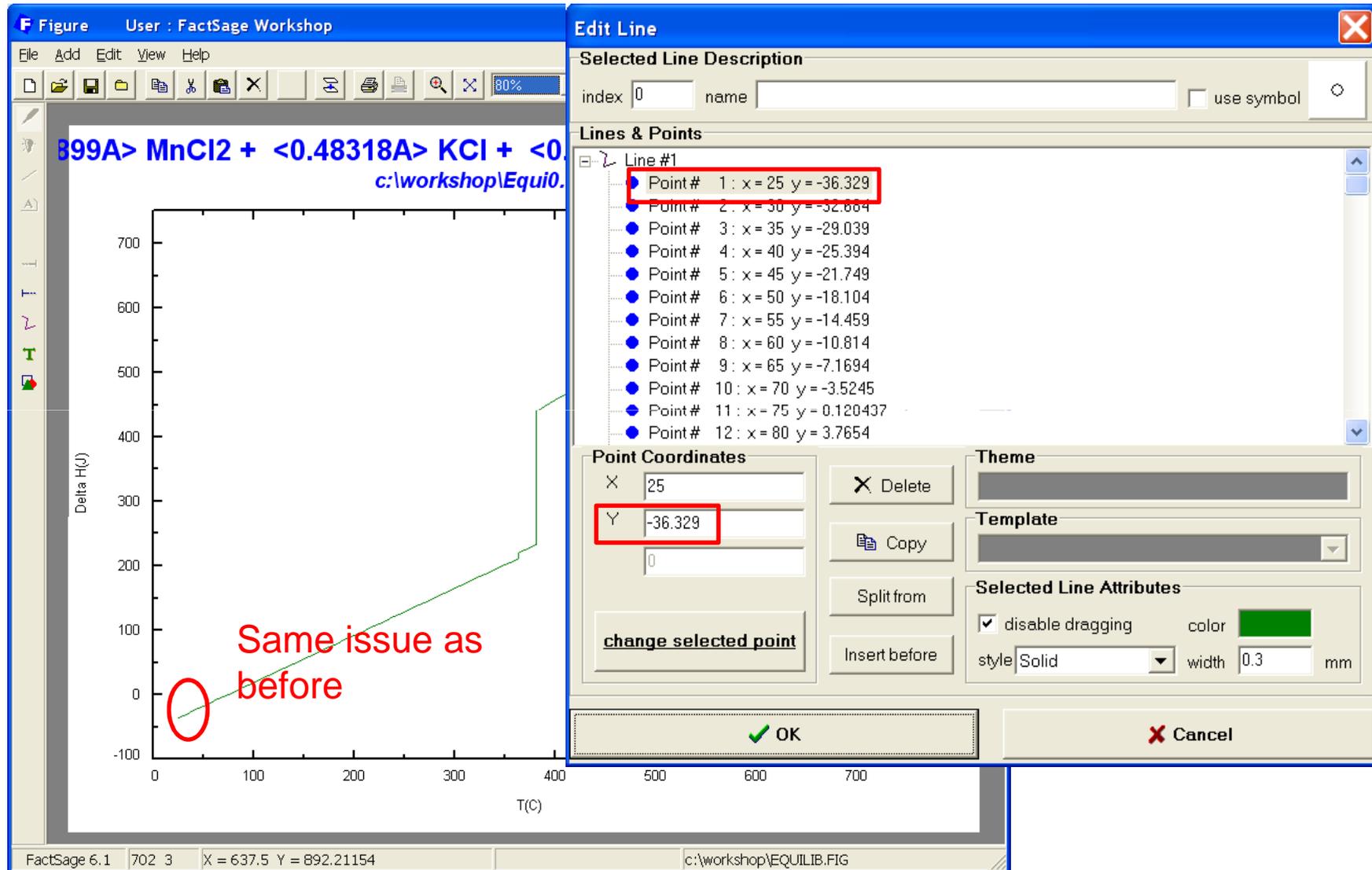
Cl 1.0000 Stoichiometry = 3.0000

System component Mole fraction Mass fraction
Mn 0.20000 0.27415
K 0.20000 0.19511
Cl 0.60000 0.53074
Na 3.5852E-19 2.0565E-19

+ 0.00000 gram AAlk2MX4#1
(25.00 C, 1 atm, a=0.99999)
(100.00 wt.% Na2MnCl4
+ 0.0673E-00 wt.% K2MnCl4)
```

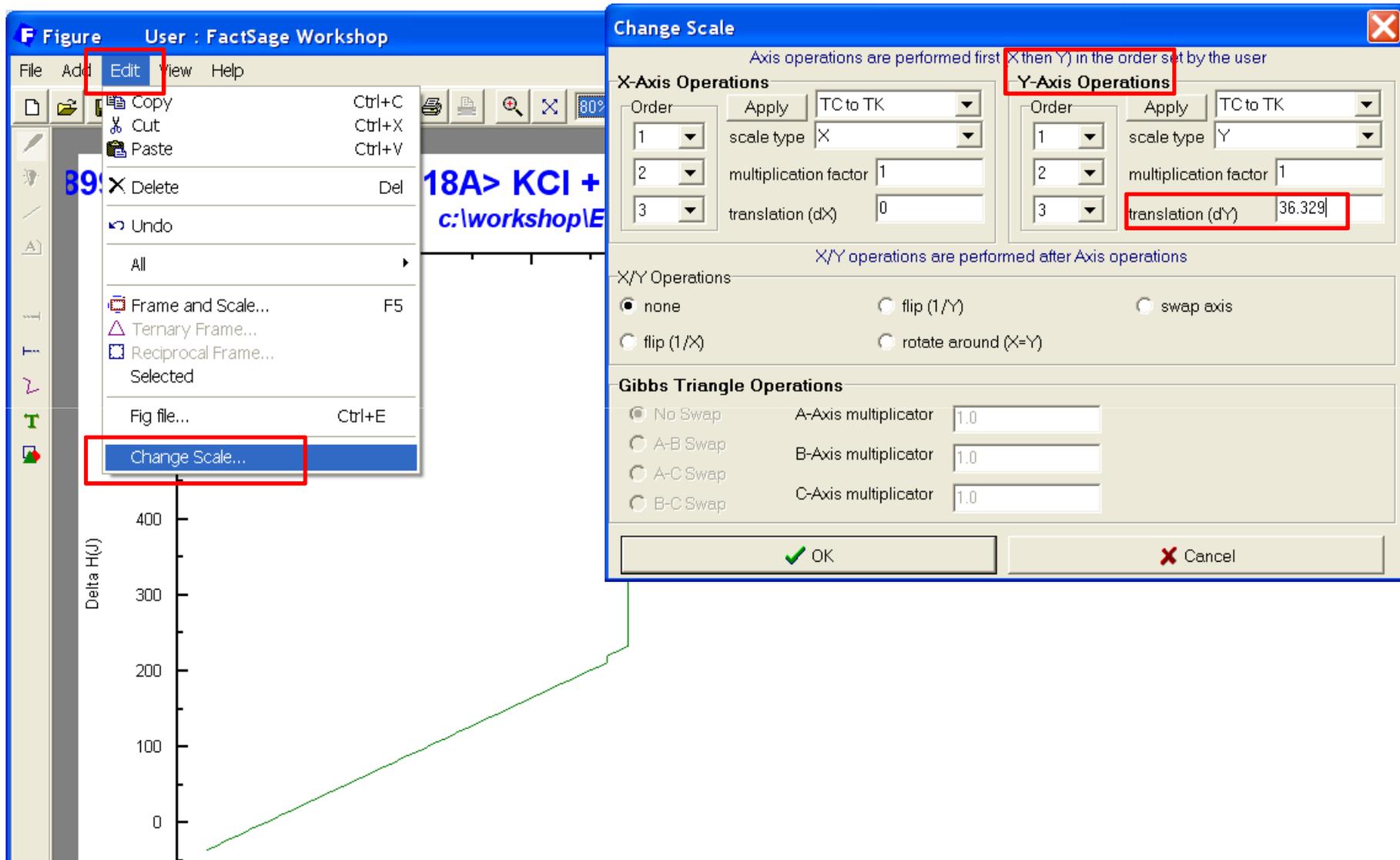
# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



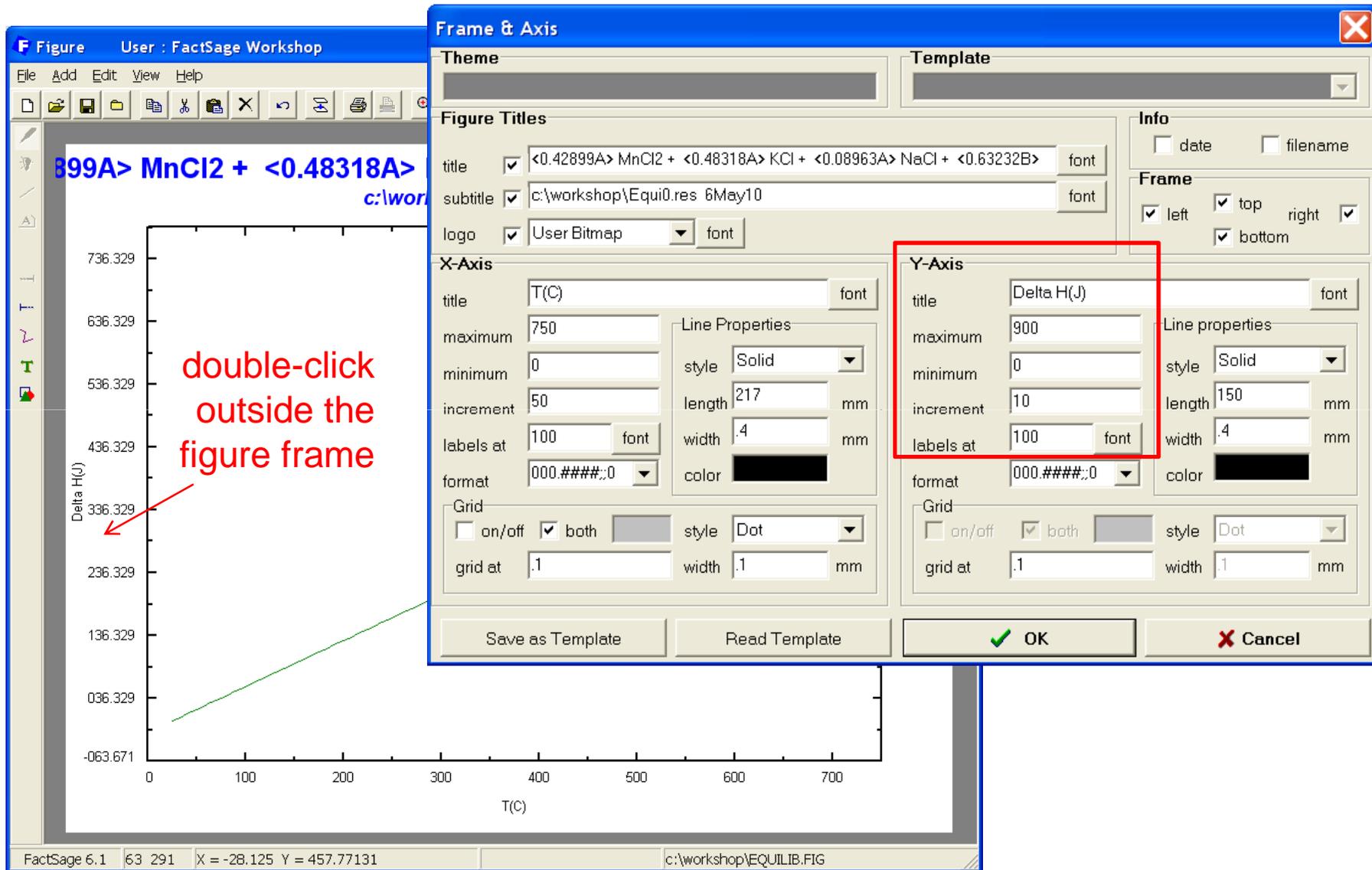
# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



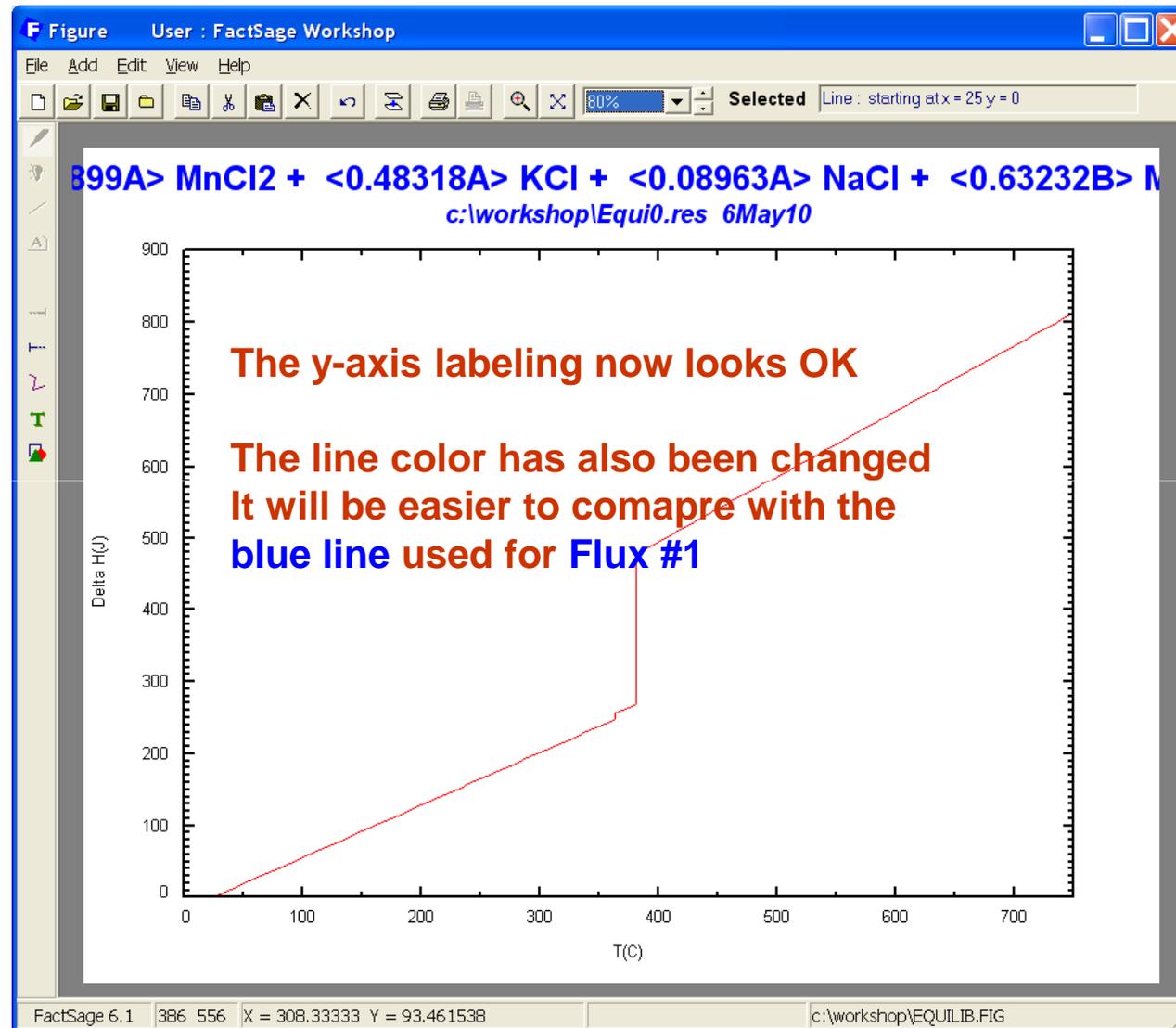
# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



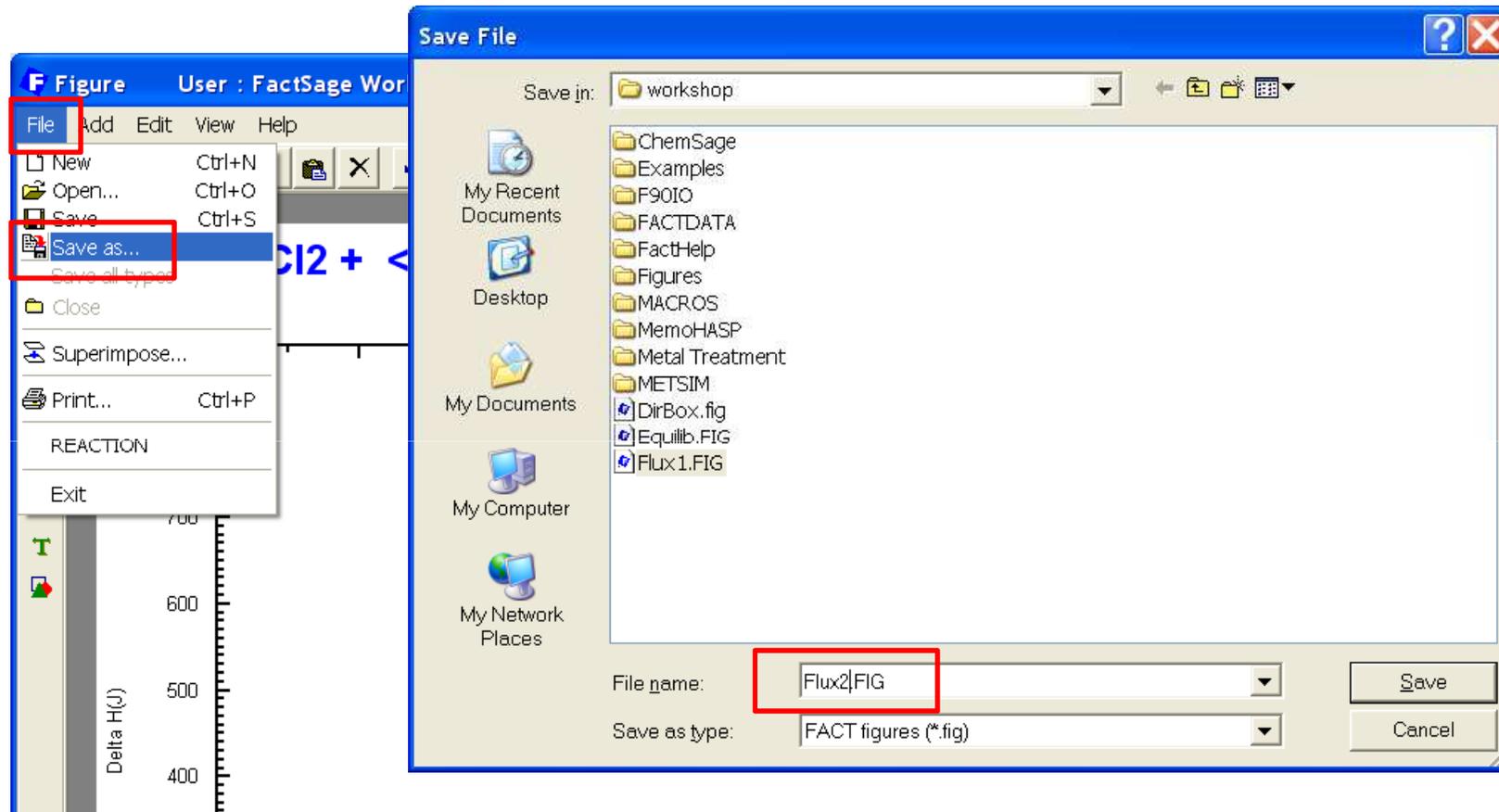
# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



**Save the file to compare with flux #1**

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

