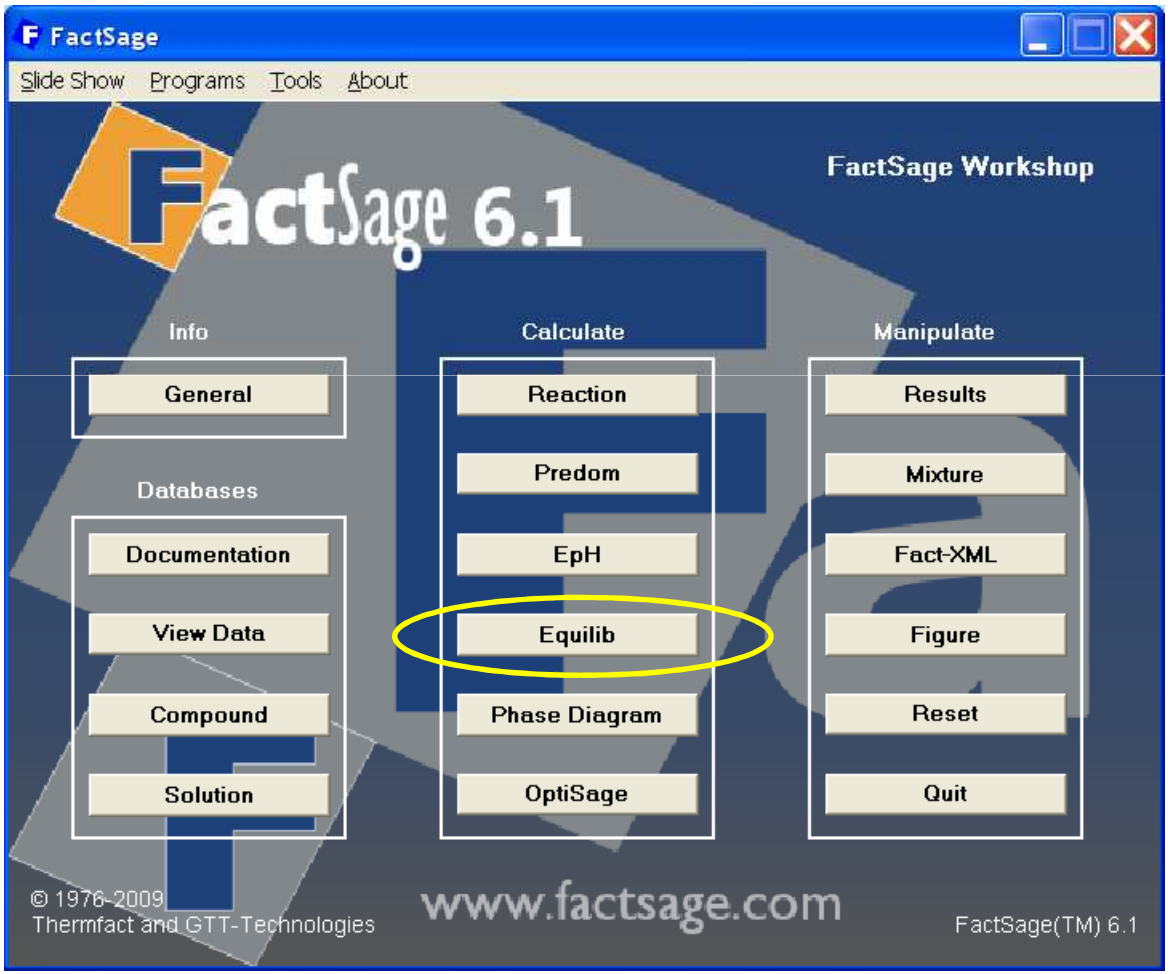
- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**

5.52% Mg

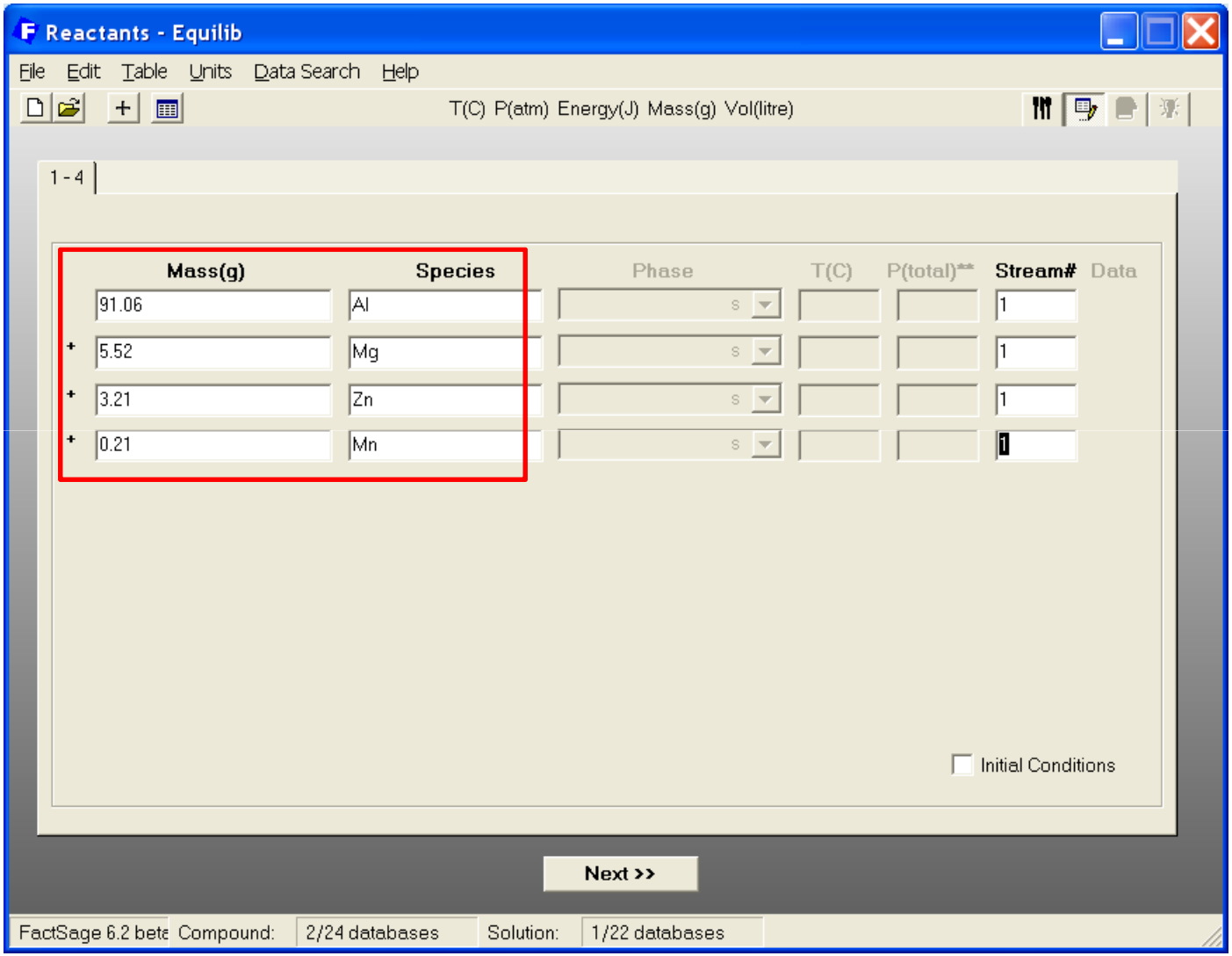
3.21% Zn

0.21% Mn

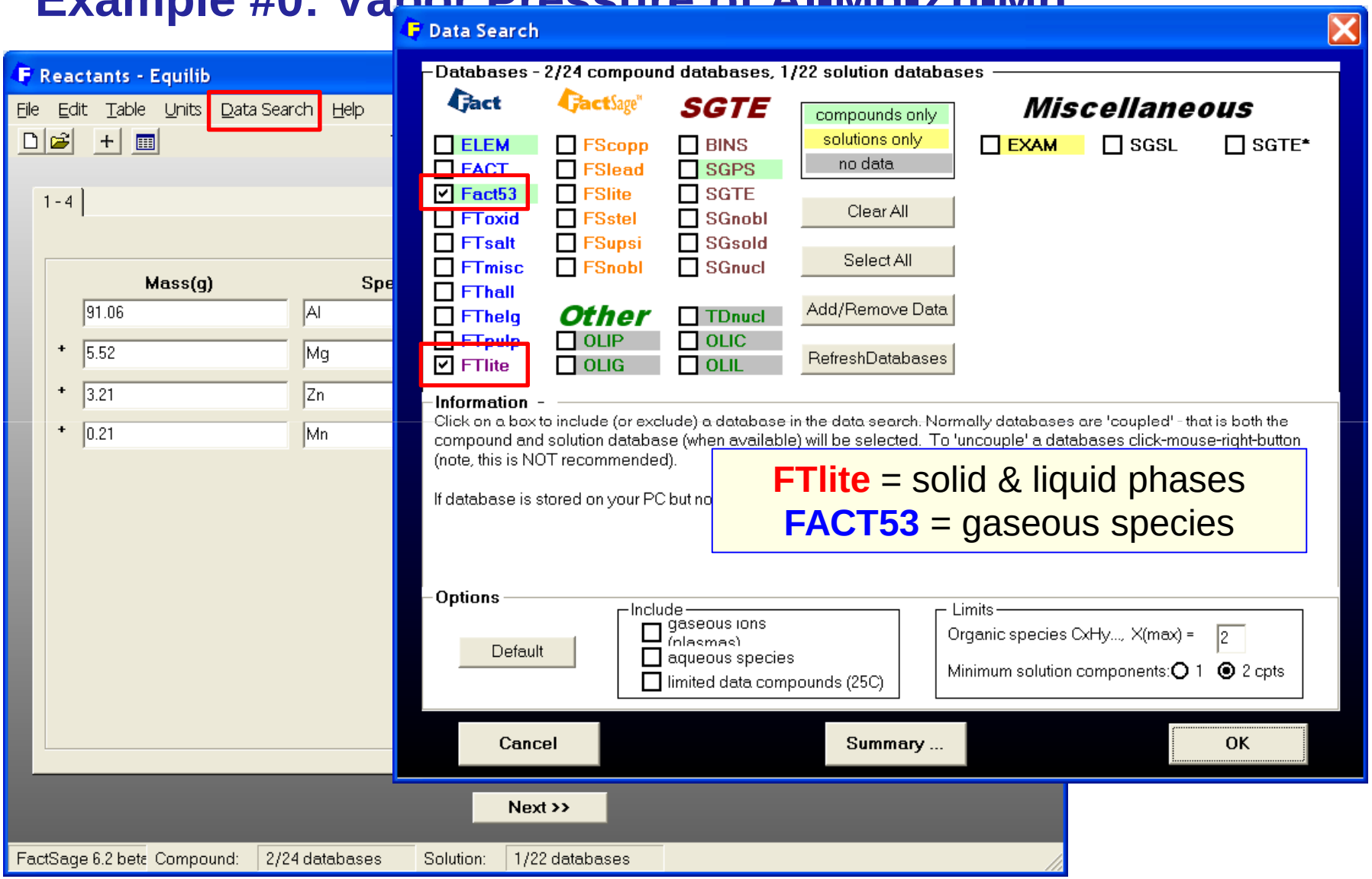
Balance Al



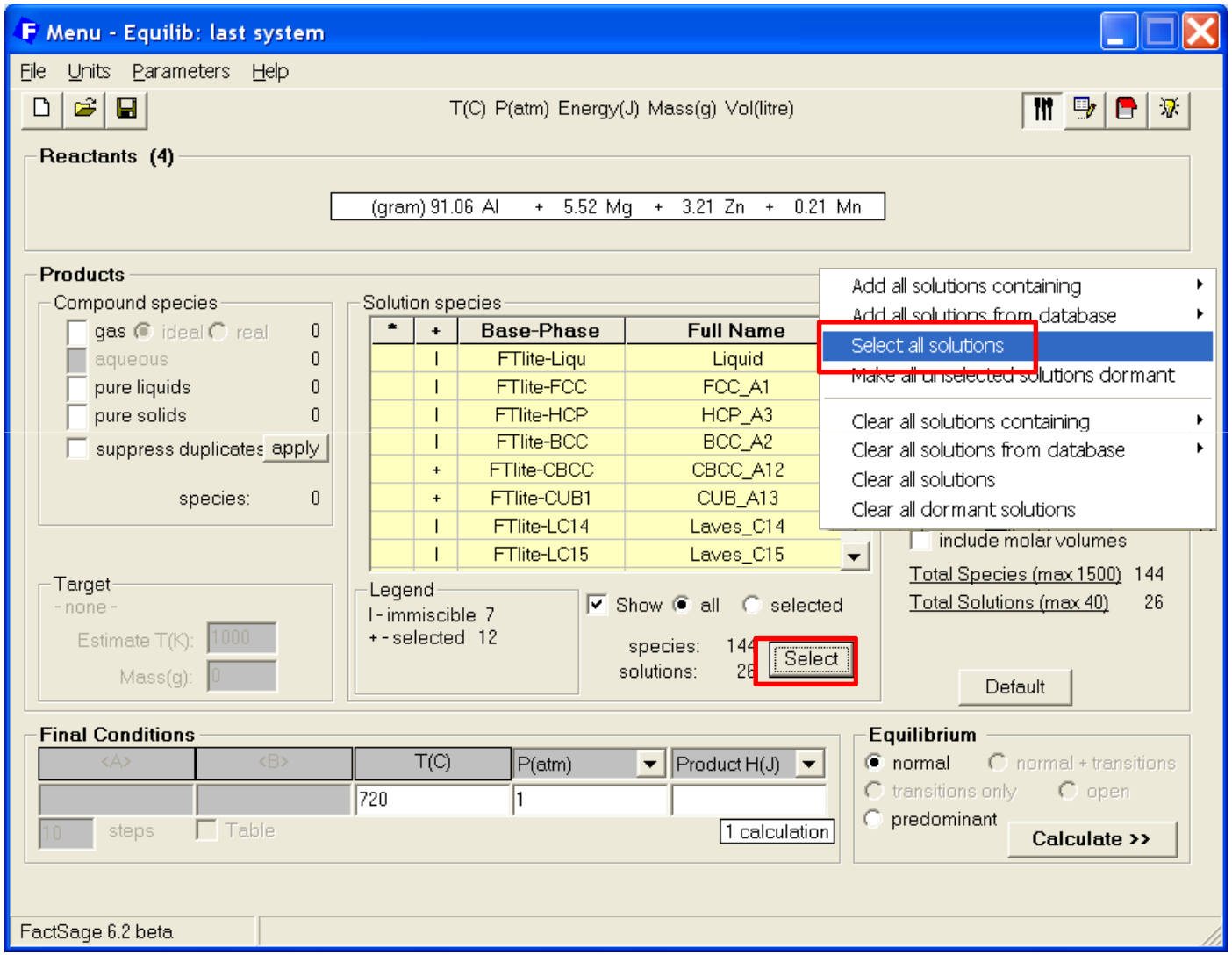
- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**



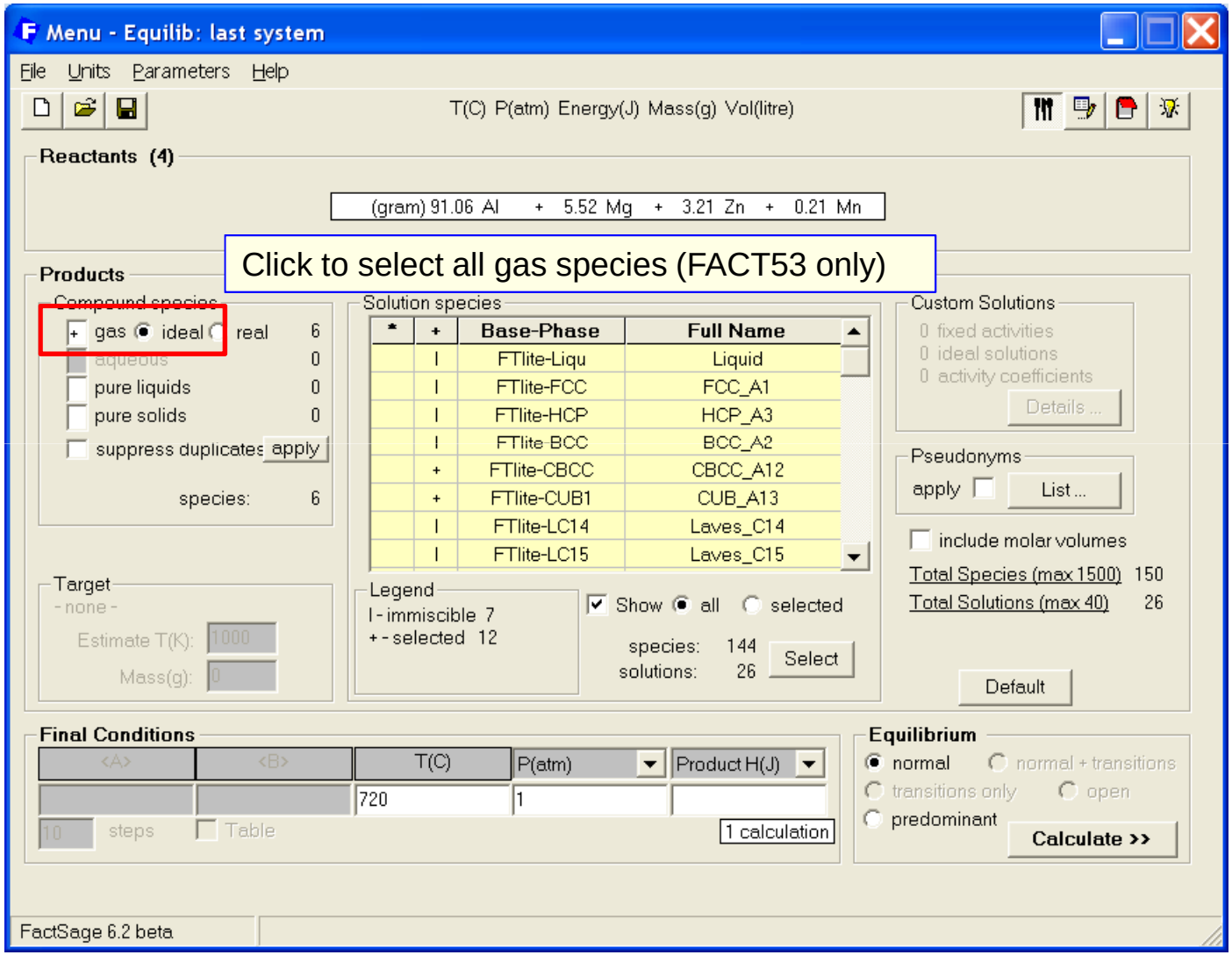
- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**



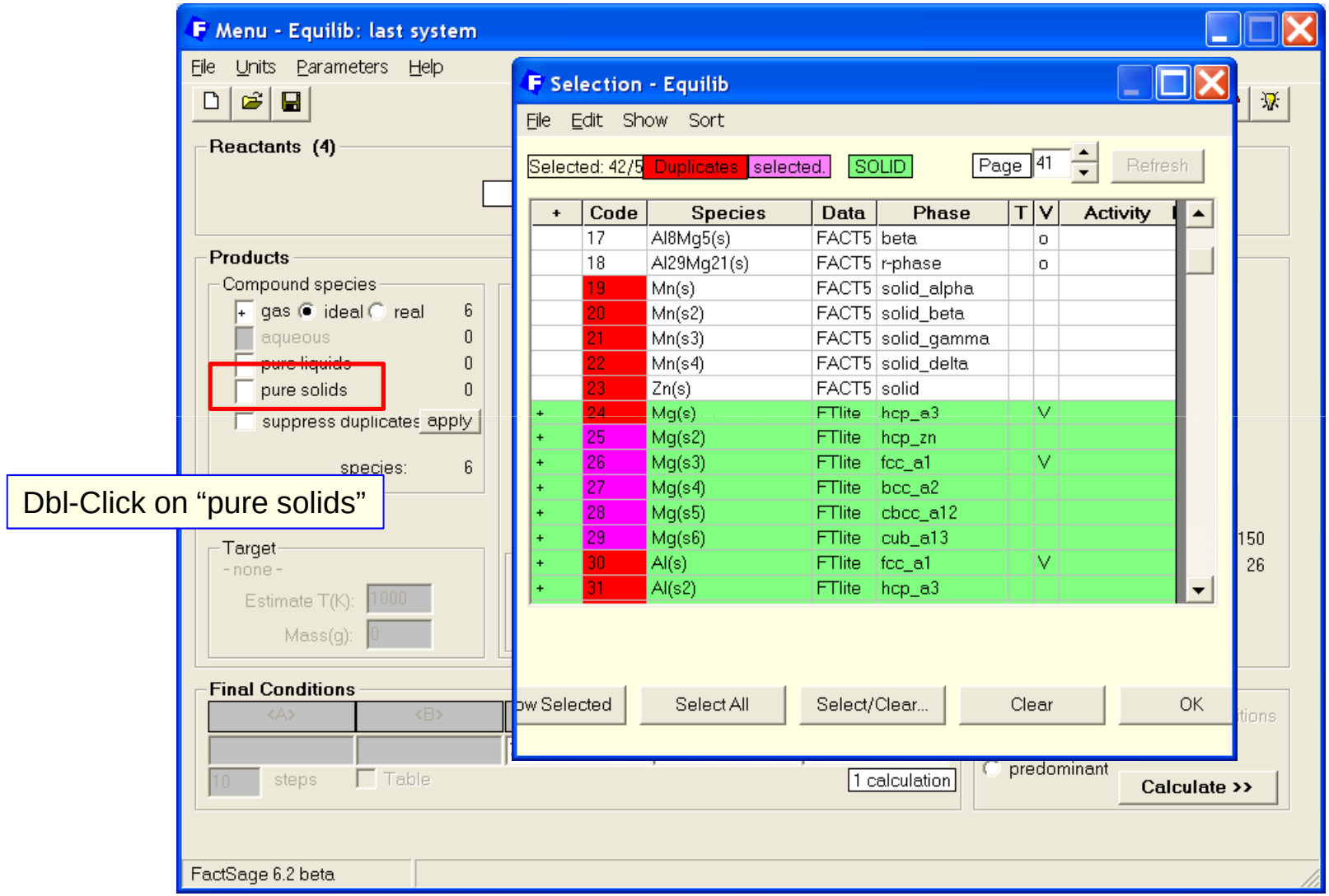
- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**



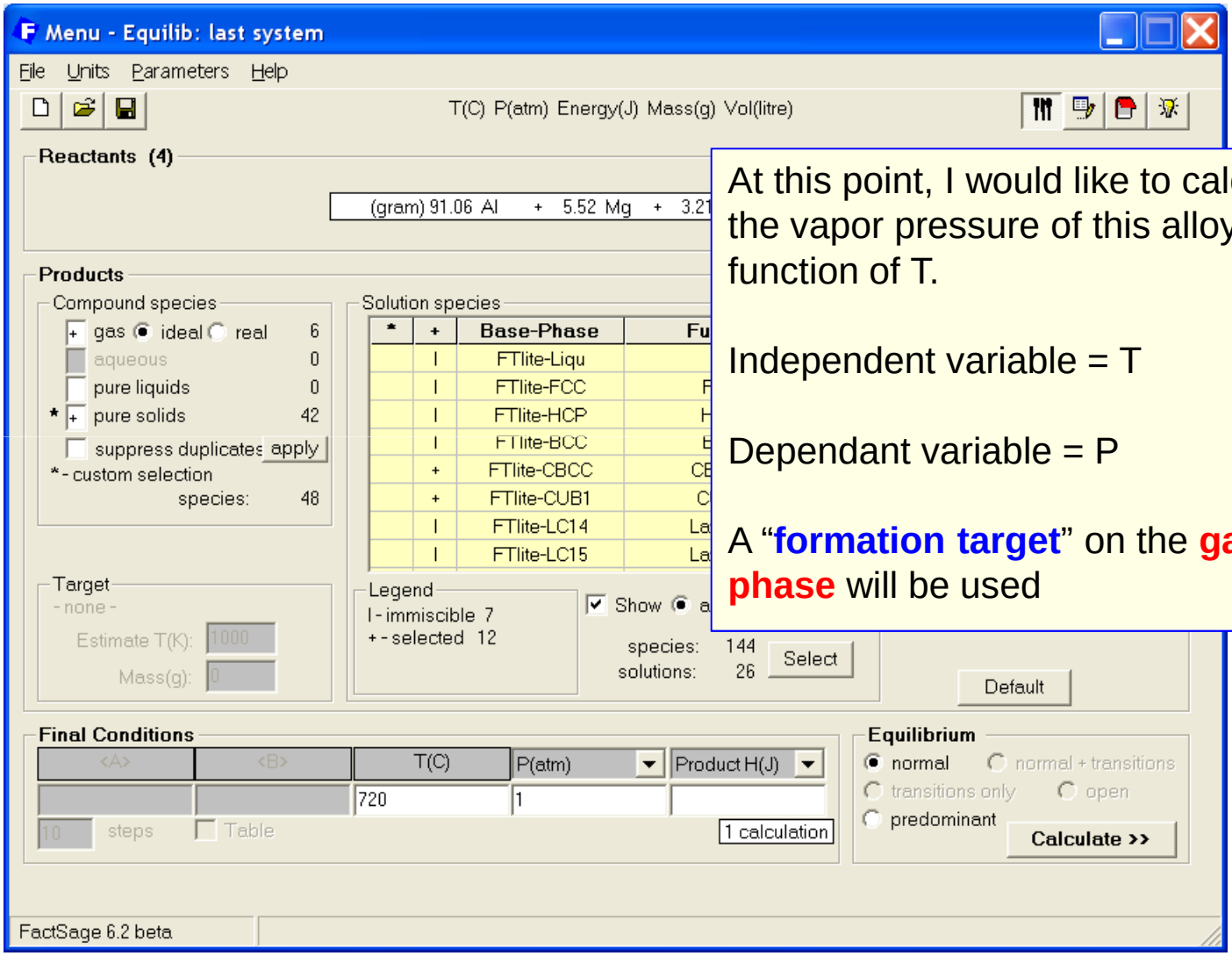
- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**



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



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



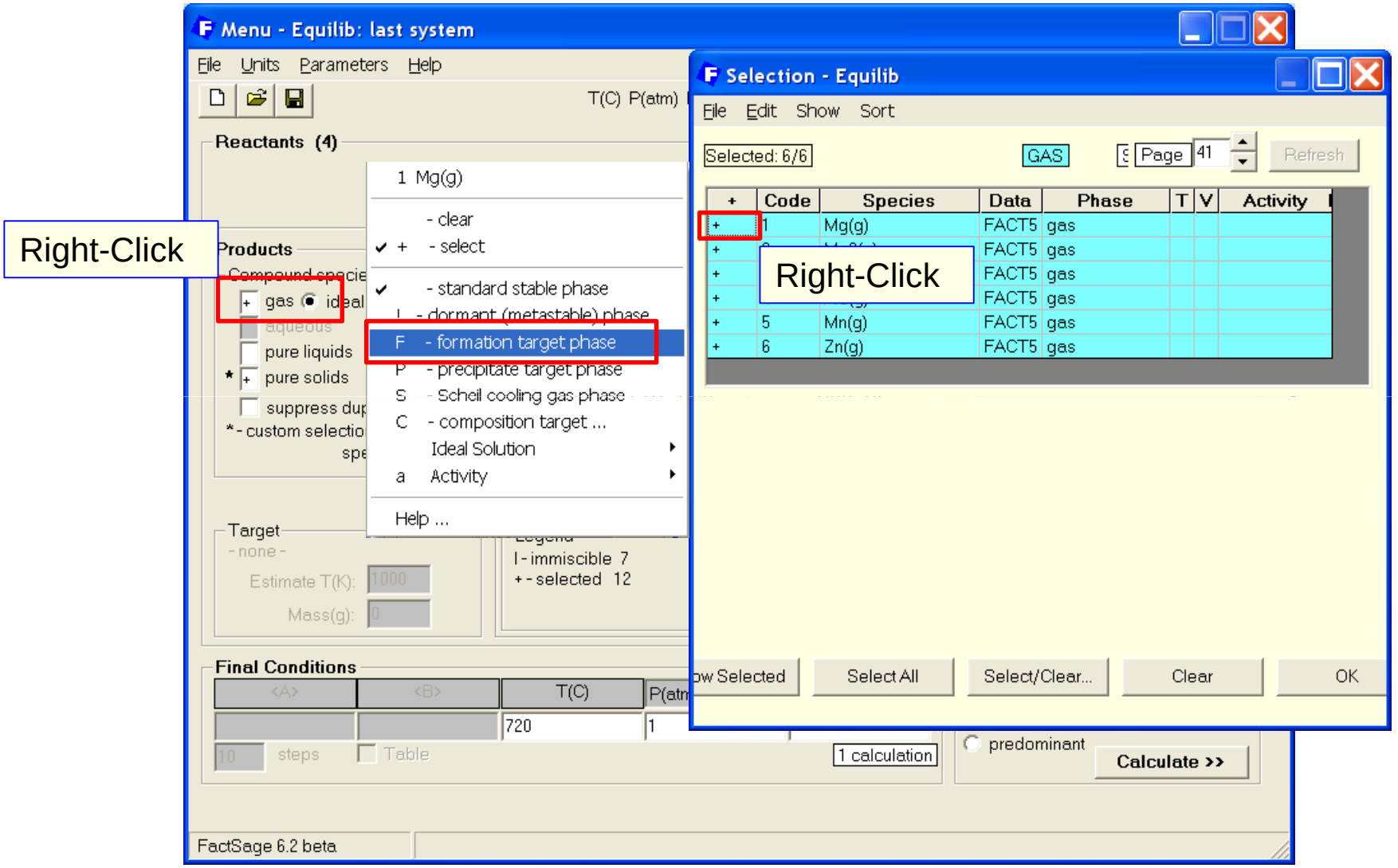
At this point, I would like to calculate the vapor pressure of this alloy as a function of T.

Independent variable = T

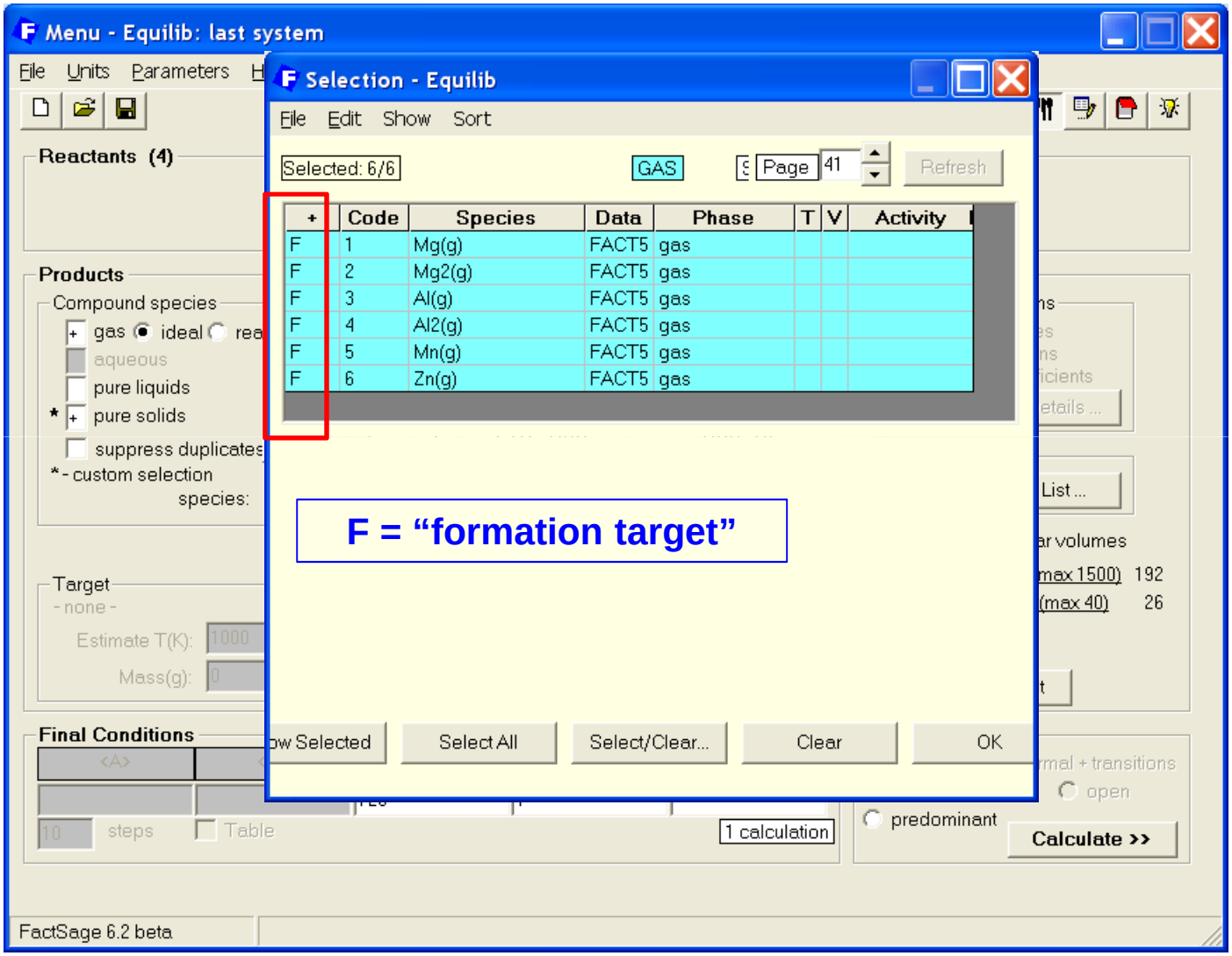
Dependant variable = P

A "**formation target**" on the **gas phase** will be used

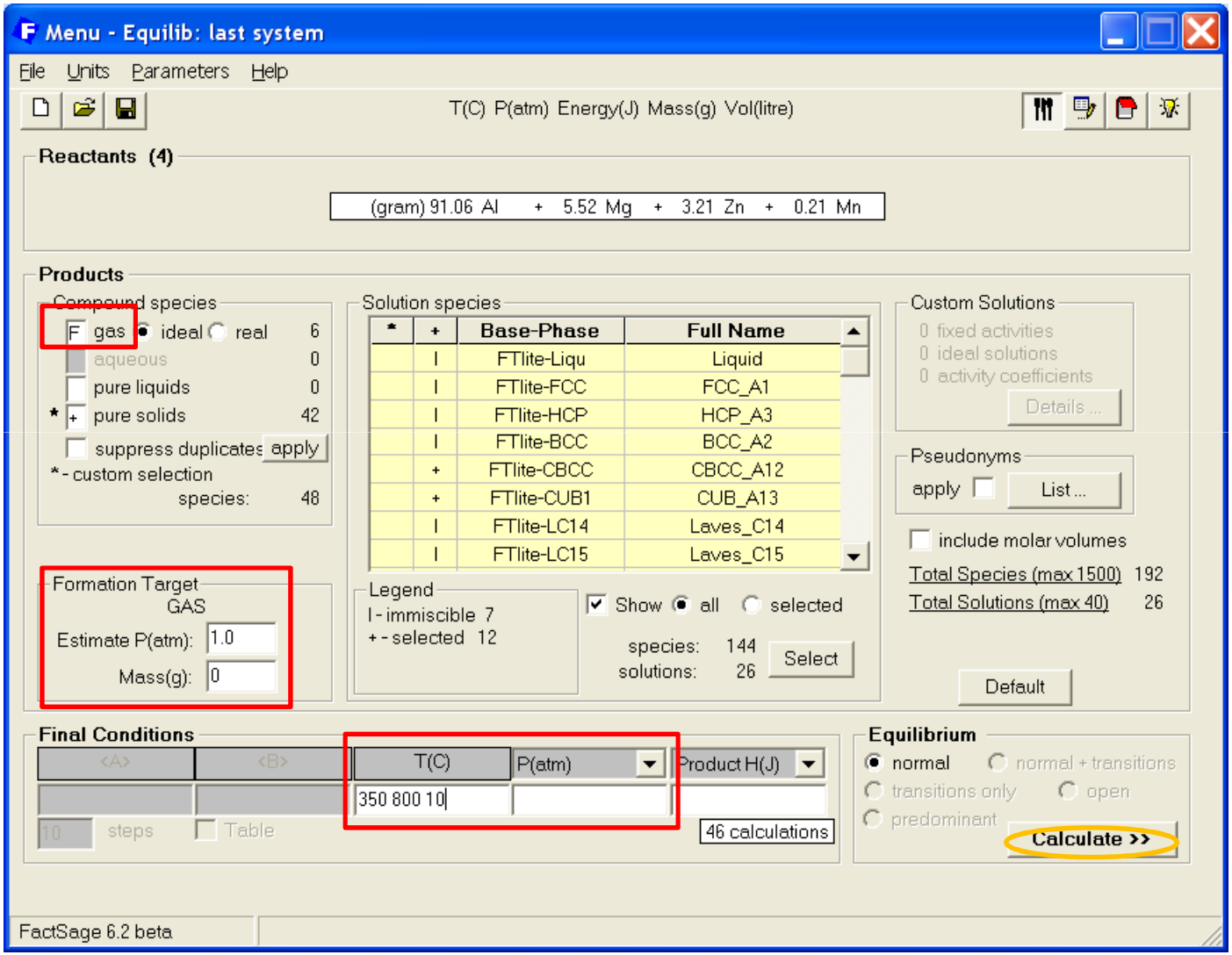
- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**



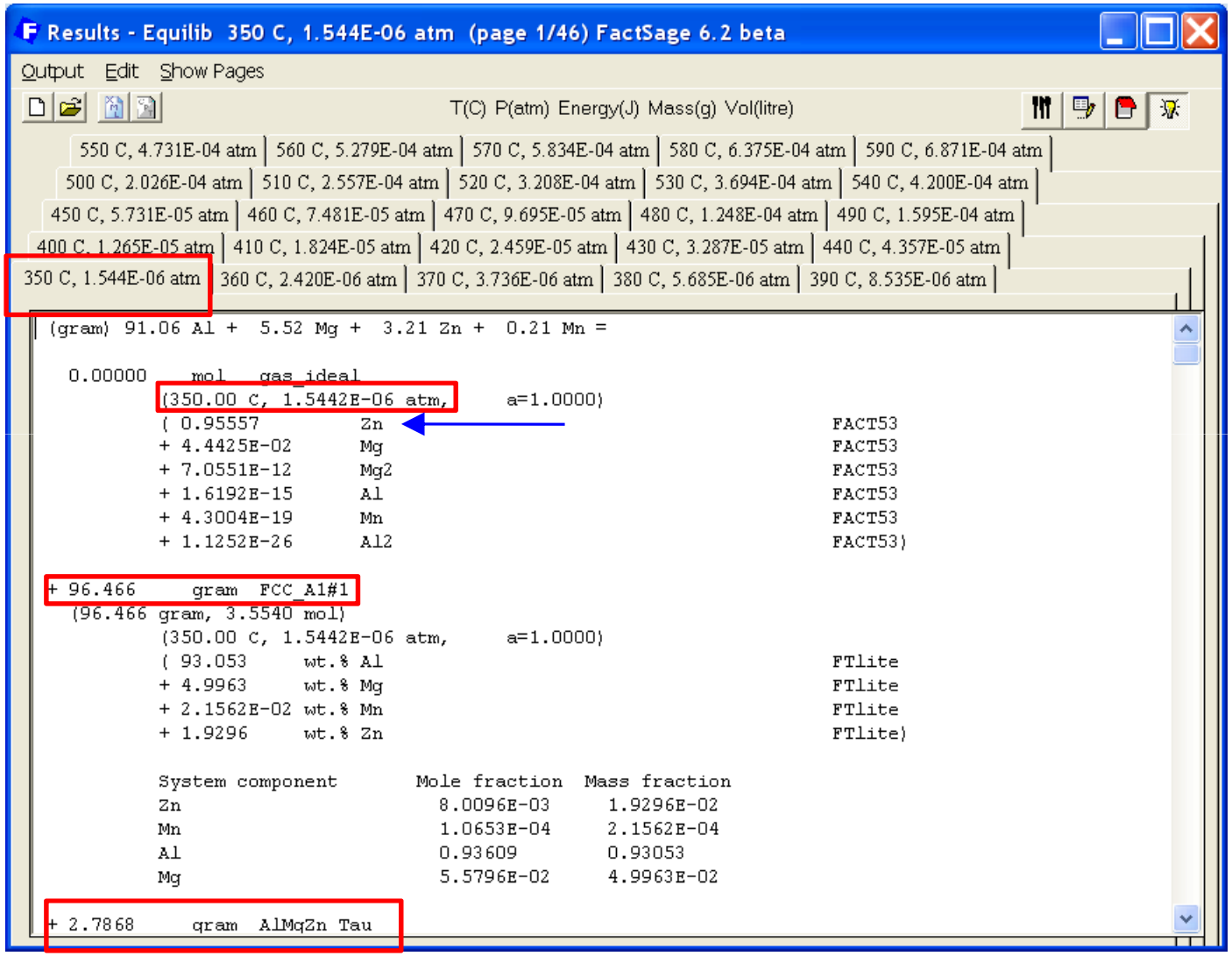
- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**