**Strategy :**

- 1) Liquidus projection  $\rightarrow$  NaCl-KCl-MnCl<sub>2</sub> :  
GOAL : identify 1 or 2 low melting compositions  
PHASE DIAGRAM
- 2)  $H_T - H_{25C}$  for the mixture(s)  $\rightarrow$  enthalpy requirement for melting  
GOAL : identify the lowest melting enthalpy  
EQUILIB
- 3) **Same for KMgCl<sub>3(s)</sub>**  
**GOAL : compare the mixture(s) with the reference flux**  
**EQUILIB**
- 4) Calculate the alkali removal from a Al-5%Mg alloy with the fluxes  
GOAL: check if the capability to remove Na and Ca is similar

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Reactants - Equilib

File Edit Table Units Data Search Help

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

1-7

| Mass(g)      | Species | Phase                    | T(C) | P(total)** | Stream# | Data |
|--------------|---------|--------------------------|------|------------|---------|------|
| <0.42899A>   | MnCl2   | solid scacchite          | 25   | 1.0        | 1       |      |
| + <0.48318A> | KCl     | solid sylvite (nacl_roc  | 25   | 1.0        | 1       |      |
| + <0.08963A> | NaCl    | solid halite (rock salt_ | 25   | 1.0        | 1       |      |
| + <0.63232B> | MnCl2   | solid scacchite          | 25   | 1.0        | 1       |      |
| + <0.15069B> | KCl     | solid sylvite (nacl_roc  | 25   | 1.0        | 1       |      |
| + <0.21698B> | NaCl    | solid halite (rock salt_ | 25   | 1.0        | 1       |      |
| + 1          | KMgCl3  | solid perovskite         | 25   | 1.0        | 1       |      |

\*\* P(total) is the hydrostatic pressure above the phase.  
For a gaseous stream this is the sum of the partial pressures of the species in that stream.

Initial Conditions

Next >>

FactSage 6.2 beta Compound: 1/24 databases Solution: 1/22 databases

Change value from 0 to 1 for the input of  $\text{KMgCl}_3$  (ref. flux)

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

**Menu - Equilib: last system**

File Units Parameters Help

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

**Reactants (7)**

(gram) <0.42899A> MnCl2 + <0.48318A> KCl + <0.08963A> NaCl + <0.63232B> MnCl2 + <0.15069B>

(25C,s,#1) (25C,s,#1) (25C,s,#1) (25C,s,#1) (25C,s,#1)

**Products**

Compound species

gas  ideal  real 0

aqueous 0

pure liquids 0

+ pure solids 17

suppress duplicates

species: 17

Solution species

| * | + | Base-Phase   | Full Name          |
|---|---|--------------|--------------------|
| J |   | FTsalt-ACL_B | BAIkCl-ss_rocksalt |
| J |   | FTsalt-AMX4A | AAIk2MX4           |
| J |   | FTsalt-PRVKA | AAMX3-Perovskite   |
| I |   | FTsalt-R-3m  | MCl2_SOLID         |
| I |   | FTsalt-SALTB | BSaltLiquid        |

Legend

I - immiscible 2

J - 3-immiscible 3

Show  all  selected

species: 48

solutions: 13

Custom Solutions

0 fixed activities

0 ideal solutions

0 activity coefficients

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 65

Total Solutions (max 40) 13

**Final Conditions**

| <A> | <B> | T(C)     | P(atm) | Delta H(J) |
|-----|-----|----------|--------|------------|
| 0   | 0   | 25 750 5 | 1      |            |

Equilibrium

normal  normal + transitions

transitions only  open

predominant

146+ calculations

**<A>=0 <B>=0 Ref. flux**

FactSage 6.2 beta

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

The screenshot displays the FactSage 6.2 beta interface. The main window shows a list of chemical species and their activities. Overlaid on this are three dialog boxes:

- Plot: Delta H(J) vs T(C)**: The main plot window, showing a dropdown menu with the selected reaction:  $\langle 0.42899A \rangle \text{MnCl}_2 + \langle 0.48318A \rangle \text{KCl} + \langle 0.08963A \rangle \text{NaCl}$ .
- Plot Results**: A menu option highlighted in red, with a sub-menu showing "Repeat Plot - Delta H(J) vs T(C)".
- Axes: Delta H(J) vs T(C)**: A dialog box for configuring the plot axes. The Y-axis is labeled "Delta H(J)" and the X-axis is labeled "T(C)". The Y-axis scale is set from 0 to 900 with major ticks every 50. The X-axis scale is set from 0 to 750 with major ticks every 50. The "Refresh" button is highlighted in red.

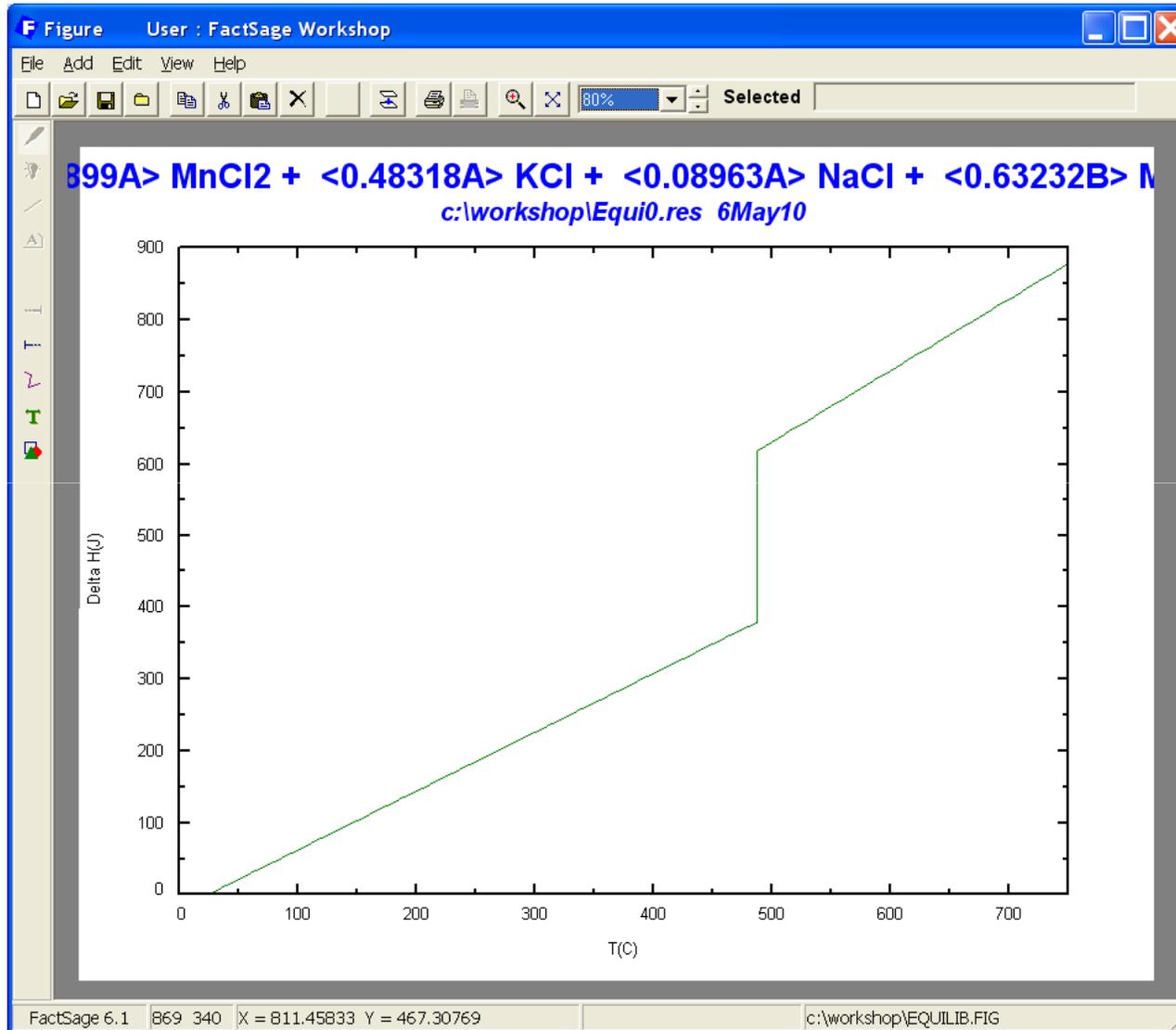
The main window also shows a list of chemical species and their activities, including:

- AAMX3-Perovskite#1
- AAMX3-Perovskite#2
- AAMX3-Perovskite#3
- MC12\_SOLID#1
- MC12\_SOLID#2
- BSalt-liquid#1

The status bar at the bottom indicates "FactSage 6.1", the file path "c:\workshop\Equi0.res", the date "6May10", and "148 sets".