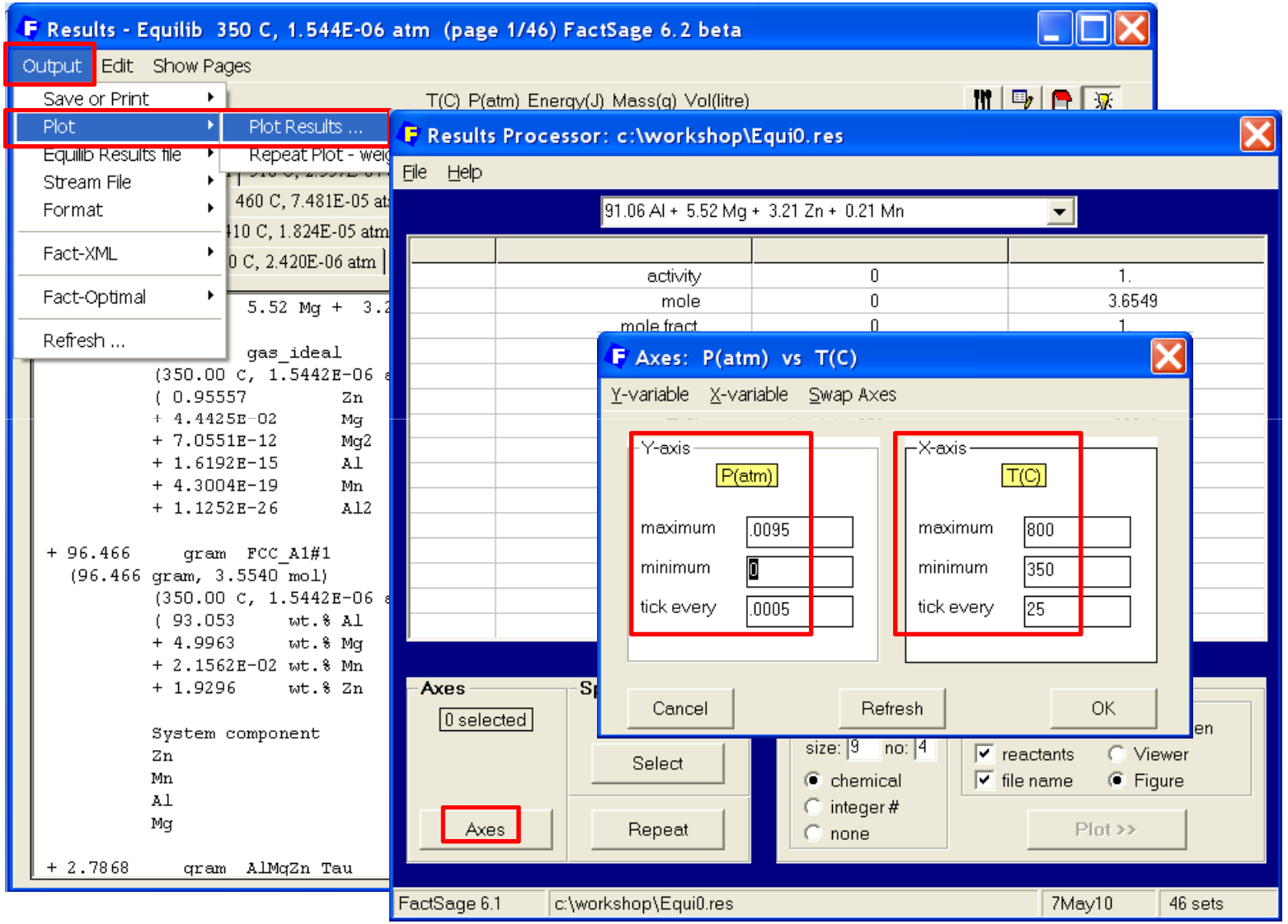
- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**



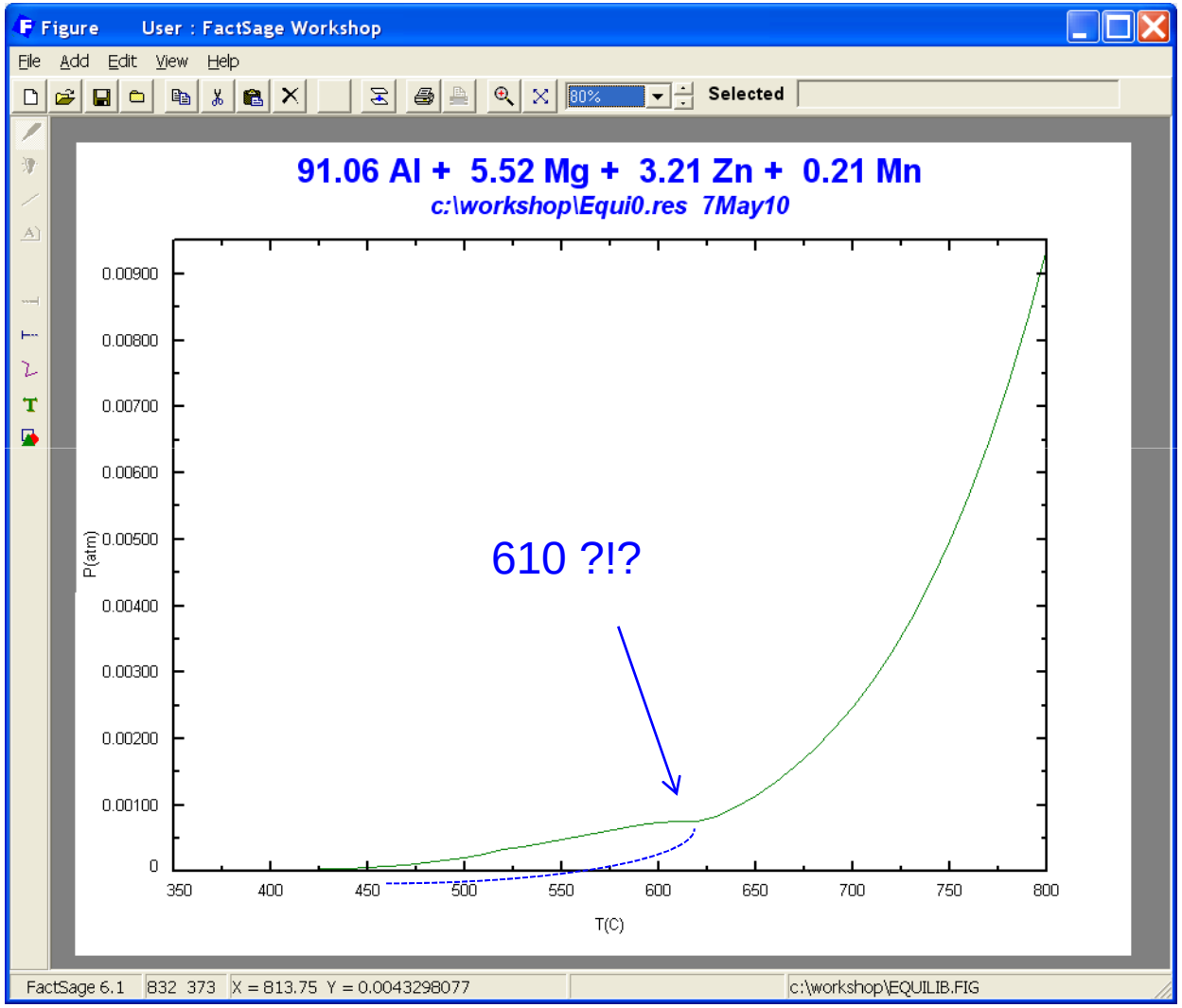
- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**



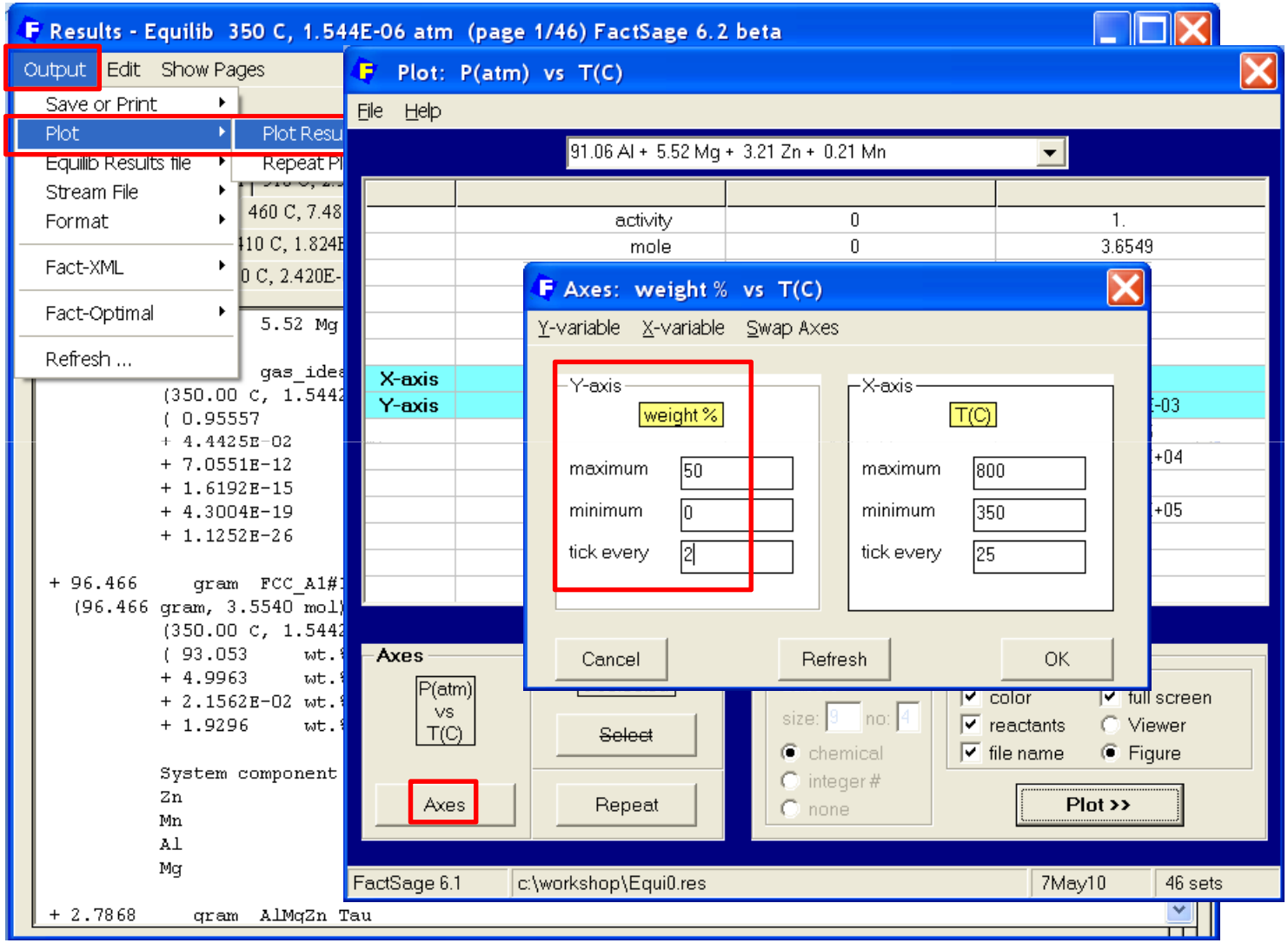
- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**



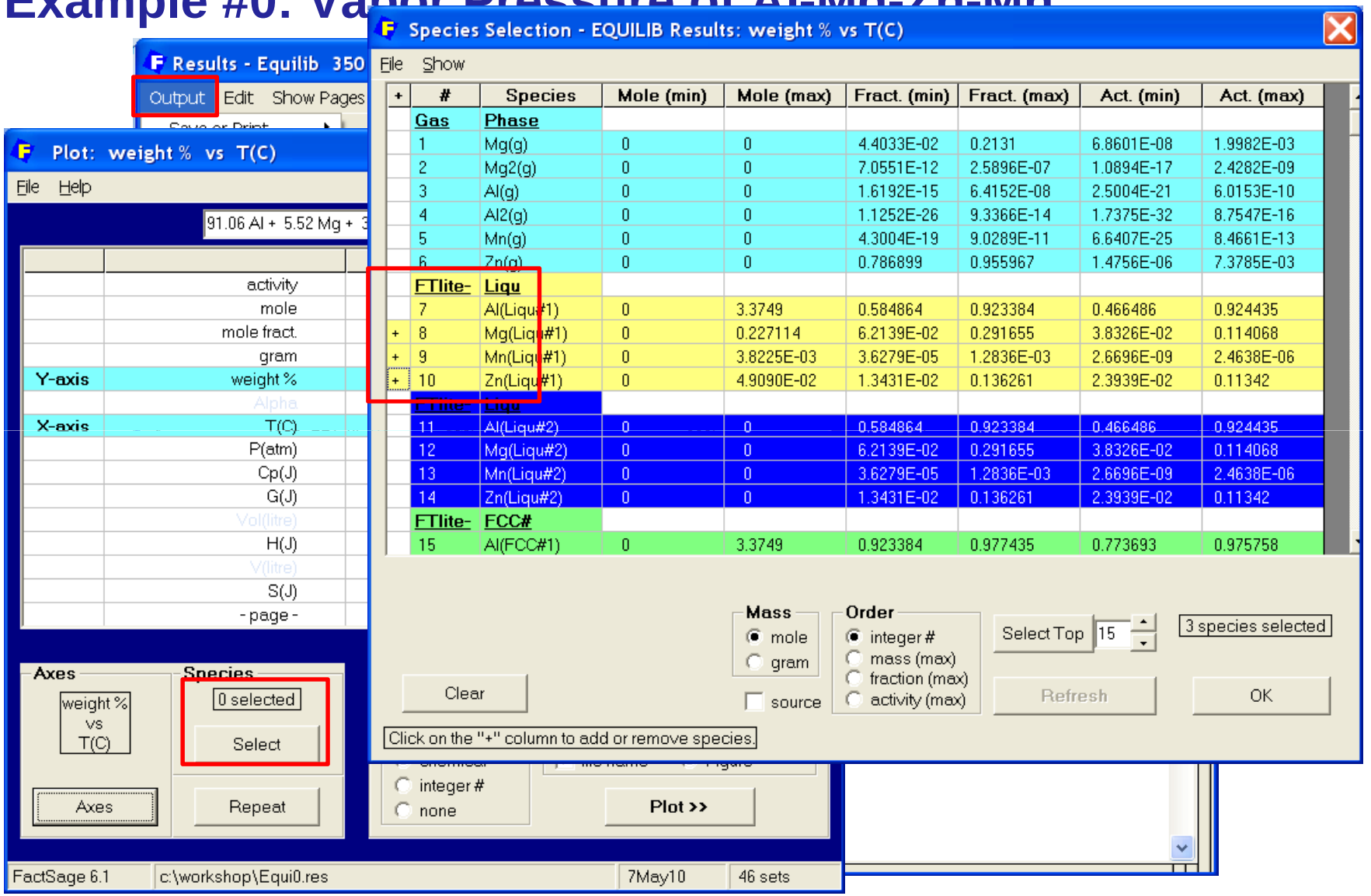
- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**



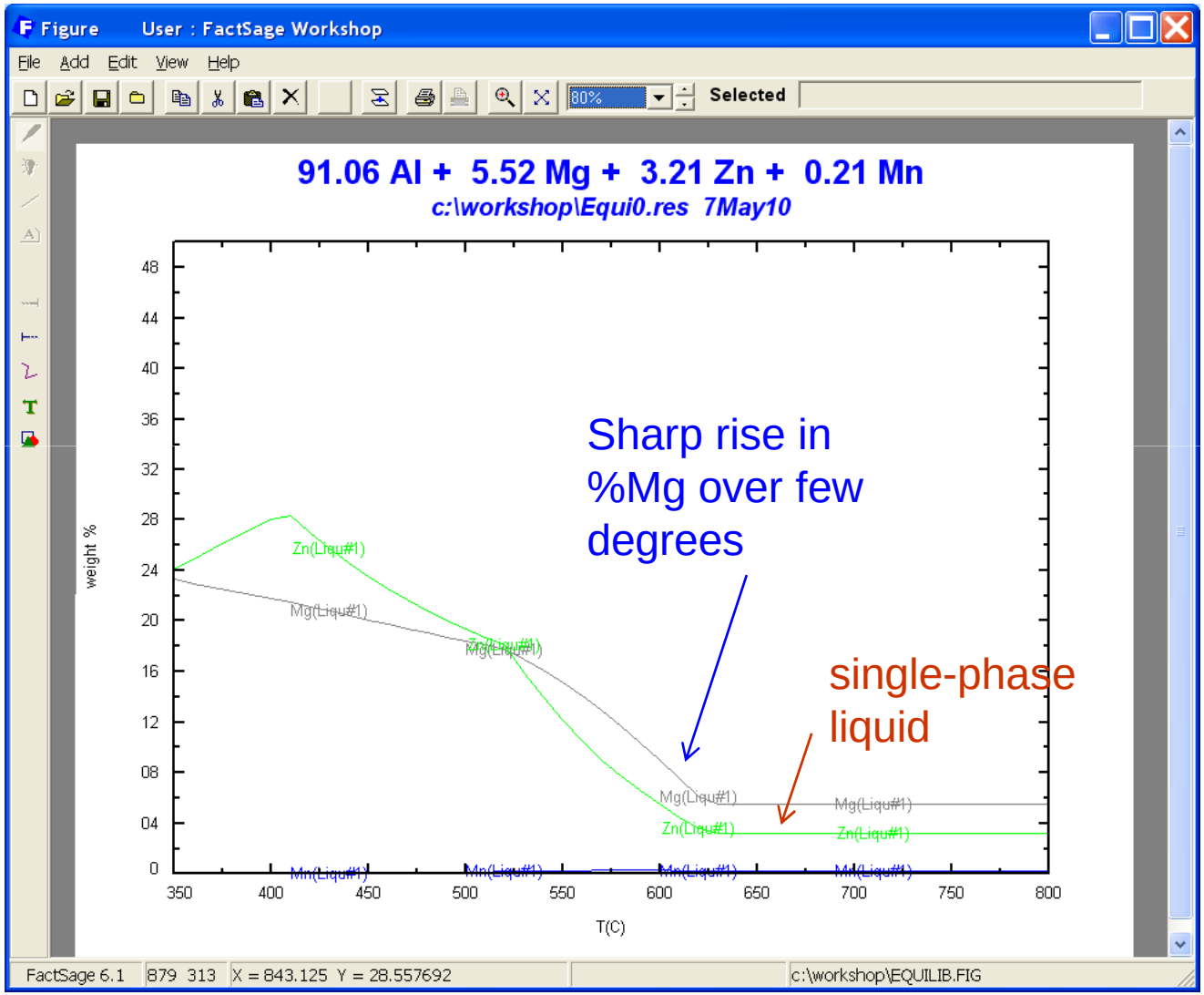
- **Example #0: Vapor Pressure of Al-Mg-Zn-Mn**