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



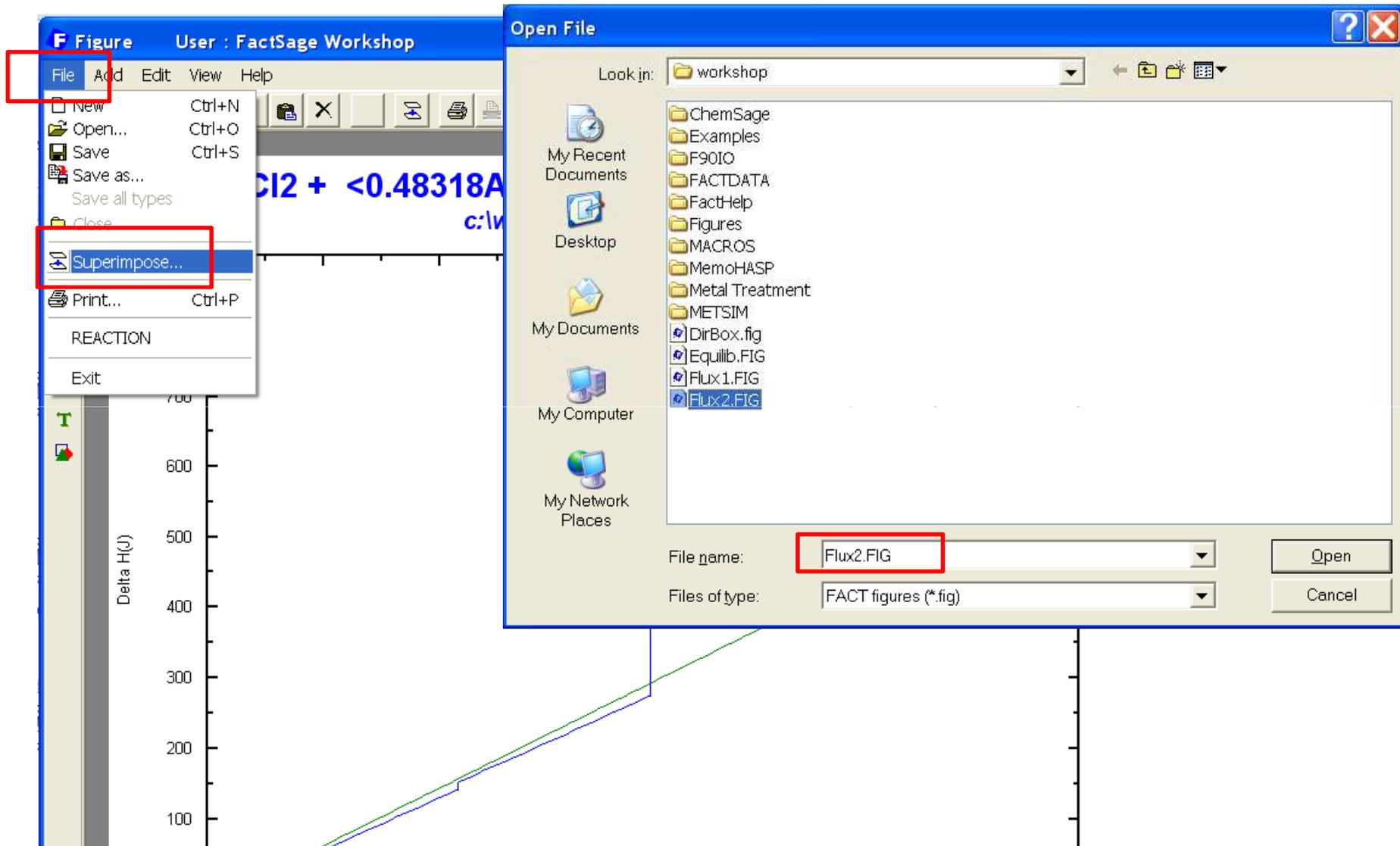
# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

The image shows a screenshot of the FactSage Workshop software interface. The main window displays a plot of Delta H(j) on the y-axis (ranging from 100 to 700) against an unlabeled x-axis. The plot title is "REACTION" and "Exit". A red box highlights the "File" menu, and another red box highlights the "Superimpose..." option. An "Open File" dialog box is open, showing the "workshop" directory. The file list includes "DirBox.fig", "Equilib.FIG", "Flux1.FIG", and "Flux2.FIG". The "File name" field is set to "Flux1.FIG" and the "Files of type" is set to "FACT figures (\*.fig)".

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



# Metal Treatment (Al & Mg)

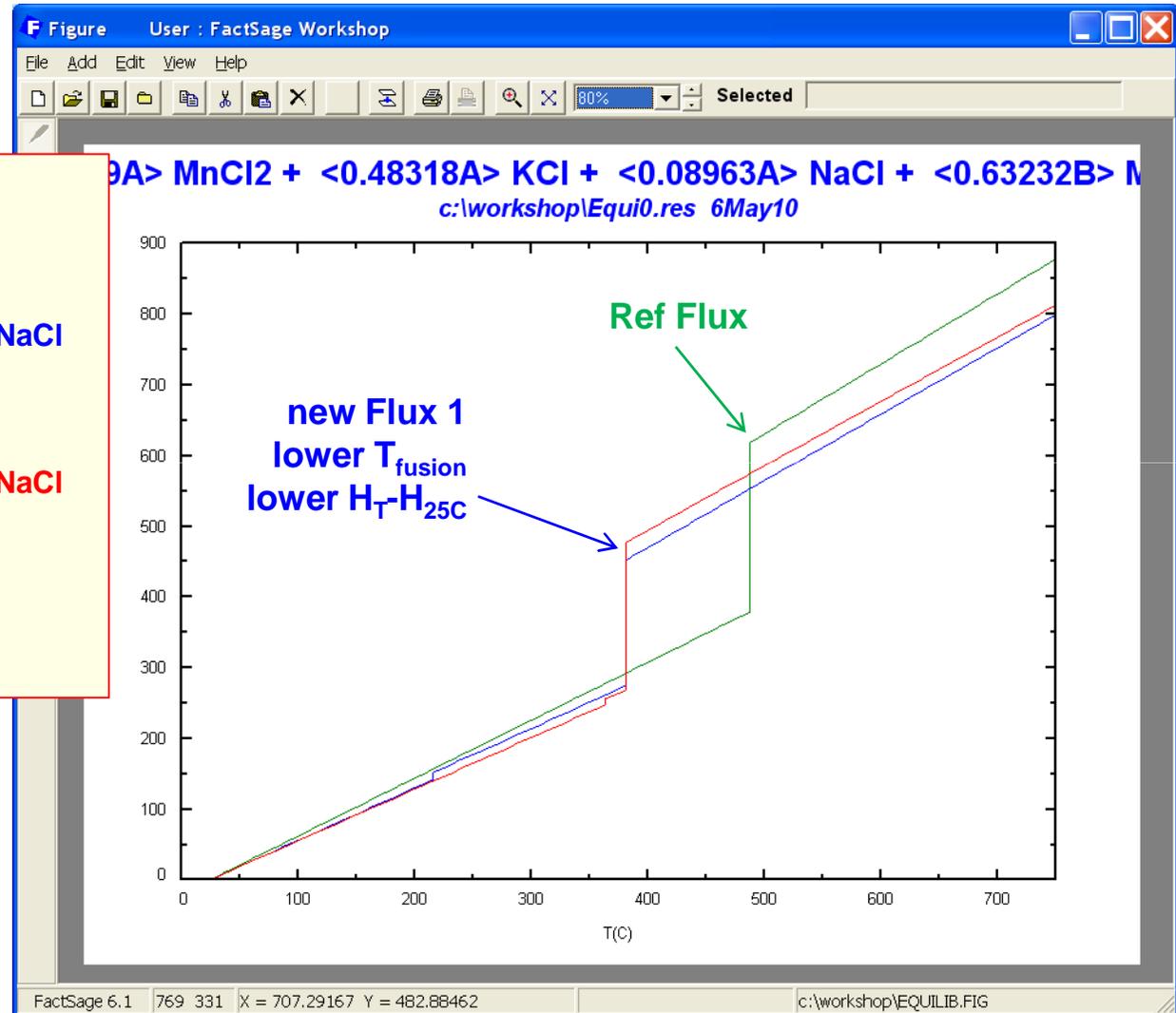
- **Example #2: Comparison of 2 salt fluxes for alkali removal**

**2 low-melting compositions**  
*wt.fractions*

**Flux 1**  
**0.42899 MnCl<sub>2</sub> + 0.48138KCl + 0.08963NaCl**  
**@ 380.95°C**

**Flux 2**  
**0.63232 MnCl<sub>2</sub> + 0.15069KCl + 0.21698NaCl**  
**@ 381.64°C**

**Ref. Flux**  
**KMgCl<sub>3</sub>**  
**@ 487°C**



- **Example #2: Comparison of 2 salt fluxes for alkali removal**

**Strategy :**

- 1) Liquidus projection  $\rightarrow$  NaCl-KCl-MnCl<sub>2</sub> :  
GOAL : identify 1 or 2 low melting compositions  
PHASE DIAGRAM
- 2)  $H_T - H_{25C}$  for the mixture(s)  $\rightarrow$  enthalpy requirement for melting  
GOAL : identify the lowest melting enthalpy  
EQUILIB
- 3) Same for KMgCl<sub>3(s)</sub>  
GOAL : compare the mixture(s) with the reference flux  
EQUILIB
- 4) **Calculate the alkali removal from a Al-5%Mg alloy with the fluxes**  
**GOAL: check if the capability to remove Na and Ca is similar**

## Metal Treatment (Al & Mg)

---

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

### Strategy :

- 4) Calculate the alkali removal from a Al-5%Mg alloy with the fluxes  
**GOAL: check if the capability to remove Na and Ca is similar**

The alloy to be treated is **Al + 5% Mg + 40 ppm Na + 20 ppm Ca**

As a light metal alloy is used, the **FTlite database** must be now activated

# Metal Treatment (Al & Mg)

- Example #2: Comparison of 2 salt fluxes for alkali removal

**F Data Search**

Databases - 2/24 compound databases, 2/22 solution databases

| Fact                                       | FactSage <sup>®</sup>           | SGTE                            |                                         | Miscellaneous                  |
|--------------------------------------------|---------------------------------|---------------------------------|-----------------------------------------|--------------------------------|
| <input type="checkbox"/> ELEM              | <input type="checkbox"/> FSopp  | <input type="checkbox"/> BINS   | <input type="checkbox"/> compounds only | <input type="checkbox"/> EXAM  |
| <input type="checkbox"/> FACT              | <input type="checkbox"/> FSlead | <input type="checkbox"/> SGPS   | <input type="checkbox"/> solutions only | <input type="checkbox"/> SGSL  |
| <input type="checkbox"/> Fact53            | <input type="checkbox"/> FSlite | <input type="checkbox"/> SGTE   | <input type="checkbox"/> no data        | <input type="checkbox"/> SGTE* |
| <input type="checkbox"/> FToxid            | <input type="checkbox"/> FSstel | <input type="checkbox"/> SGnobl | Clear All                               |                                |
| <input checked="" type="checkbox"/> FTsalt | <input type="checkbox"/> FSupsi | <input type="checkbox"/> SGsold | Select All                              |                                |
| <input type="checkbox"/> FTmisc            | <input type="checkbox"/> FSnobl | <input type="checkbox"/> SGnucl | Add/Remove Data                         |                                |
| <input type="checkbox"/> FThall            | <b>Other</b>                    | <input type="checkbox"/> TDnucl | RefreshDatabases                        |                                |
| <input type="checkbox"/> FTheig            | <input type="checkbox"/> OLIP   | <input type="checkbox"/> OLIC   |                                         |                                |
| <input type="checkbox"/> FTpulp            | <input type="checkbox"/> OLIG   | <input type="checkbox"/> OLIL   |                                         |                                |
| <input checked="" type="checkbox"/> FTlite |                                 |                                 |                                         |                                |

**Information** -  
Click on a box to include (or exclude) a database in the data search. Normally databases are 'coupled' - that is both the compound and solution database (when available) will be selected. To 'uncouple' a databases click-mouse-right-button (note, this is NOT recommended).  
If database is stored on your PC but not listed here then you must 'add the database to the list' - click on 'Add/Remove ...'.

**Options**

Default

Include

- gaseous ions (in aemas)
- aqueous species
- limited data compounds (25C)

Limits

Organic species C<sub>x</sub>H<sub>y</sub>... X(max) =

Minimum solution components:  1  2 cpts

Cancel Summary ... OK

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Al-5%Mg with (40 ppm Na and 20 ppm Ca)

| Mass(g)      | Species | Phase | T(C) | P(total)** | Stream# | Data |
|--------------|---------|-------|------|------------|---------|------|
| <0.42899A>   | MnCl2   | s     |      |            | 1       |      |
| + <0.48318A> | KCl     | s     |      |            | 1       |      |
| + <0.08963A> | NaCl    | s     |      |            | 1       |      |
| + <0.63232B> | MnCl2   | s     |      |            | 2       |      |
| + <0.15069B> | KCl     | s     |      |            | 2       |      |
| + <0.21698B> | NaCl    | s     |      |            | 2       |      |
| + 94.994     | Al      | s     |      |            | 3       |      |
| + 5          | Mg      | s     |      |            | 3       |      |
| + 40E-4      | Na      | s     |      |            | 3       |      |
| + 20E-4      | Ca      | s     |      |            | 3       |      |

Initial Conditions

Next >>

FactSage 6.2 beta Compound: 1/24 databases Solution: 1/22 databases

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

Warning message due to the addition of the new element Ca

The selection of phases might have to be updated

Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 10

| Mass(g)      | Species | Phase | T(C) | P(total)** | Stream# | Data |
|--------------|---------|-------|------|------------|---------|------|
| <0.42899A>   | MnCl2   | s     |      |            | 1       |      |
| + <0.48318A> |         |       |      |            | 1       |      |
| + <0.08963A> |         |       |      |            | 1       |      |
| + <0.63232B> |         |       |      |            | 2       |      |
| + <0.15069B> |         |       |      |            | 2       |      |
| + <0.21698B> |         |       |      |            | 2       |      |
| + 94.994     |         |       |      |            | 3       |      |
| + 5          |         |       |      |            | 3       |      |
| + 40E-4      | Na      |       |      |            | 3       |      |
| + 20E-4      | Ca      |       |      |            | 3       |      |

Initial Conditions

Next >>

FactSage 6.2 beta Compound: 1/24 databases Solution: 1/22 databases

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

**F Menu - Equilib: last system**

File Units Parameters Help

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

**Reactants (10)**

(gram) <0.42899A> MnCl2 + <0.48318A> KCl + <0.08963A> NaCl + <0.63232B> MnCl2 + <0.15069B>

**Products**

Compound species

- gas  ideal  real 0
- aqueous 0
- pure liquids 0
- pure solids 70

suppress duplicates

species: 70

**Solution species**

| * | + | Base-Phase  | Full Name |
|---|---|-------------|-----------|
|   | I | FTlite-Liqu | Liquid    |
|   | I | FTlite-FCC  | FCC_A1    |
|   | I | FTlite-HCP  | HCP_A3    |
|   | I | FTlite-BCC  | BCC_A2    |
|   | + | FTlite-CBCC | CBCC_A12  |
|   | + | FTlite-CUB1 | CUB_A13   |
|   | I | FTlite-LC14 | Laves_C14 |
|   | I | FTlite-LC15 | Laves_C15 |

Legend

- I - immiscible 10
- J - 3-immiscible 3
- + - selected 8

Show  all  selected

species: 20  
solutions: 37

**Final Conditions**

| <A> | <B> | T(C)     | P(atm) | Product H(J) |
|-----|-----|----------|--------|--------------|
| 0   | 0   | 25 750 5 | 1      |              |

10 steps  Table 146 calculations

**Equilibrium**

- normal  normal + transitions
- transitions only  open
- predominant

FactSage 6.2 beta

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

**F Menu - Equilib: last system**

File Units Parameters Help

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

**Reactants (10)**

(gram) <0.42899A> MnCl2 + <0.48318A> KCl + <0.08963A> NaCl + <0.63232B> MnCl2 + <0.15089B>

**Products**

Compound species

- gas  ideal  real 0
- aqueous 0
- pure liquids 0
- pure solids 70
- suppress duplicates

species: 70

Solution species

| * | + | Base-Phase  | Full Name |
|---|---|-------------|-----------|
|   | I | FTlite-Liqu | Liquid    |
|   | I | FTlite-FCC  | FCC_A1    |
|   | I | FTlite-HCP  | HCP_A3    |
|   | I | FTlite-BCC  | BCC_A2    |
|   | + | FTlite-CBCC | CBCC_A12  |
|   | + | FTlite-CUB1 | CUB_A13   |
|   | I | FTlite-LC14 | Laves_C14 |
|   | I | FTlite-LC15 | Laves_C15 |

Legend

- I - immiscible 10
- J - 3-immiscible 3
- + - selected 8

Show  all  selected

species: 201  
solutions: 37

Custom Solutions

- 0 fixed activities
- 0 ideal solutions
- 0 activity coefficients

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 271  
Total Solutions (max 40) 37

Target

- none -

Estimate T(K): 1000  
Mass(g): 0

**Final Conditions**

| <A> | <B> | T(C) | P(atm) | Product H(J) |
|-----|-----|------|--------|--------------|
| 0   | 0   | 720  | 1      |              |

41 calculations

**Equilibrium**

- normal  normal + transitions
- transitions only  open
- predominant

FactSage 6.2 beta

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



Liquid Alloy  
100 grams

Molten Salt  
0.0288 grams

Output Edit Show Pages

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

A=0.12 |  
 A=0.06 | A=0.065 | A=0.07 | A=0.075 | A=0.08 | A=0.085 | A=0.09 | A=0.095 | A=0.1 | A=0.105 | A=0.11 | A=0.115 |  
 A=0 | A=0.005 | A=0.01 | A=0.015 | A=0.02 | A=0.025 | **A=0.03** | A=0.035 | A=0.04 | A=0.045 | A=0.05 | A=0.055

(gram) <0.42899A> MnCl2 + <0.48318A> KCl + <0.08963A> NaCl + <0.63232 (0)> ...