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



- **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-$MnCl_2$

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

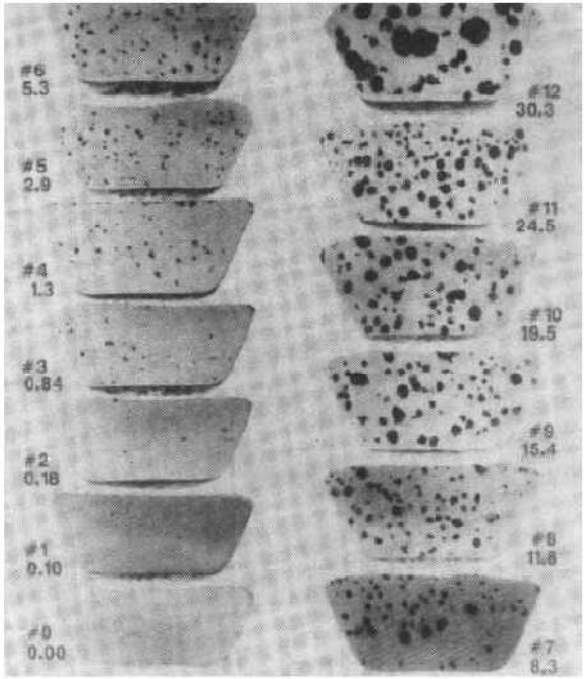
Solubility of H_2 in Liquid Alloys

$$2Al + 3H_2O \rightarrow Al_2O_3 + 3H_2$$

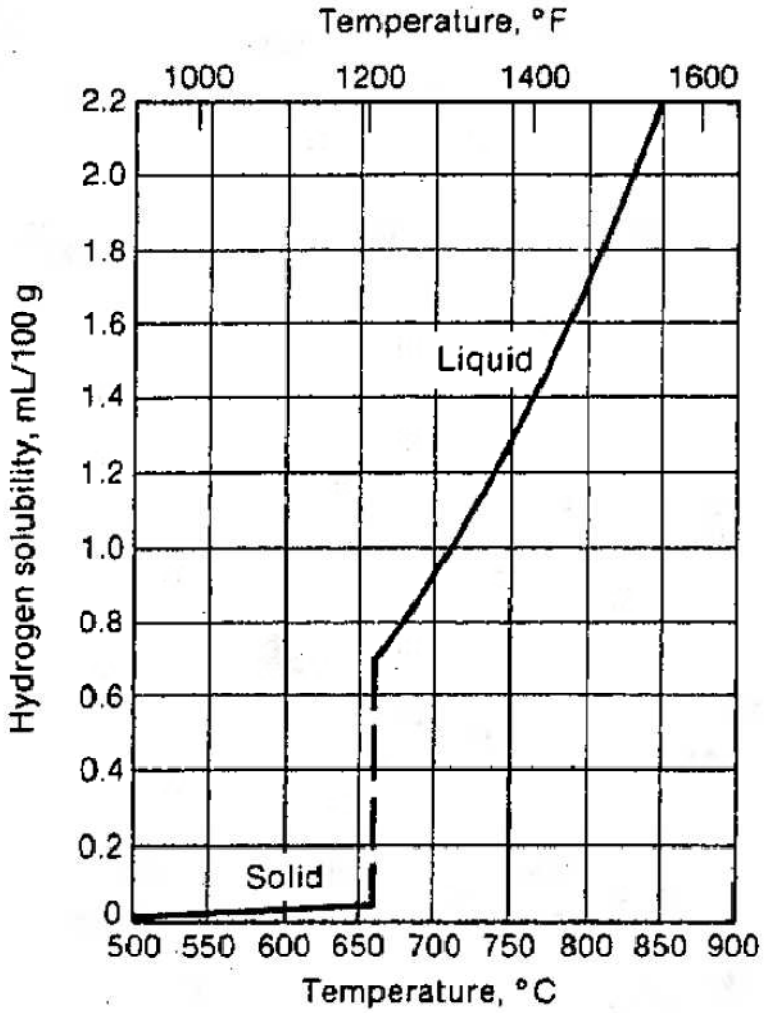
$$Mg + H_2O \rightarrow MgO + H_2$$

$$\tfrac{1}{2}H_2 \leftrightarrow \underline{H}$$

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



Porosity in Al alloys as a function of the H_2-solubility in mL/100 g



- **Example #1: Solubility of hydrogen (H_2) in liquid alloys**

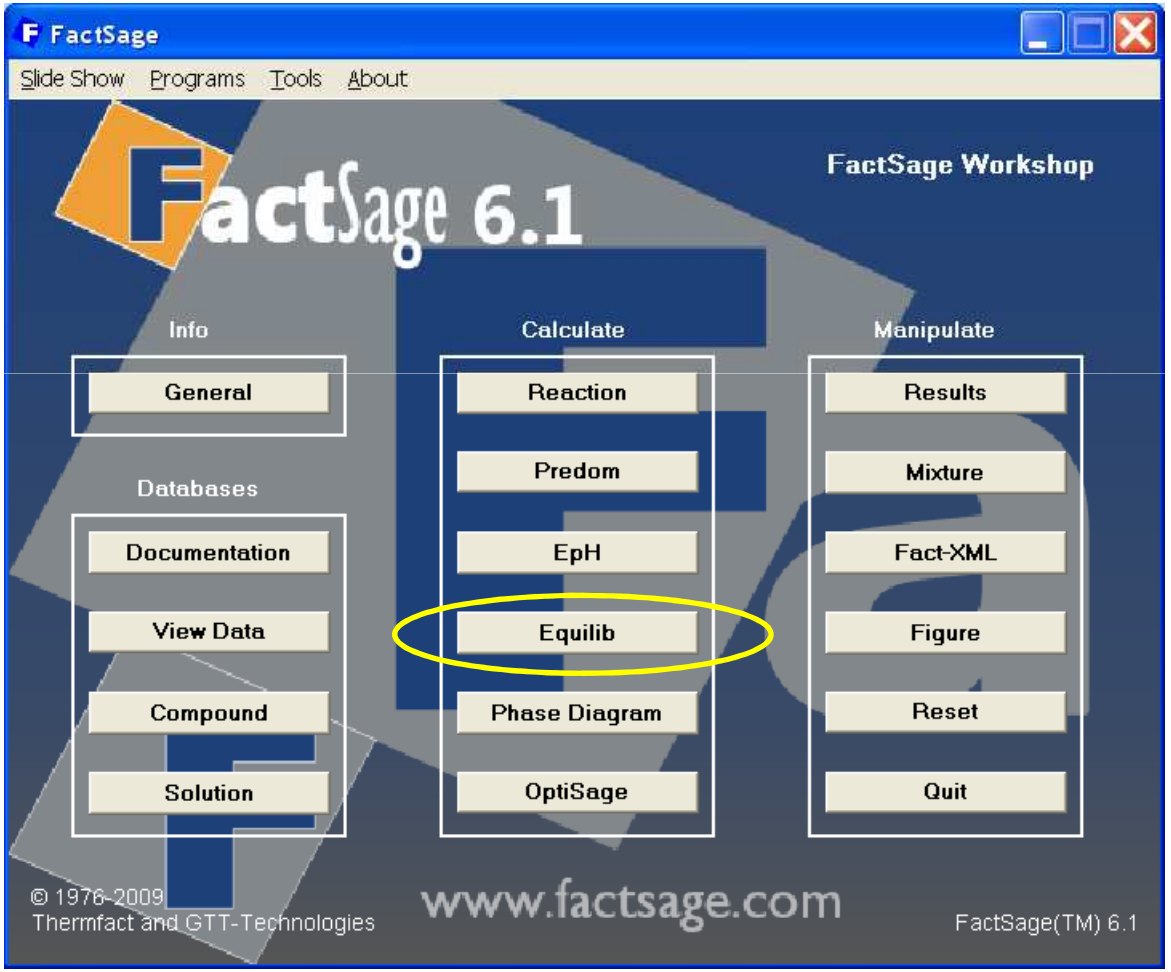
  a) Mg alloys : AZ91 @ fixed $P(H_2)$

9% Al

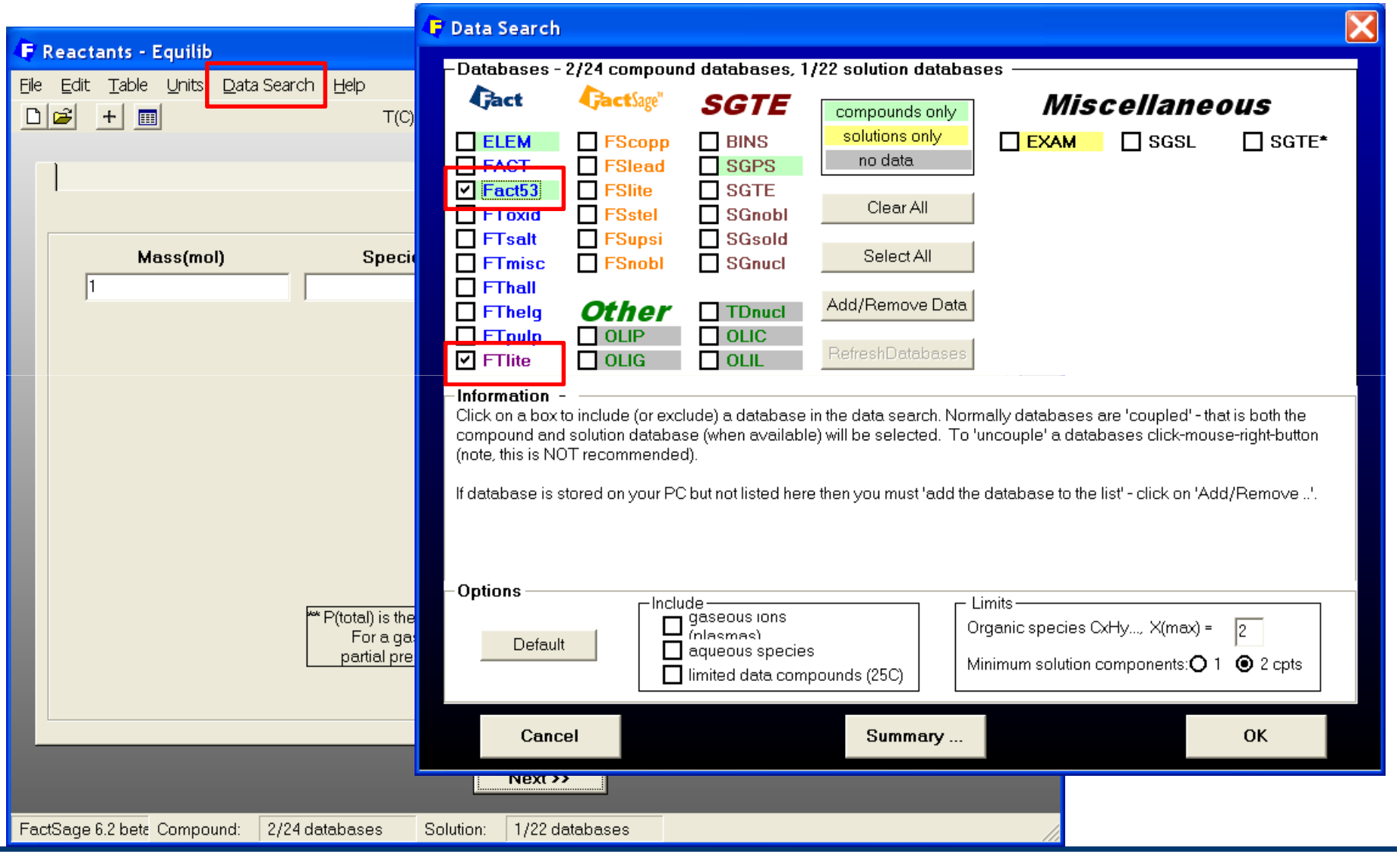
1% Zn

Bal. Mg

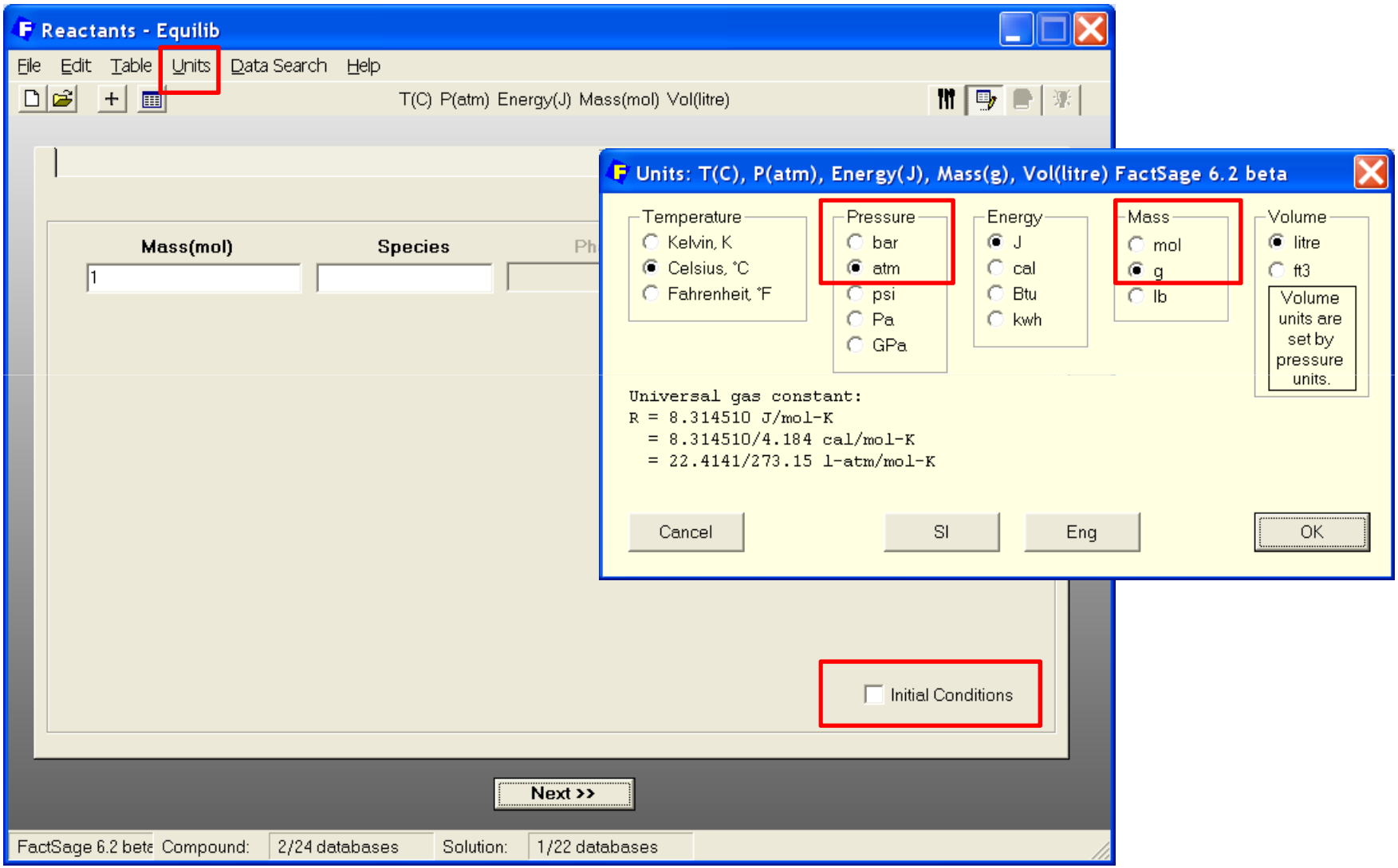
700°C



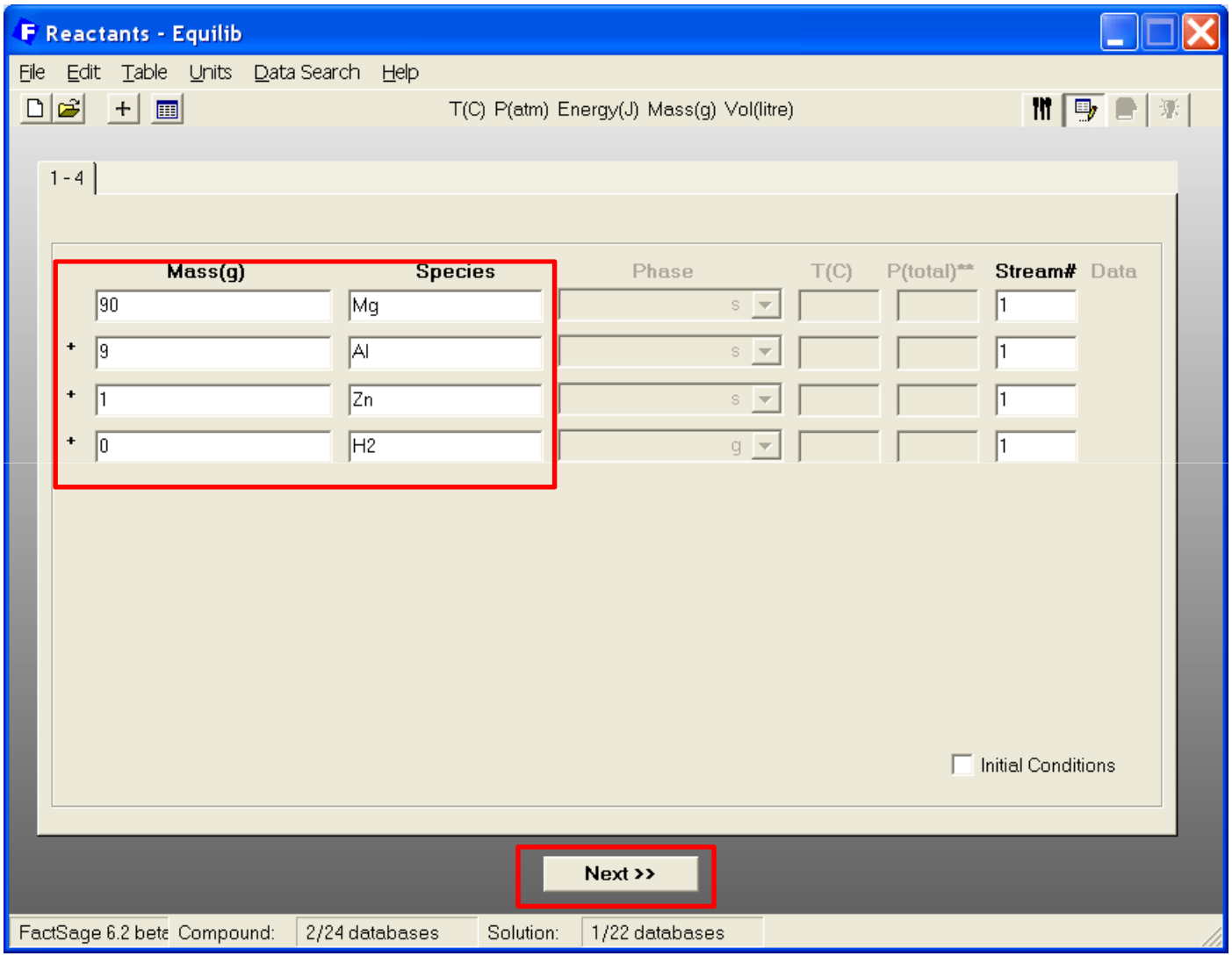
- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



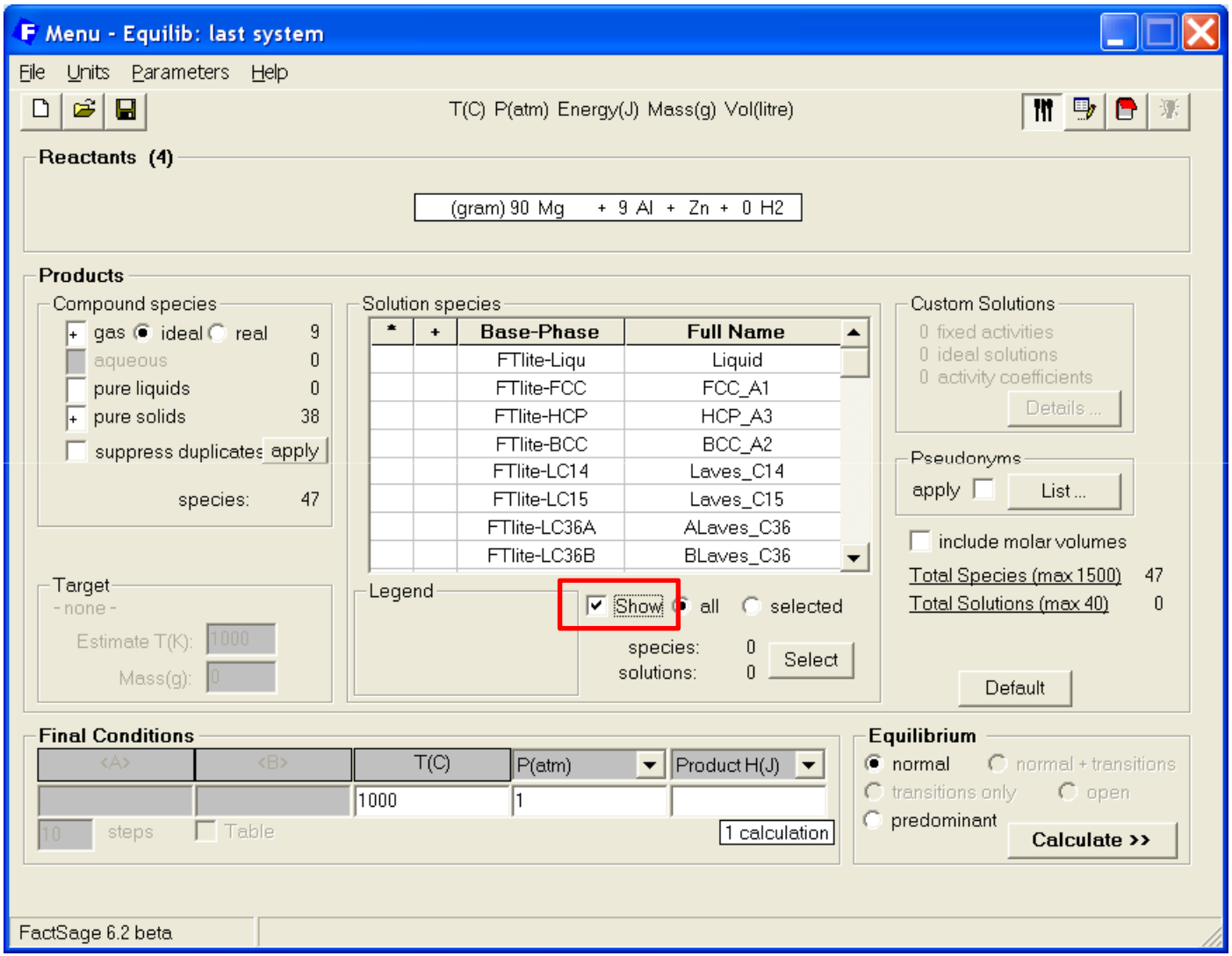
- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



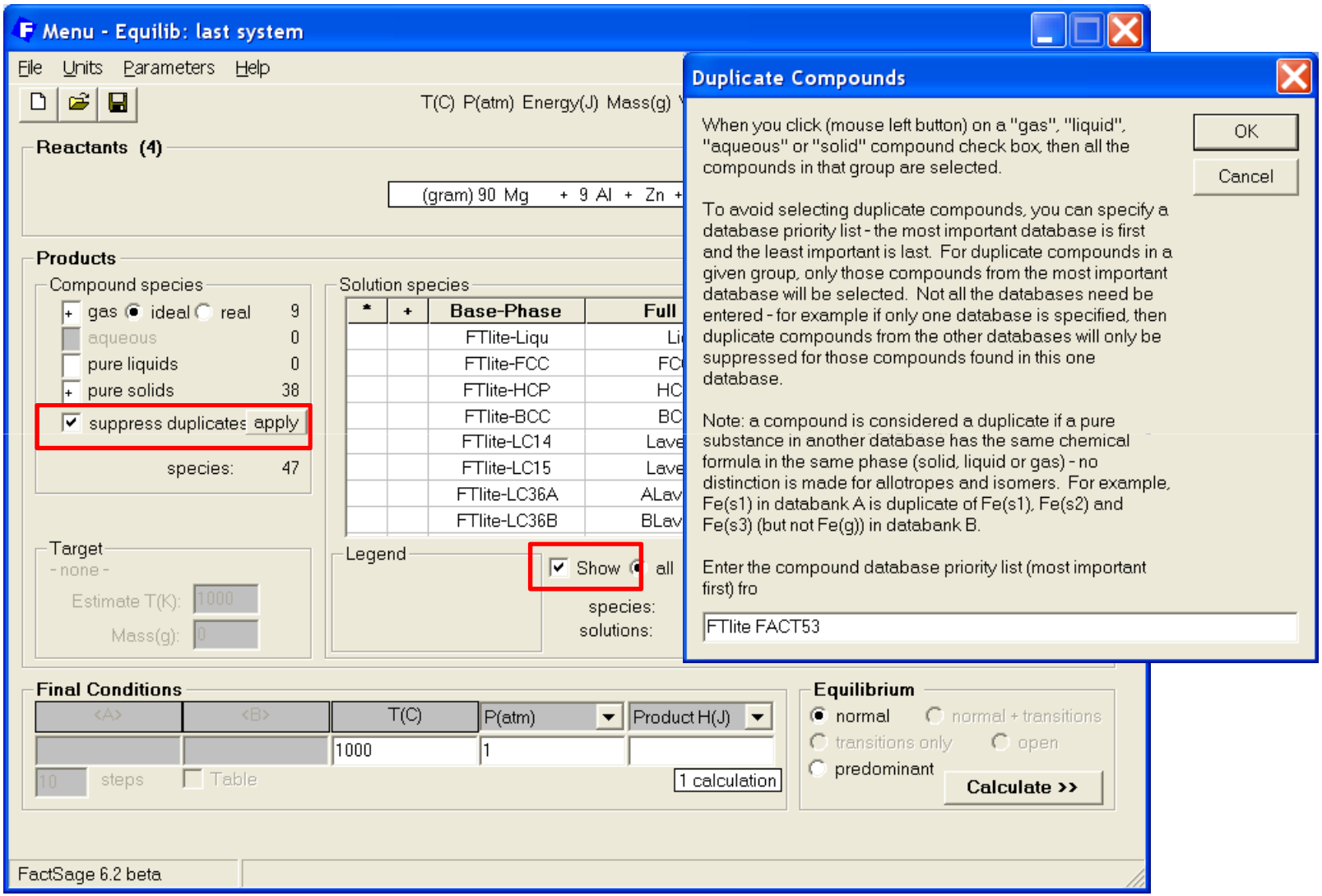
- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



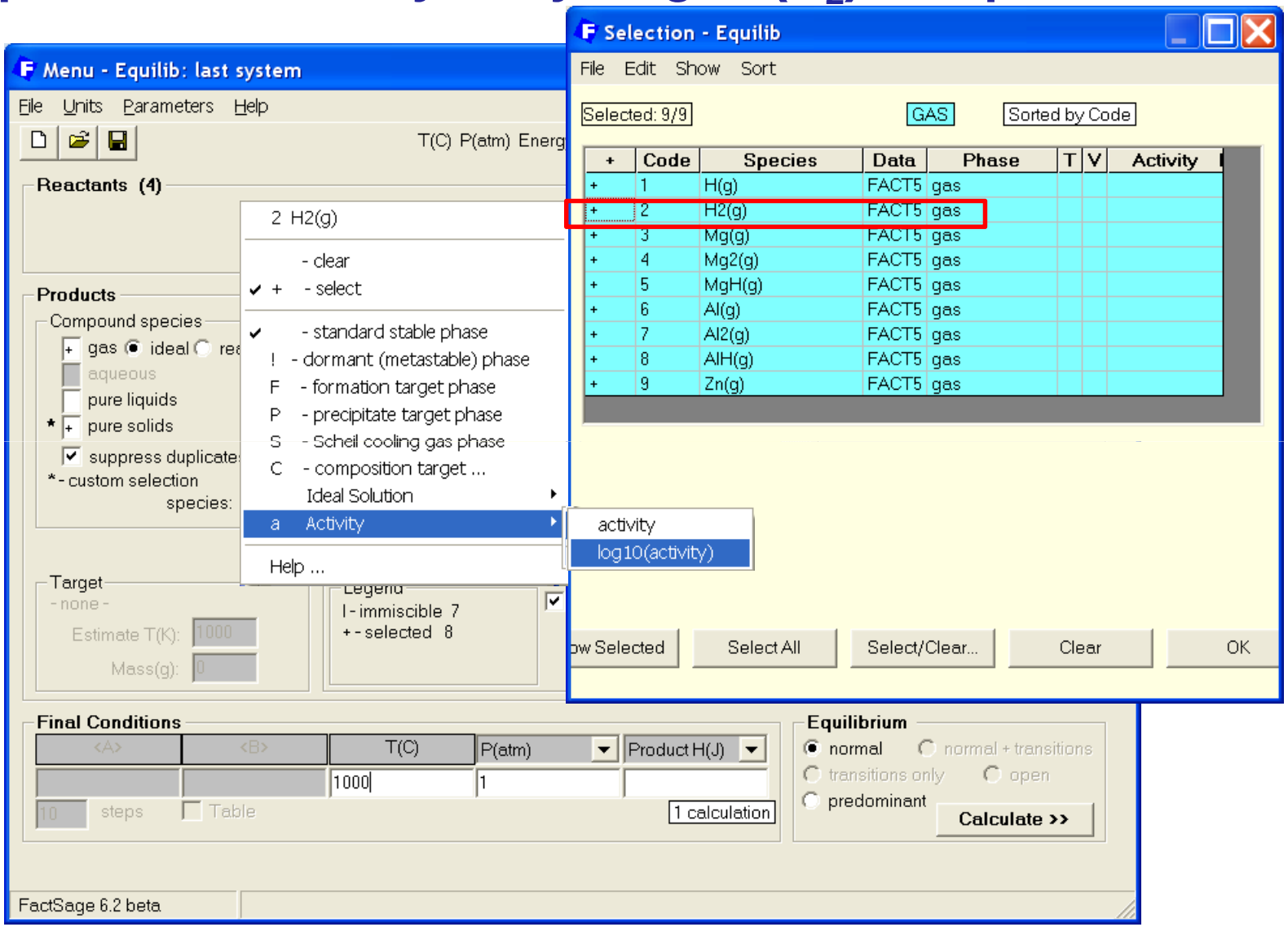
- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



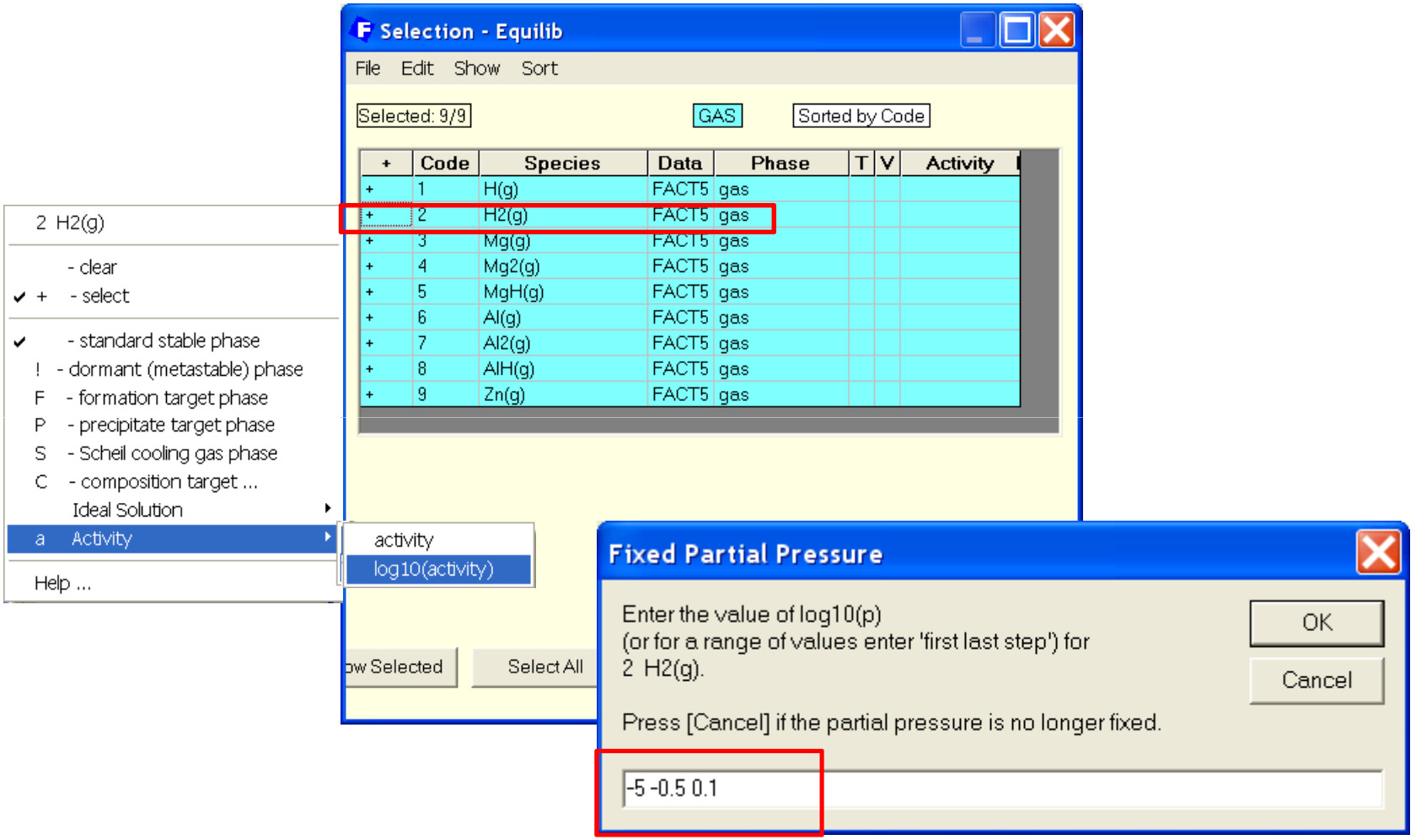
- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**