(gram) <0.15069 (0)> KCl + <0.21698 (0)> NaCl + 94.994 Al + 5 Mg +

(gram) 40E-4 Na + 20E-4 Ca =

**100.00 gram Liquid#1**  
 (100.00 gram, 3.7266 mol)  
 (720.00 C, 1 atm, a=1.0000)  
 ( 94.993 wt.% Al FTLite  
 + 1.5711E-03 wt.% Ca FTLite  
 + 2.0515E-18 wt.% Cl FTLite  
 + 1.6323E-05 wt.% K FTLite  
 + 4.9997 wt.% Mg FTLite  
 + 5.6183E-03 wt.% Mn FTLite  
 + 2.0448E-04 wt.% Na FTLite)

| System component | Mole fraction | Mass fraction |
|------------------|---------------|---------------|
| Mn               | 2.7443E-05    | 5.6183E-05    |
| Ca               | 1.0520E-05    | 1.5711E-05    |
| K                | 1.1203E-07    | 1.6323E-07    |
| Cl               | 1.5528E-20    | 2.0515E-20    |
| Al               | 0.94476       | 0.94993       |
| Mg               | 5.5201E-02    | 4.9997E-02    |
| Na               | 2.3868E-06    | 2.0448E-06    |

+ **2.8868E-02 gram CSalt-liquid#1**  
 (2.8868E-02 gram, 4.2505E-04 mol)  
 (720.00 C, 1 atm, a=1.0000)  
 ( 42.738 wt.% NaCl FTsalt  
 + 50.105 wt.% KCl FTsalt  
 + 3.0434 wt.% MgCl2 FTsalt  
 + 4.1139 wt.% CaCl2 FTsalt  
 + 5.9107E-13 wt.% MnCl2 FTsalt  
 + 1.8303E-10 wt.% AlCl3\_4coord FTsalt  
 + 2.3247E-24 wt.% Al2Cl6 FTsalt  
 + 3.5110E-19 wt.% AlCl3\_5coord FTsalt)

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

The screenshot displays the FactSage 6.2 interface. The main window is titled "Results Processor: c:\workshop\Equi0.res" and shows a chemical reaction:  $\langle 0.42899A \rangle \text{MnCl}_2 + \langle 0.48318A \rangle \text{KCl} + \langle 0.08963A \rangle \text{NaCl}$ . A table of data is visible in the background, with columns for activity and mole. A dialog box titled "F Axes: weight % vs Alpha" is open, allowing for plot configuration. The Y-axis is set to "weight %" and the X-axis is set to "Alpha". The Y-axis scale is from 0 to  $45 \times 10^{-4}$  with ticks every  $5 \times 10^{-4}$ . The X-axis scale is from 0 to 2 with ticks every 0.01. The "Axes" button in the main window is highlighted with a red box. The "Plot" menu in the "Results - Equilib" window is also highlighted with a red box.

**Results - Equilib A=0.03 (page 7/41) FactSage 6.2 be**

Output Edit Show Pages

Save or Print T(C) P(atm) Energy

Plot Plot Results ...