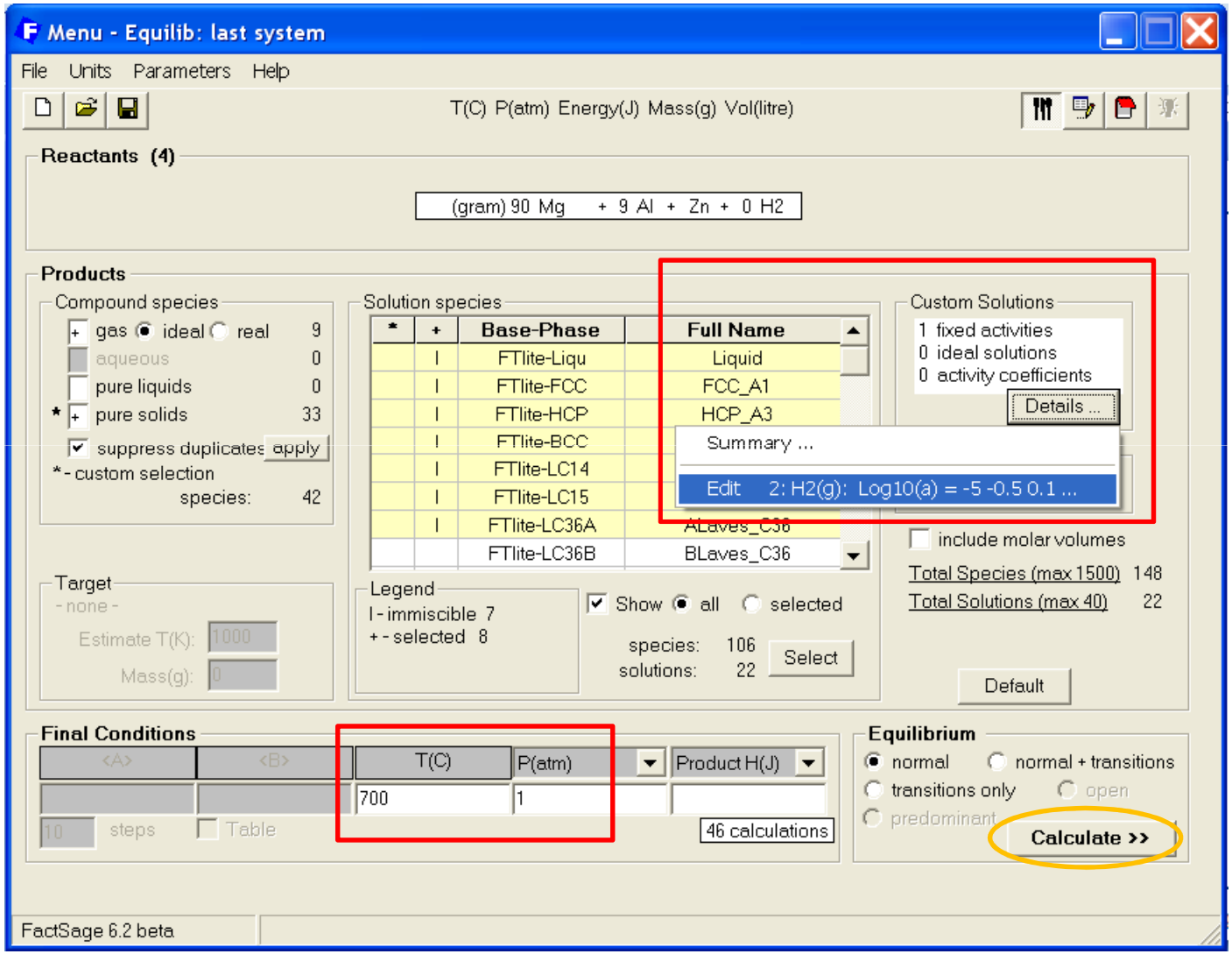


- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**

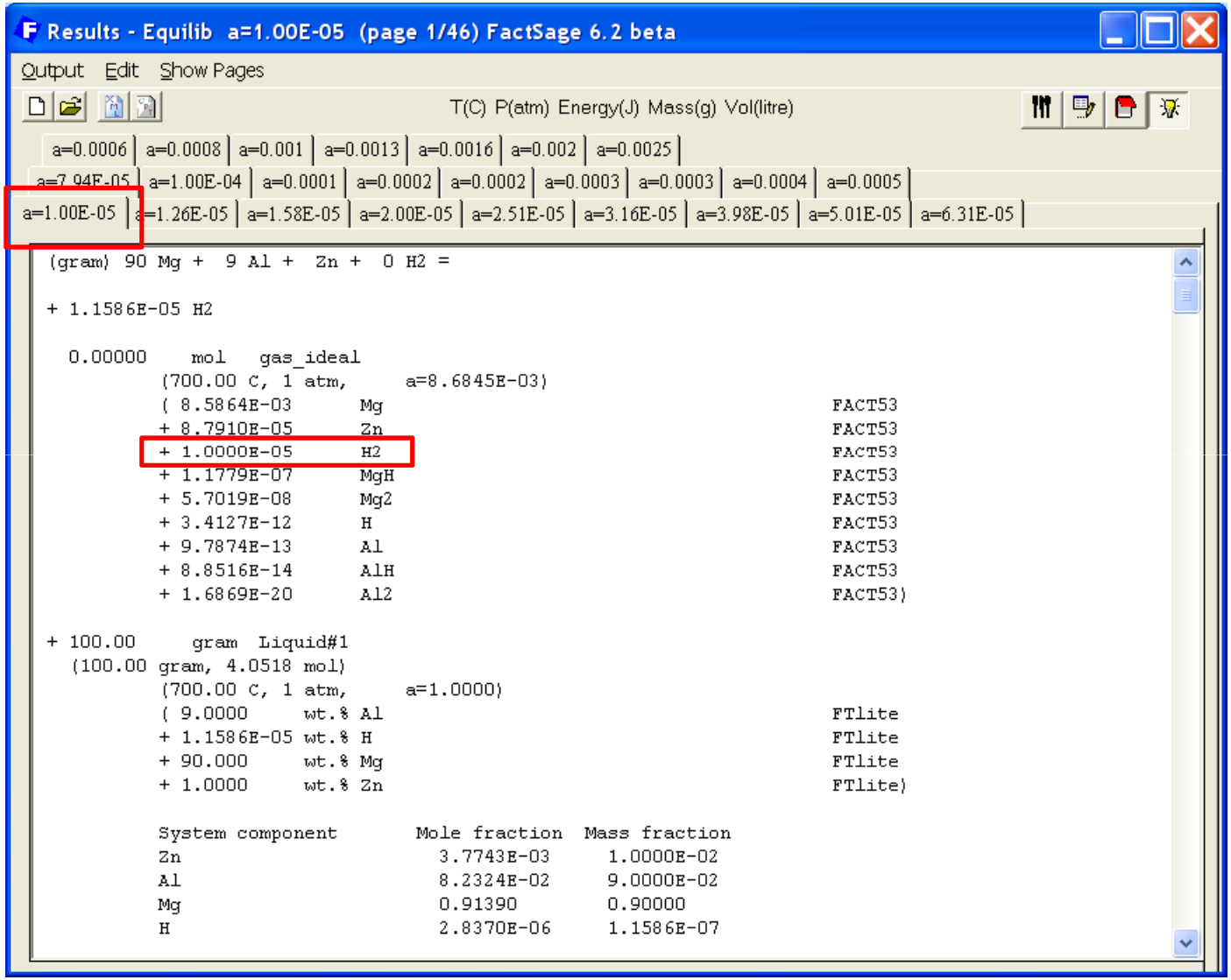


$-5 < \log_{10}P(H_2) < -0.5$ by step of 0.1

- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



- **Example #1a: Solubility of hydrogen (H_2) 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
```

- **Example #1a: Solubility of hydrogen (H_2) 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)

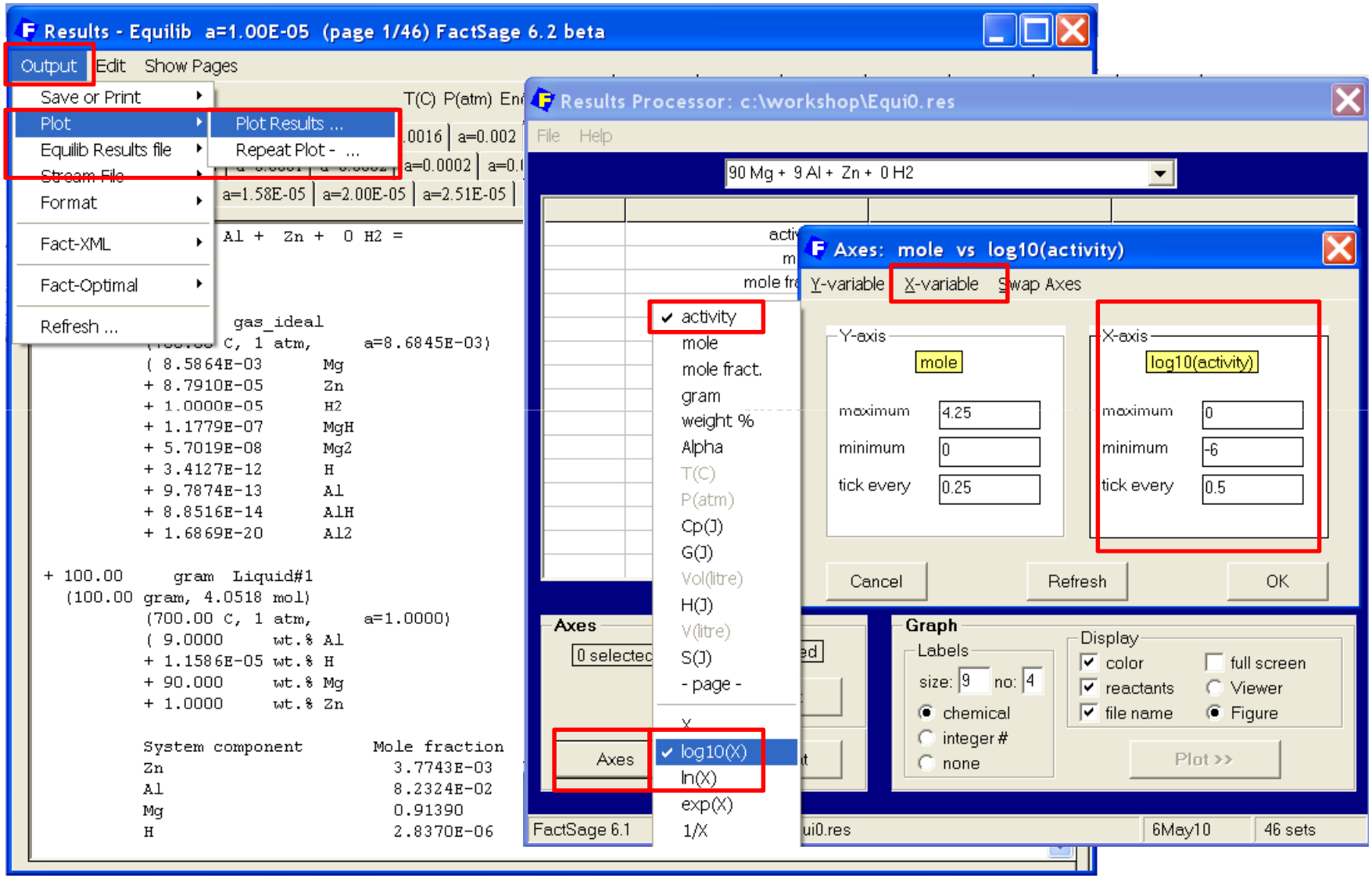
a=0.0006 | a=0.0008 | a=0.001 | a=0.0013 | a=0.0016 | a=0.002 | a=0.0025

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

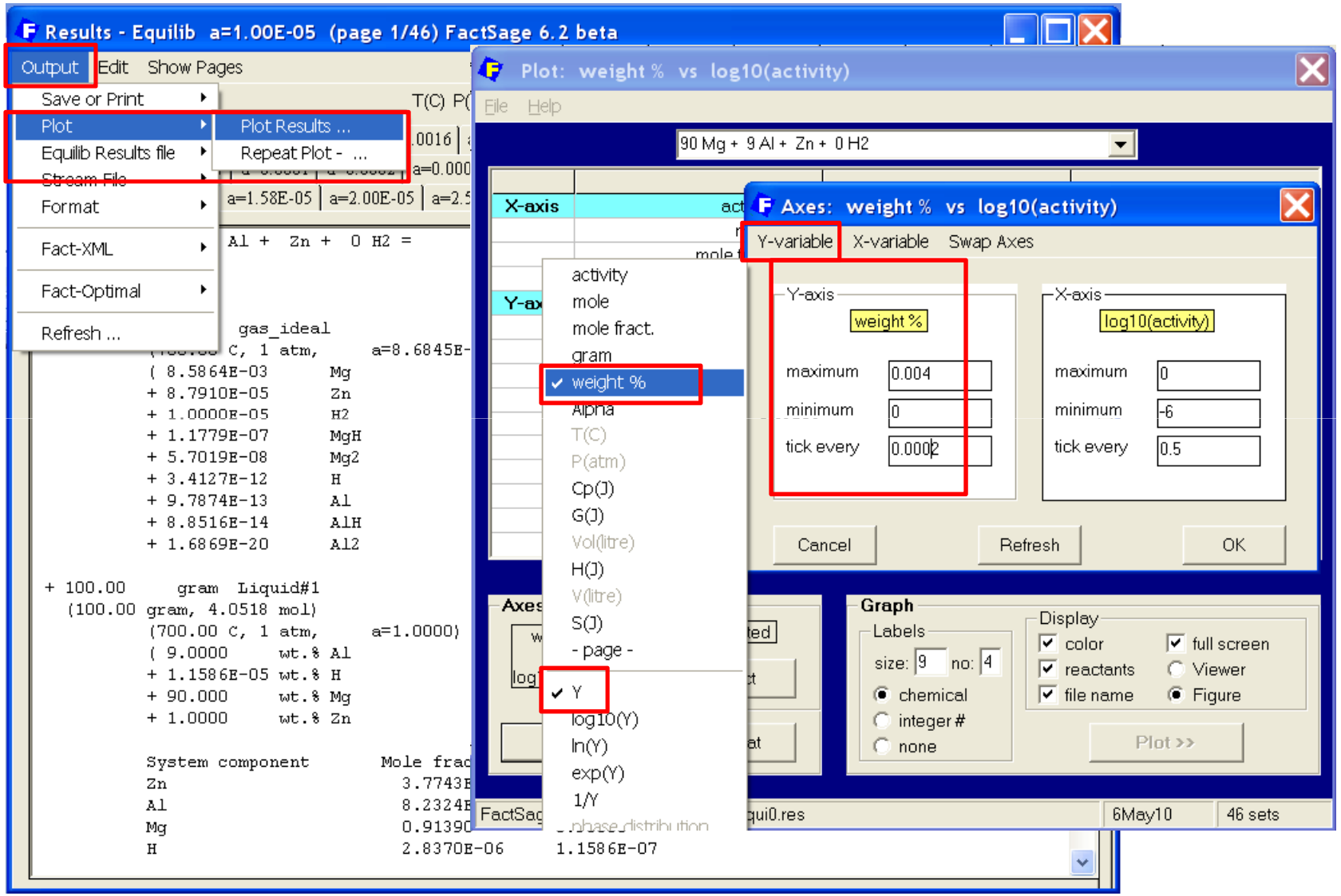
a=1.00E-05 | a=1.26E-05 | a=1.58E-05 | a=2.00E-05 | a=2.51E-05 | a=3.16E-05 | a=3.98E-05 | a=5.01E-05 | a=6.31E-05

```
(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
```

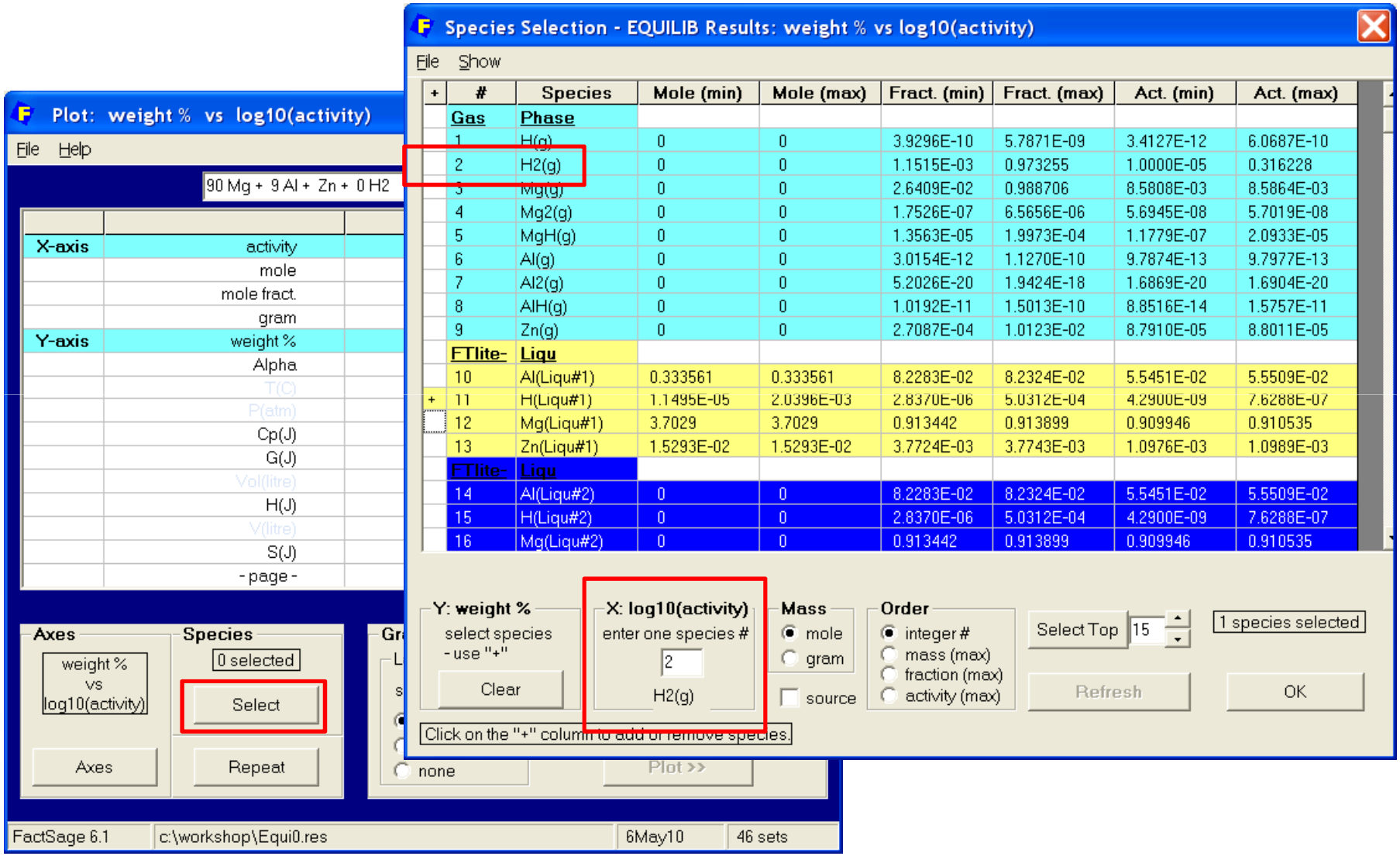
- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



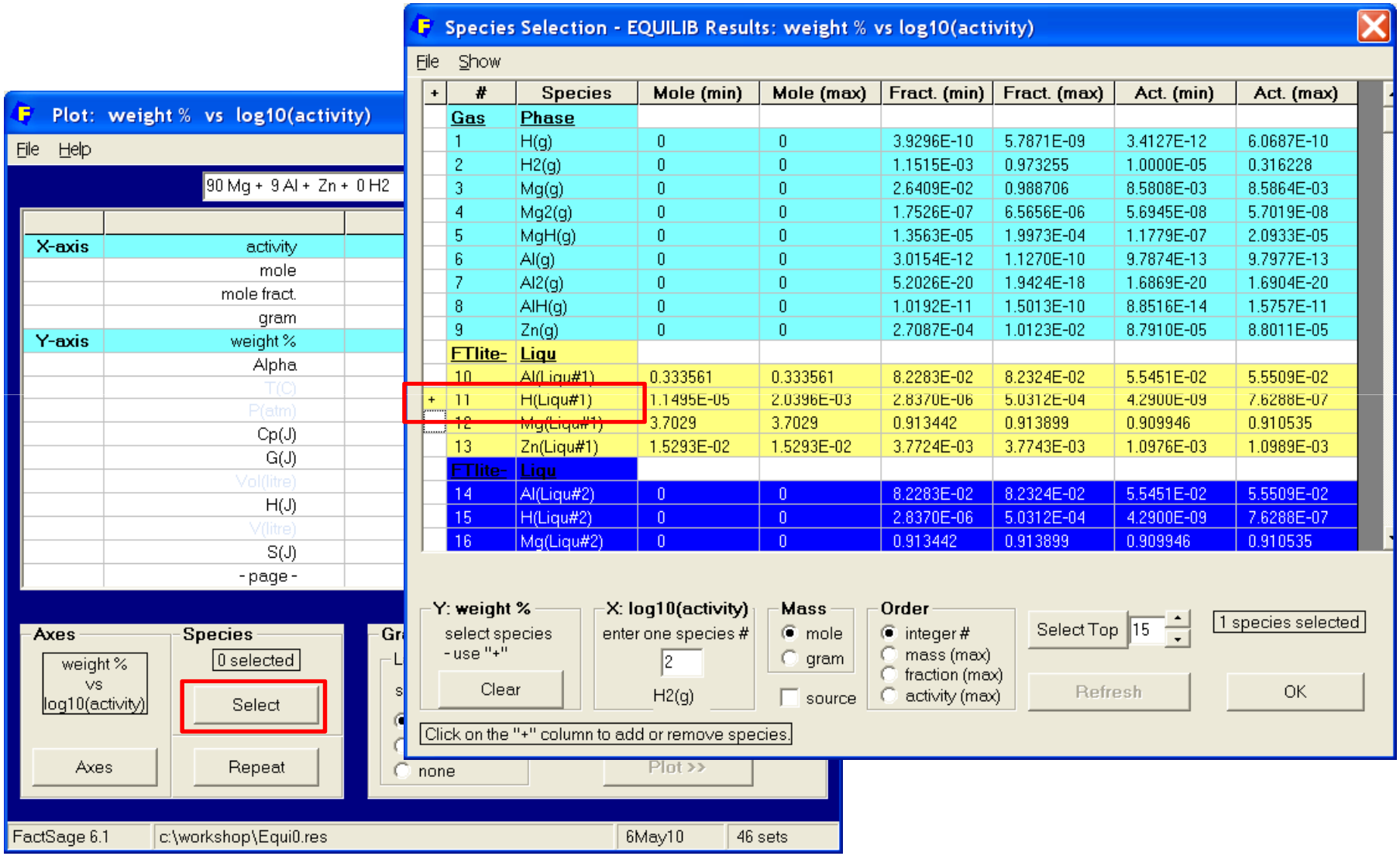
- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



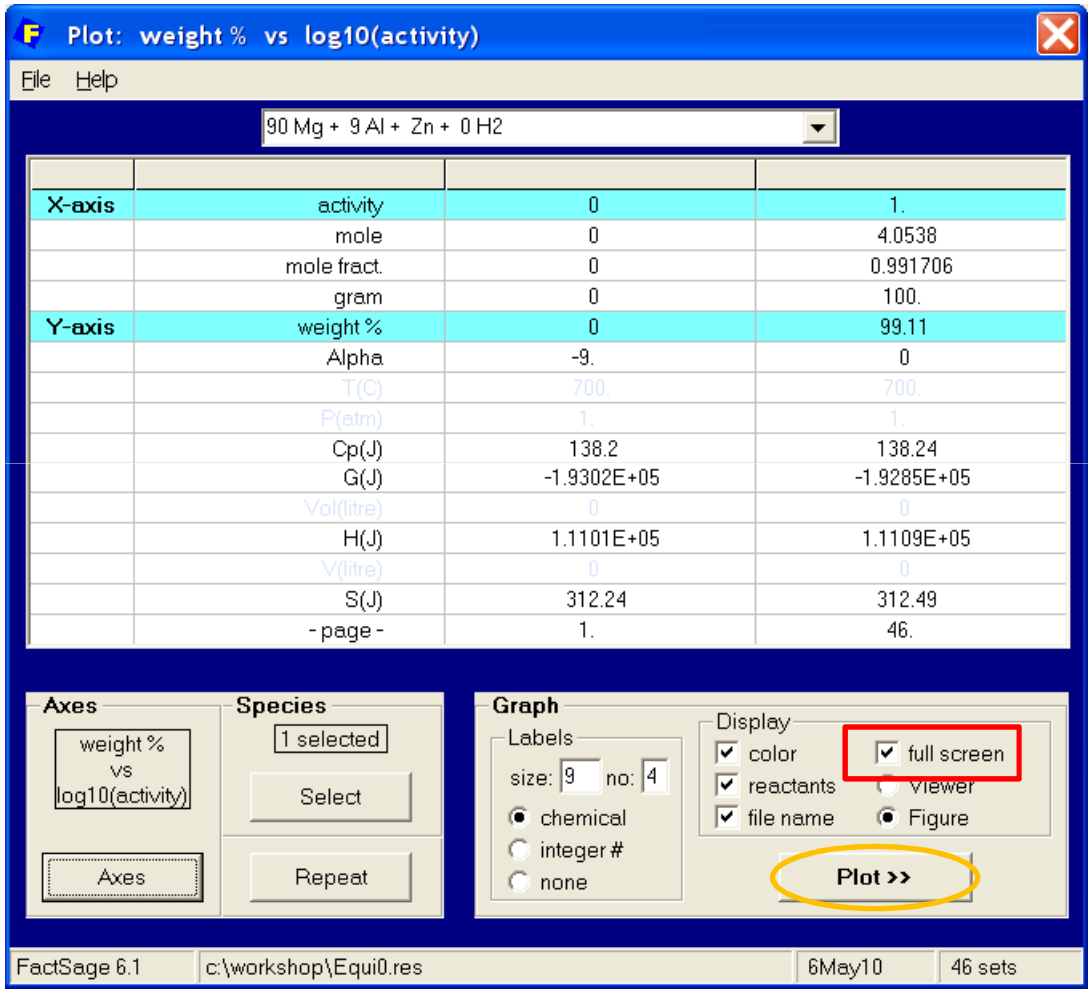
- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



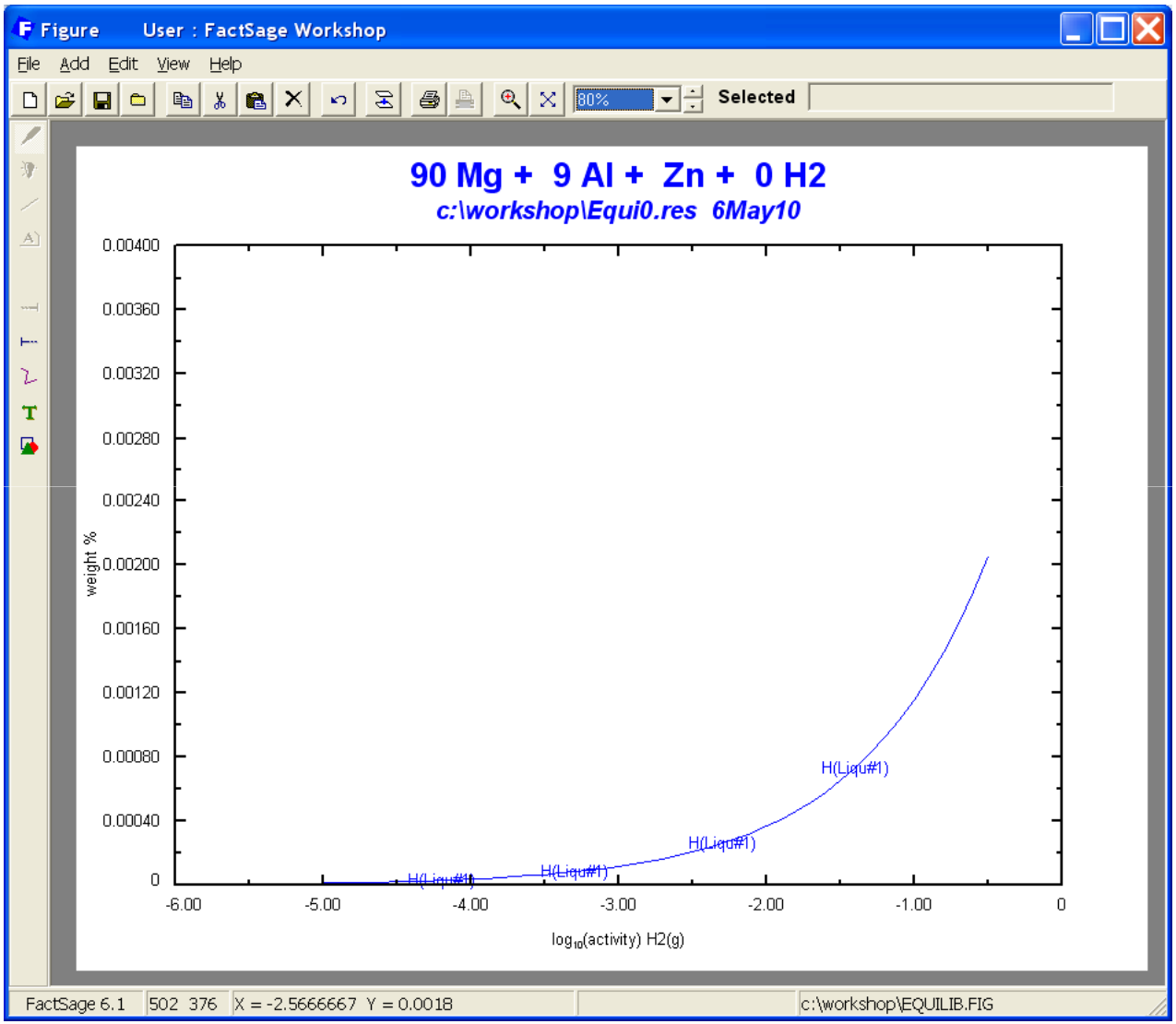
- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



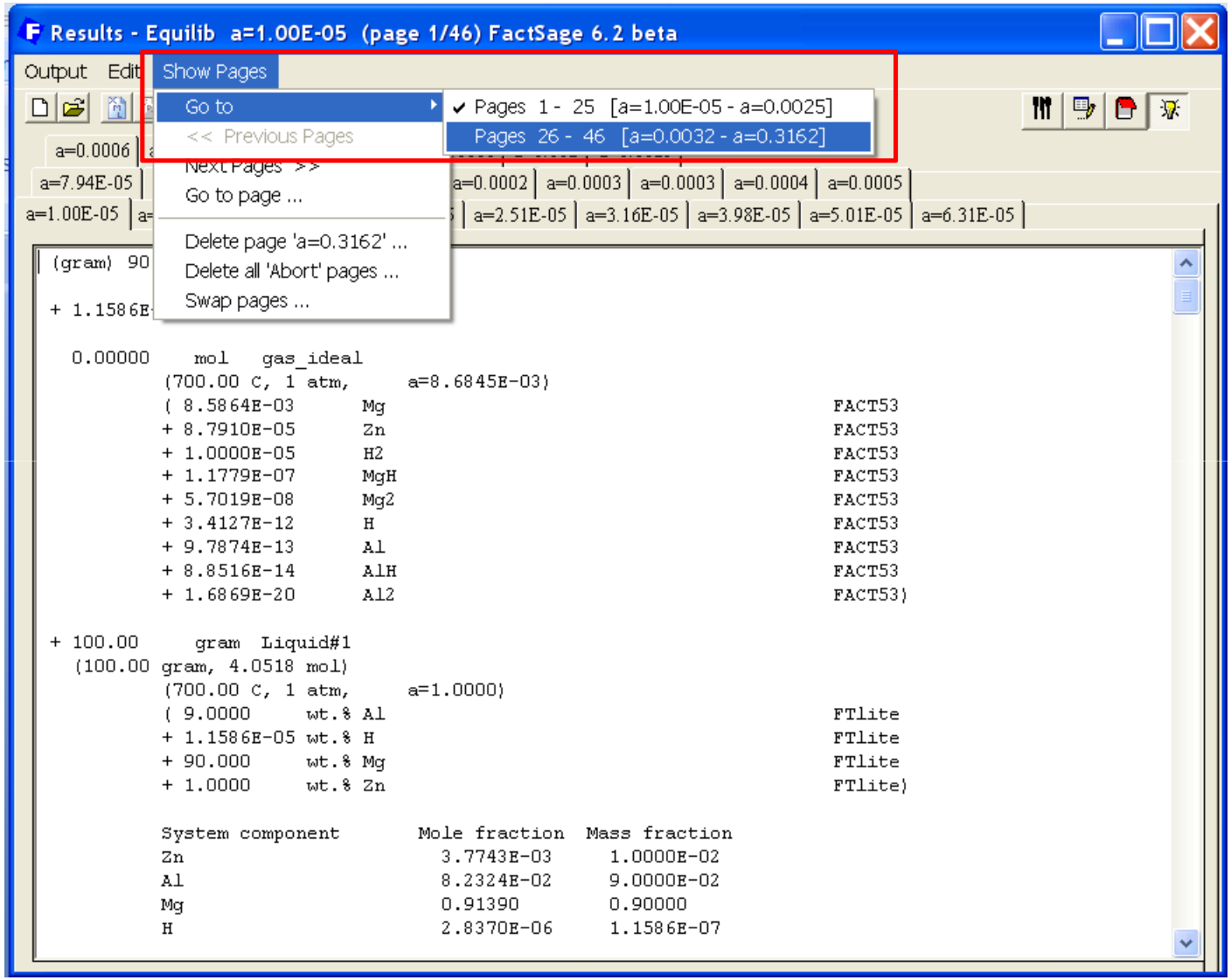
- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



- **Example #1a: Solubility of hydrogen (H_2) 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)

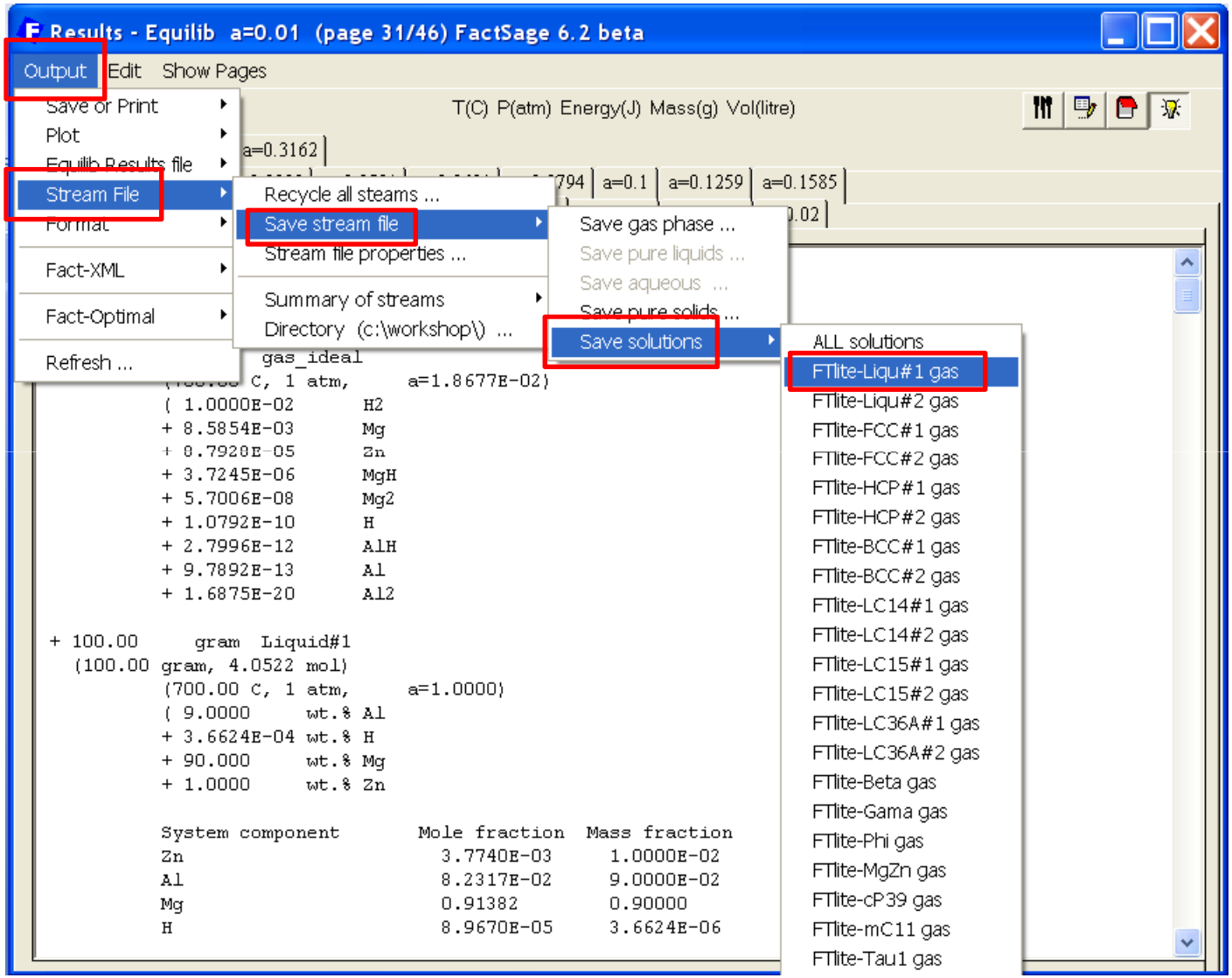
a=0.1995 | a=0.2512 | a=0.3162

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
          + 90.000      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
```

- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



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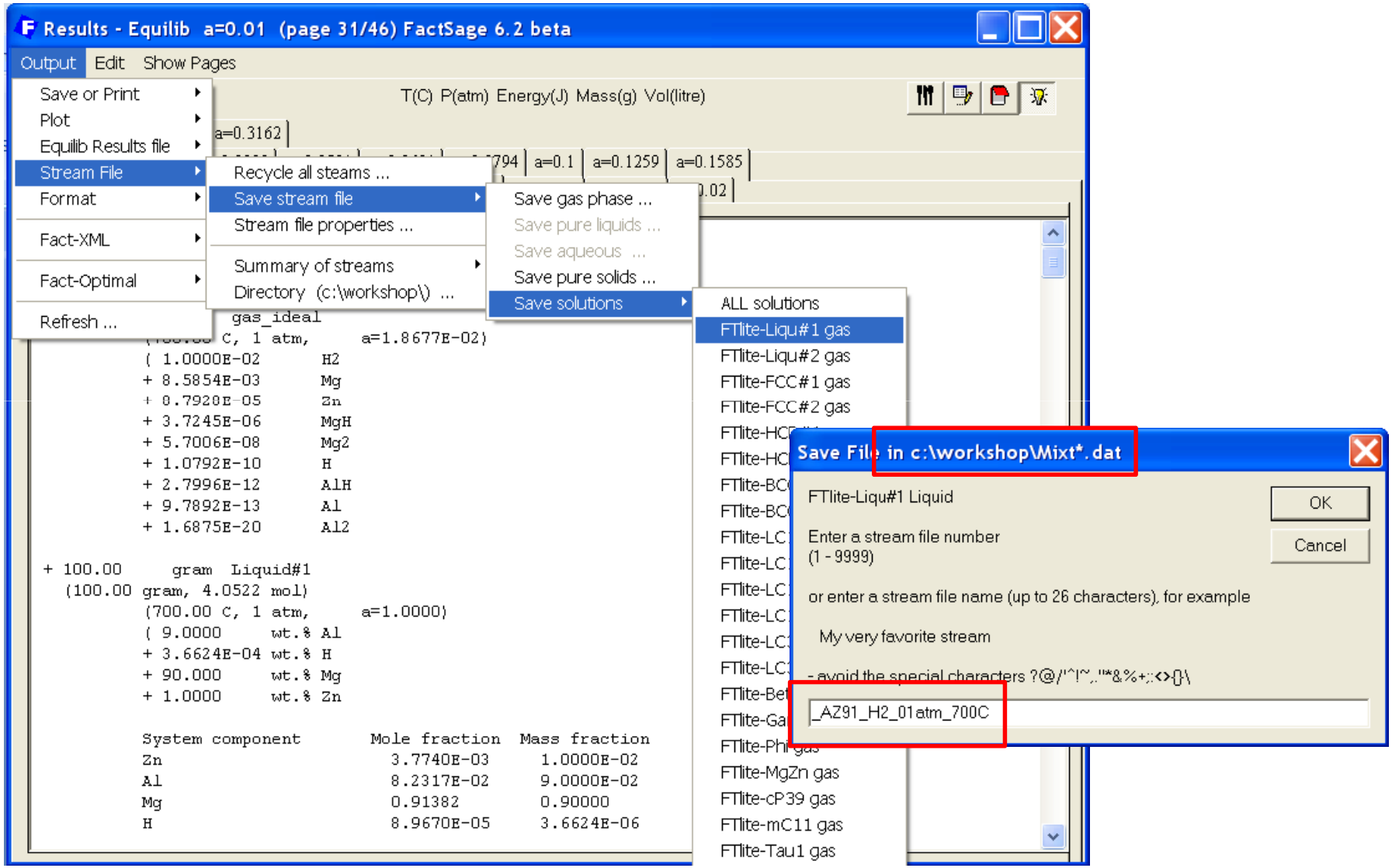
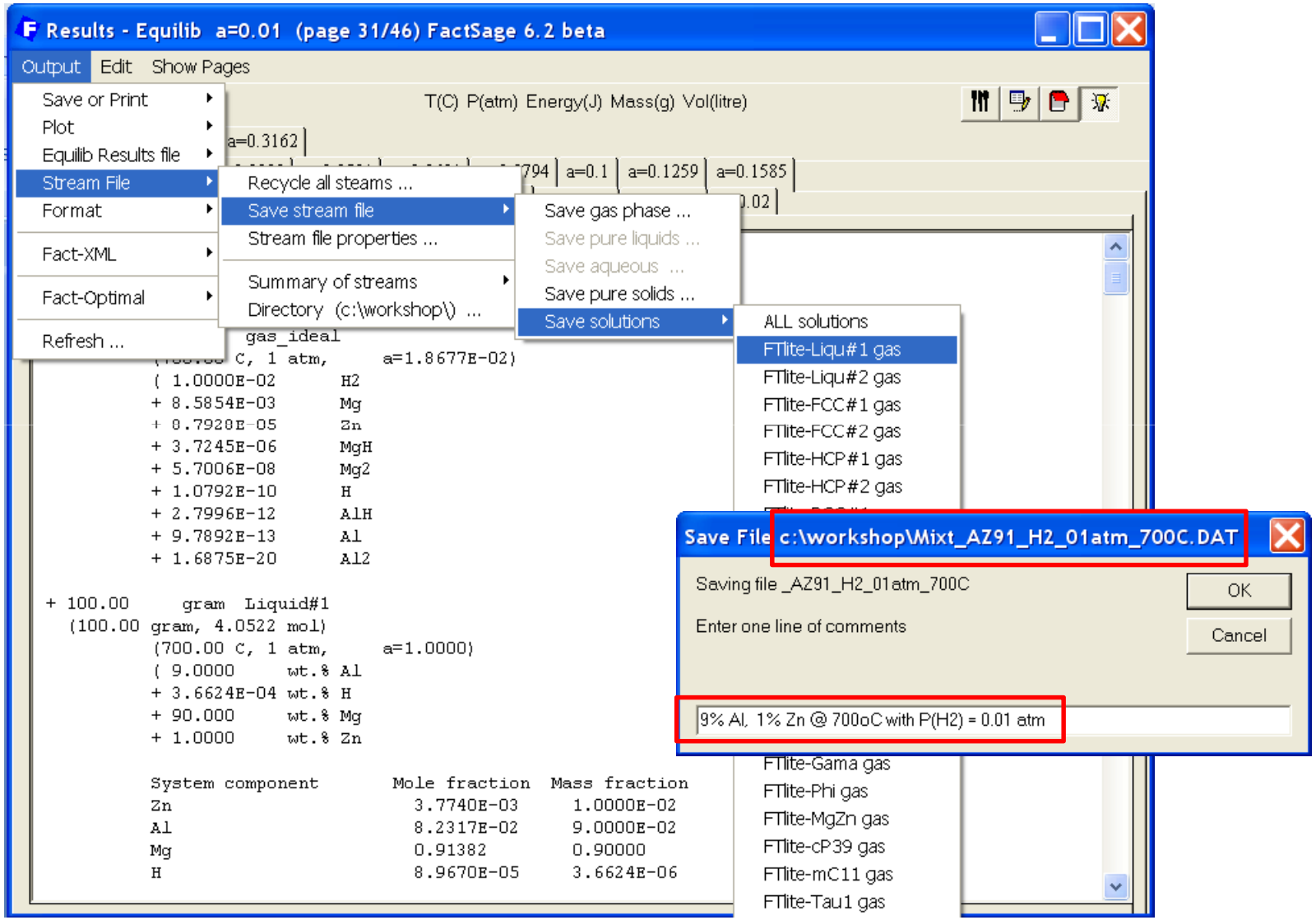
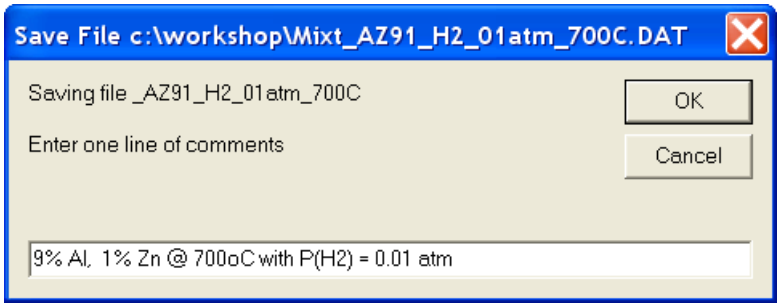


- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



- **Example #1a: Solubility of hydrogen (H_2) in liquid AZ91**



The liquid AZ91 saturated with H at $P(H_2)$ = 0.01 atm & 700°C is now stored in the **stream file**

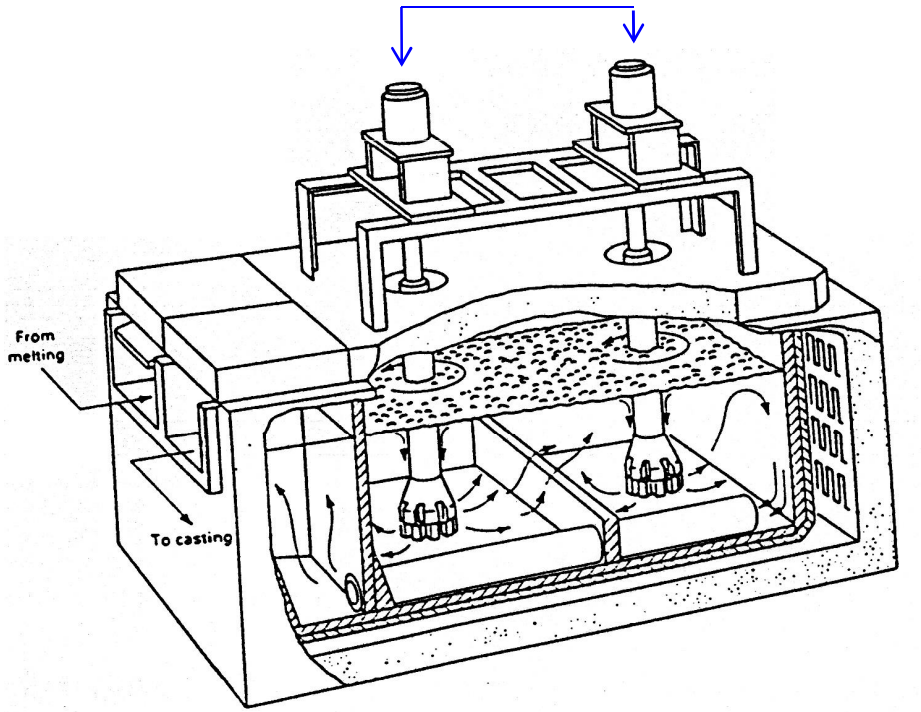
C:\workshop\Mixt_AZ91_H2_01atm_700C.dat

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

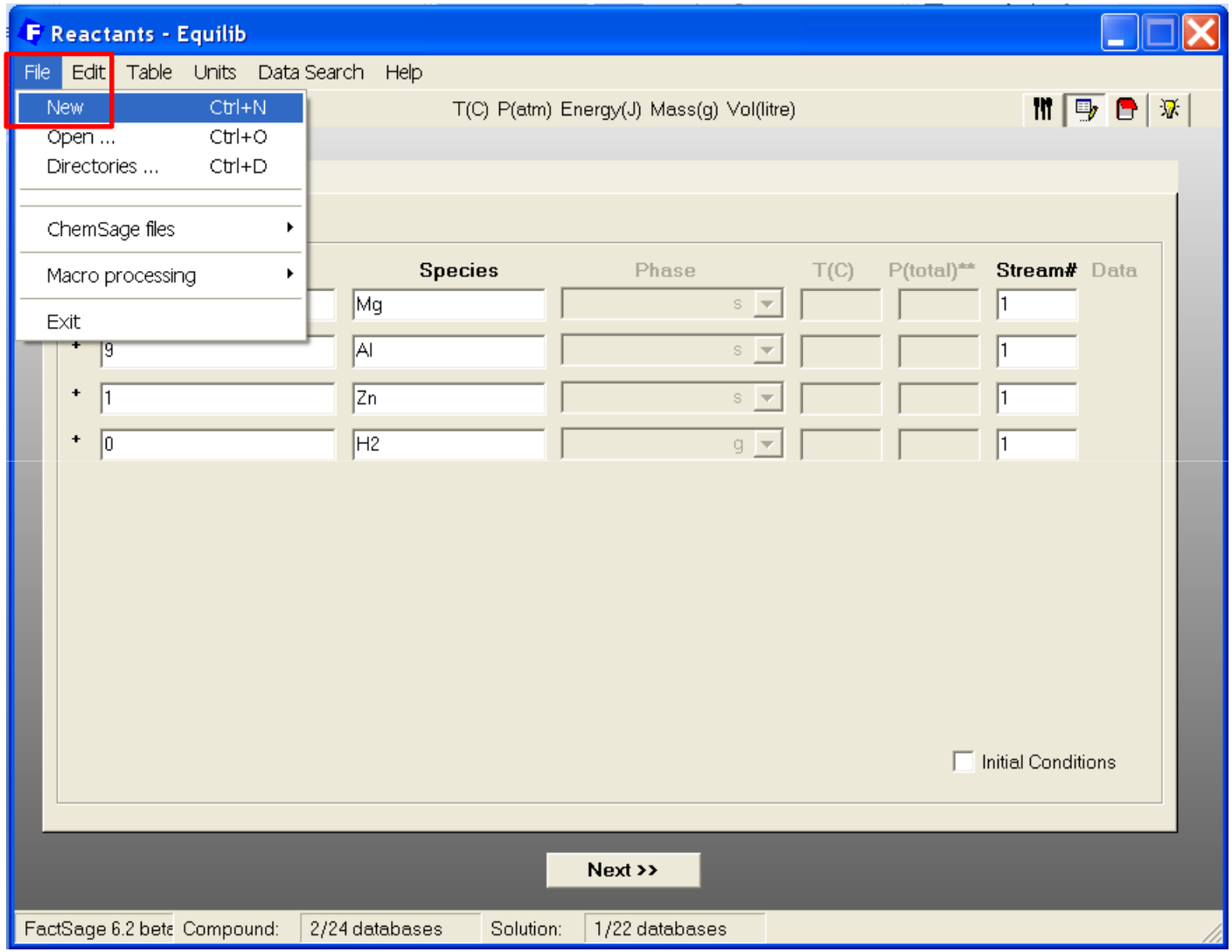
- Examples
  1) Solubility of hydrogen (H_2) in liquid alloys