Equilib Results file Repeat Plot - Delta H(T) vs T(C)

Stream File A=0.015 | A=0.02 | A=0.025 | - A=0.03 - A

Format MnCl<sub>2</sub> +  $\langle 0.48318A \rangle$  KCl +  $\langle 0.08963A \rangle$

Fact-XML MnCl<sub>2</sub> +  $\langle 0.48318A \rangle$  KCl +  $\langle 0.08963A \rangle$

Fact-Optimal  $\rangle$  KCl +  $\langle 0.21698(0) \rangle$  NaCl + 94

Refresh ... 20E-4 Ca =

100.00 gram Liquid#1  
(100.00 gram, 3.7266 mol)  
(720.00 C, 1 atm, a=1.0000)

94.993 wt.% Al  
+ 1.5711E-03 wt.% Ca  
+ 2.0515E-18 wt.% Cl  
+ 1.6323E-05 wt.% K  
+ 4.9997 wt.% Mg  
+ 5.6183E-03 wt.% Mn  
+ 2.0448E-04 wt.% Na

System component Mole fraction Mass

Mn 2.7443E-05

Ca 1.0520E-05

K 1.1203E-07

Cl 1.5528E-20

Al 0.94476

**Results Processor: c:\workshop\Equi0.res**

File Help

$\langle 0.42899A \rangle$  MnCl<sub>2</sub> +  $\langle 0.48318A \rangle$  KCl +  $\langle 0.08963A \rangle$  NaCl

|  | activity | mole   |
|--|----------|--------|
|  | 0        | 1.     |
|  | 0        | 3.7266 |
|  |          | 0.02   |
|  |          | 00.    |
|  |          | 2      |
|  |          | 0      |
|  |          | 0      |
|  |          | 9.07   |
|  |          | 28E+05 |
|  |          | 0      |
|  |          | 27E+05 |
|  |          | 0      |
|  |          | 9.93   |
|  |          | 1.     |

**F Axes: weight % vs Alpha**

Y-variable X-variable Swap Axes

Y-axis X-axis

weight % Alpha

maximum 45E-4 maximum 2

minimum 0 minimum 0

tick every 5E-4 tick every .01

Cancel Refresh OK

0 selected

Select

Repeat

size: 9 no: 4

color  full screen

reactants  Viewer

file name  Figure

chemical

integer #

none

Plot >>

FactSage 6.1 c:\workshop\Equi0.res 6May10 41 sets

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

**Species Selection - EQUILIB Results: weight % vs Alpha**

| #                   | Species    | Mole (min) | Mole (max) | Fract. (min) | Fract. (max) | Act. (min) | Act. (max) |
|---------------------|------------|------------|------------|--------------|--------------|------------|------------|
| <b>FTlite- Liqu</b> |            |            |            |              |              |            |            |
| 1                   | Al(Liqu#1) | 3.5207     | 3.5207     | 0.944738     | 0.94476      | 0.944044   | 0.944081   |
| + 2                 | Ca(Liqu#1) | 3.0322E-06 | 4.9903E-05 | 8.1366E-07   | 1.3391E-05   | 3.6498E-10 | 6.0042E-09 |
| 3                   | Cl(Liqu#1) | 0          | 3.2292E-19 | 0            | 8.6655E-20   | 0          | 8.7856E-20 |
| + 4                 | K(Liqu#1)  | 0          | 4.4085E-06 | 0            | 1.1830E-06   | 0          | 5.1386E-04 |
| 5                   | Mg(Liqu#1) | 0.205171   | 0.205719   | 5.5056E-02   | 5.5203E-02   | 3.8692E-02 | 3.8767E-02 |
| 6                   | Mn(Liqu#1) | 0          | 6.8178E-04 | 0            | 1.8295E-04   | 0          | 2.1283E-07 |
| + 7                 | Na(Liqu#1) | 5.2463E-07 | 1.7399E-04 | 1.4078E-07   | 4.6688E-05   | 5.7744E-05 | 1.9107E-02 |
| <b>FTlite- Liqu</b> |            |            |            |              |              |            |            |
| 8                   | Al(Liqu#2) | 0          | 0          | 2.2051E-09   | 0.944738     | 0.944044   | 0.944081   |
| 9                   | Ca(Liqu#2) | 0          | 0          | 6.4911E-17   | 1.3391E-05   | 3.6498E-10 | 6.0042E-09 |
| 10                  | Cl(Liqu#2) | 0          | 0          | 0            | 0.494477     | 0          | 8.7856E-20 |
| 11                  | K(Liqu#2)  | 0          | 0          | 0            | 3.7726E-08   | 0          | 5.1386E-04 |
| 12                  | Mg(Liqu#2) | 0          | 0          | 1.9142E-09   | 5.5202E-02   | 3.8692E-02 | 3.8767E-02 |
| 13                  | Mn(Liqu#2) | 0          | 0          | 0            | 9.3676E-13   | 0          | 2.1283E-07 |
| 14                  | Na(Liqu#2) | 0          | 0          | 4.6688E-05   | 0.53232      | 5.7744E-05 | 1.9107E-02 |
| <b>FTlite- FCC#</b> |            |            |            |              |              |            |            |
| 15                  | Al(FCC#1)  | 0          | 0          | 0.979952     | 0.979987     | 0.869269   | 0.869303   |
| 16                  | Ca(FCC#1)  | 0          | 0          | 1.5862E-12   | 2.6115E-11   | 3.9499E-10 | 6.4979E-09 |

Mass:  mole  gram  source

Order:  integer #  mass (max)  fraction (max)  activity (max)

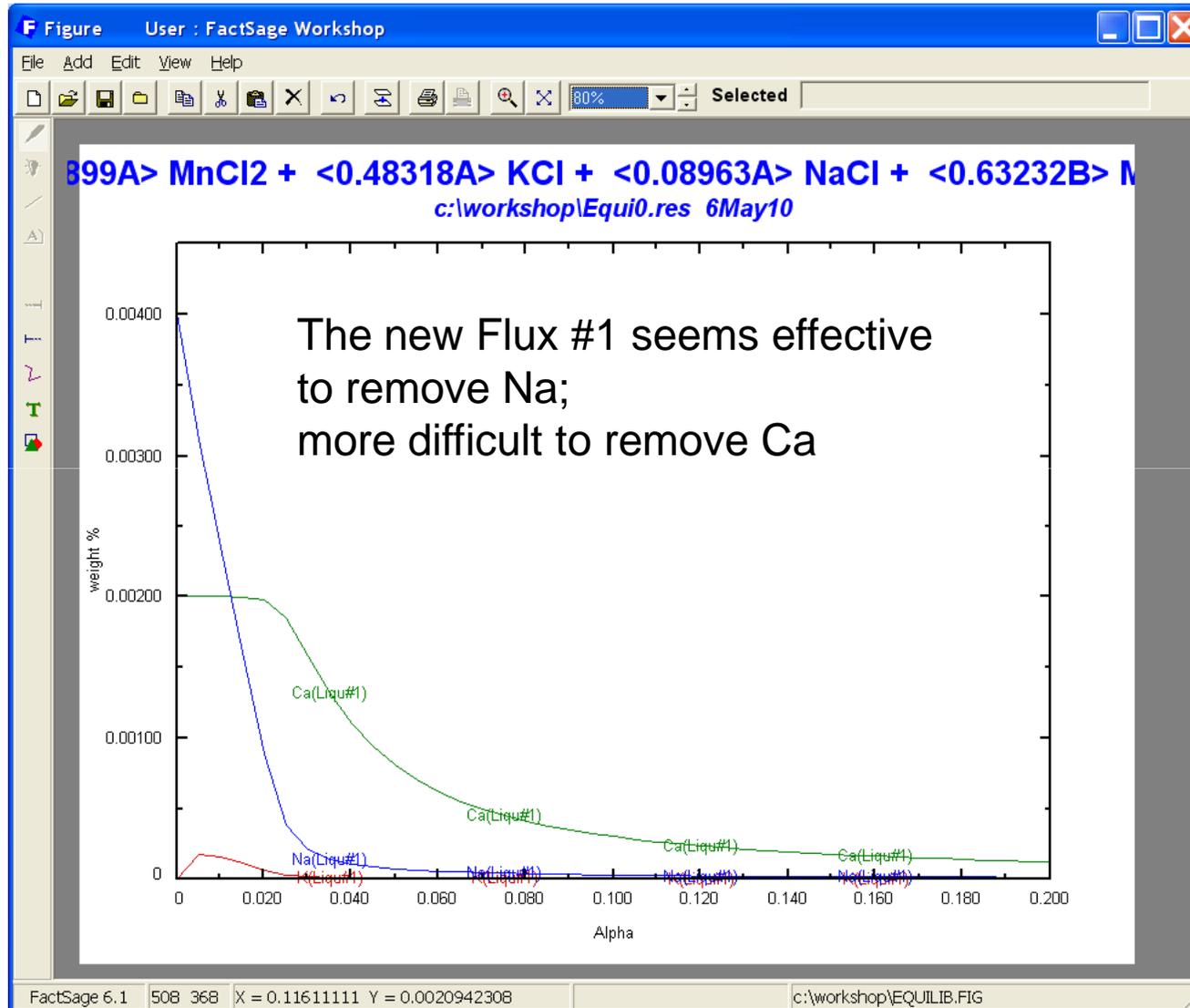
Select Top: 15 (dropdown) 3 species selected

Buttons: Clear, Refresh, OK

Footer: FactSage 6.1 | c:\workshop\Equi0.res | 6May10 | 41 sets

# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**



# Metal Treatment (Al & Mg)

- **Example #2: Comparison of 2 salt fluxes for alkali removal**

## Alkali Treatment

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