b) Degassing AZ91 with Ar

In-line Degassing Unit for Al-Treatment



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



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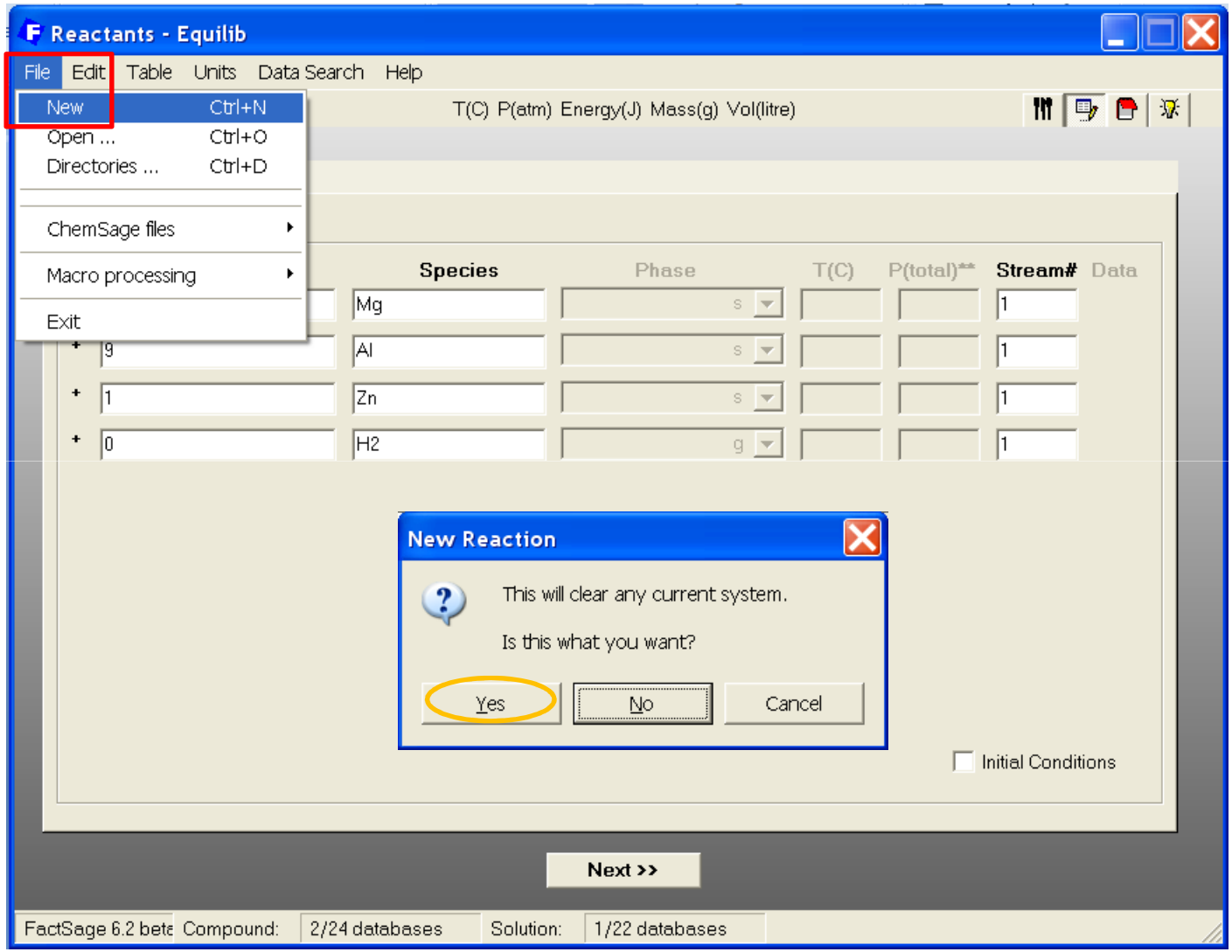

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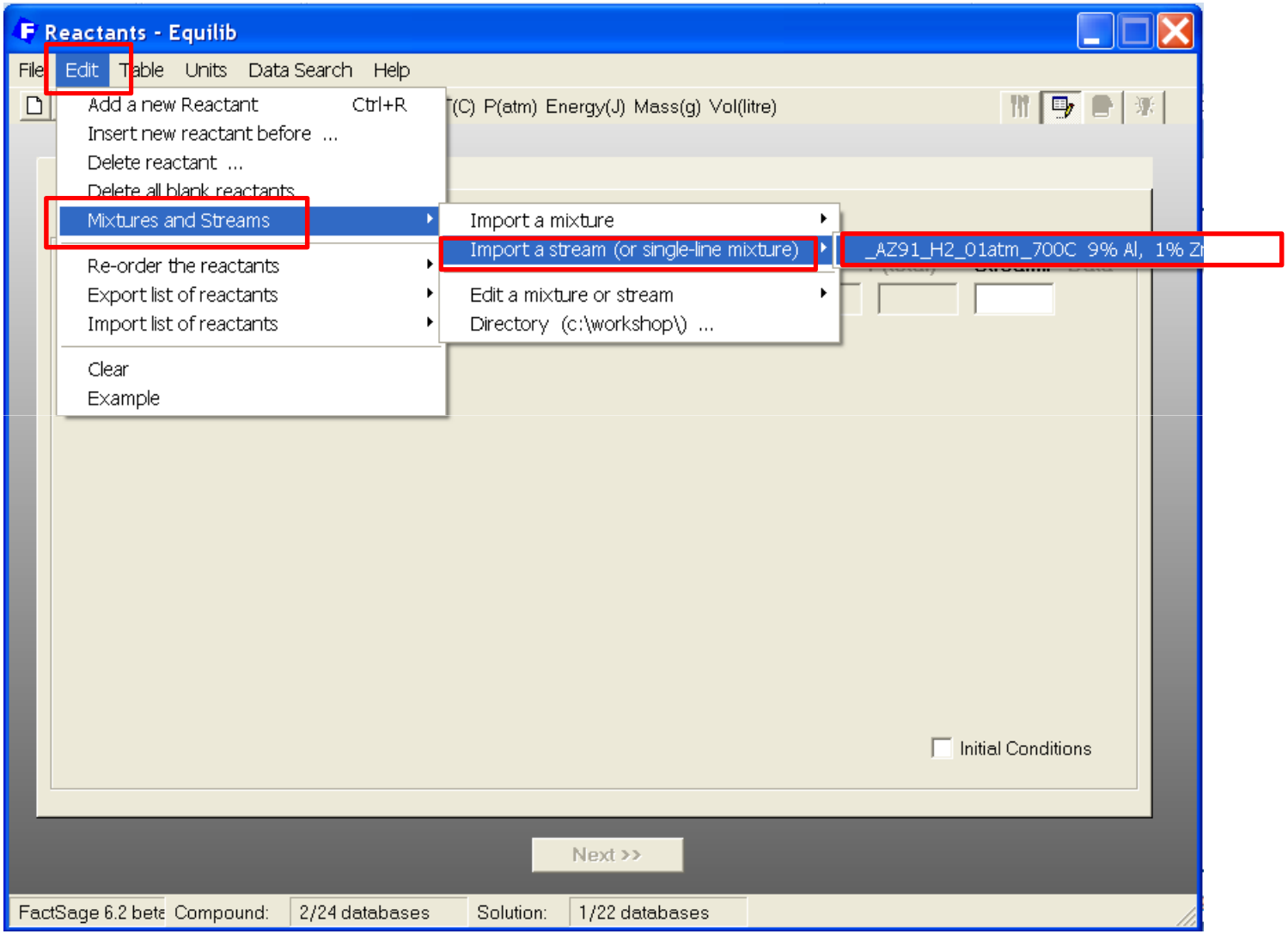

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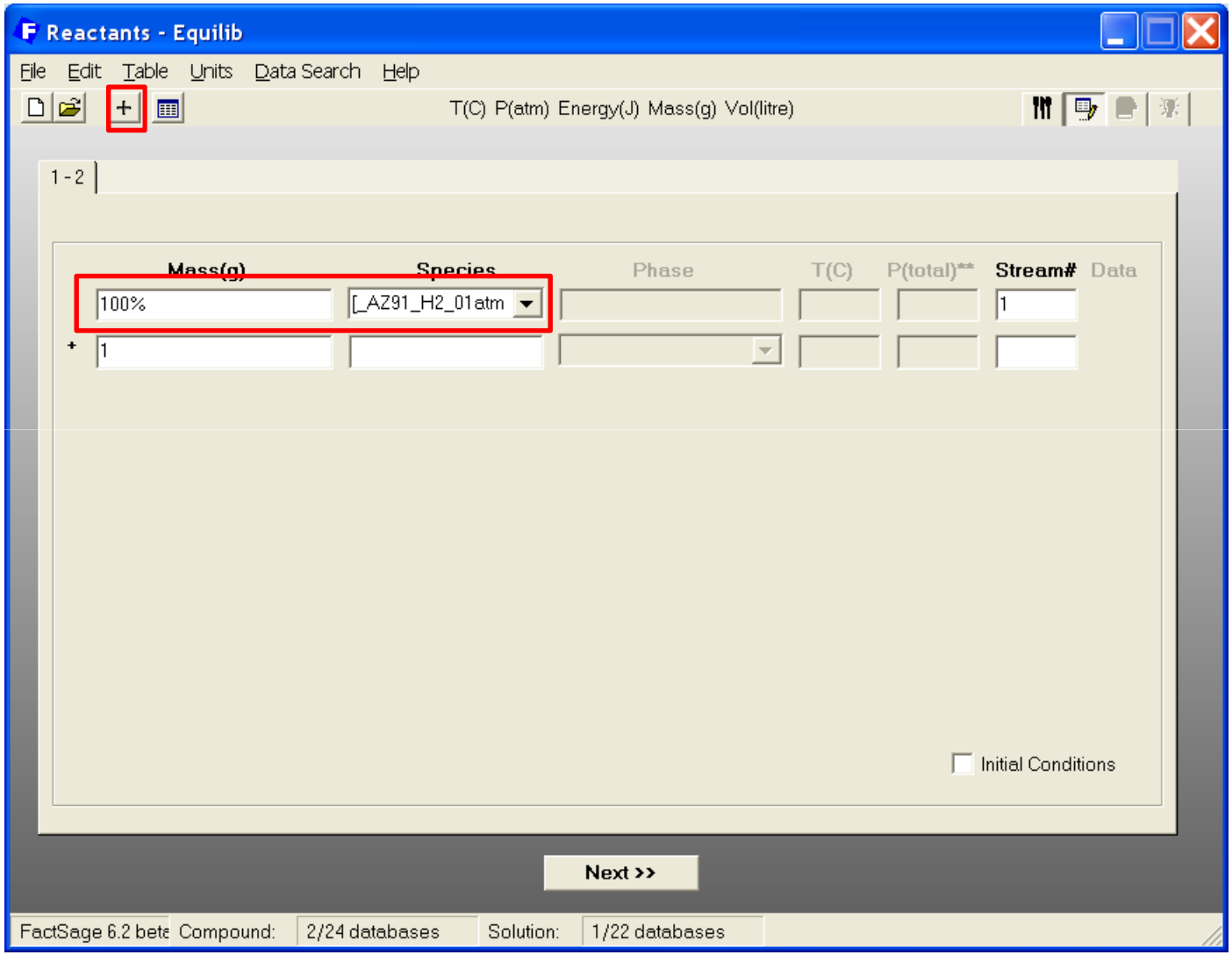

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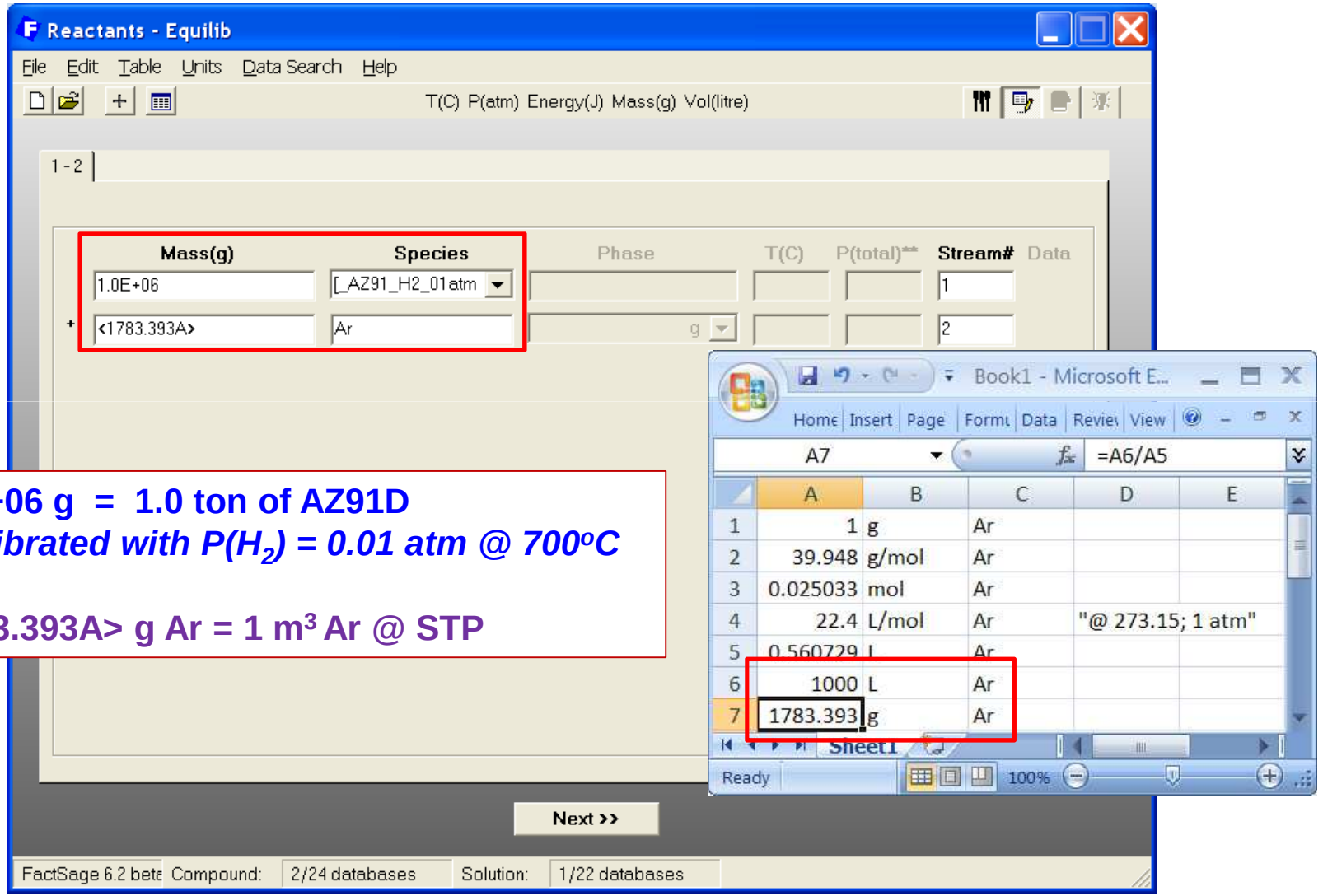
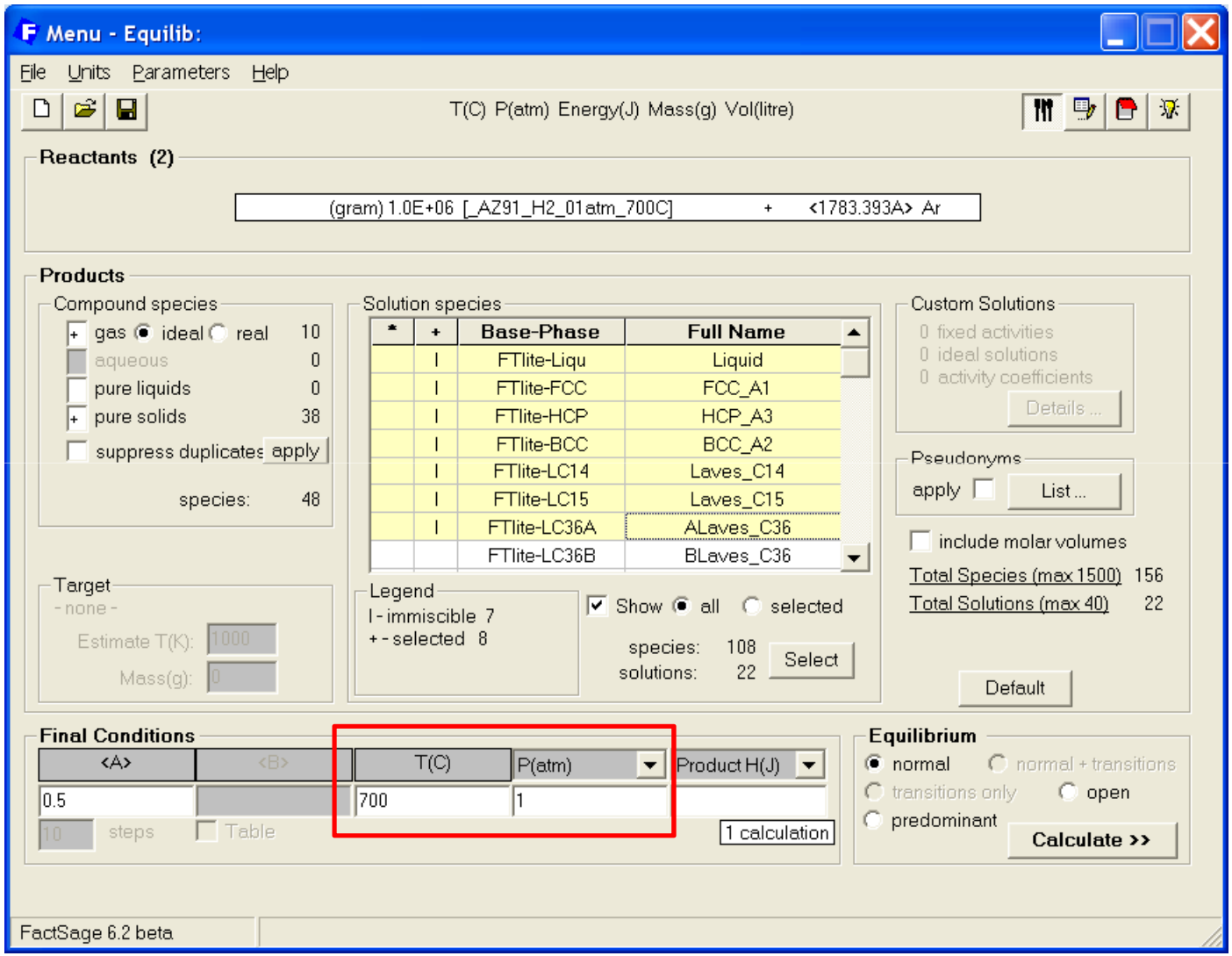


1.0E+06 g = 1.0 ton of AZ91D
equilibrated with $P(H_2)$ = 0.01 atm @ 700°C

<1783.393A> g Ar = 1 m^3 Ar @ STP

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



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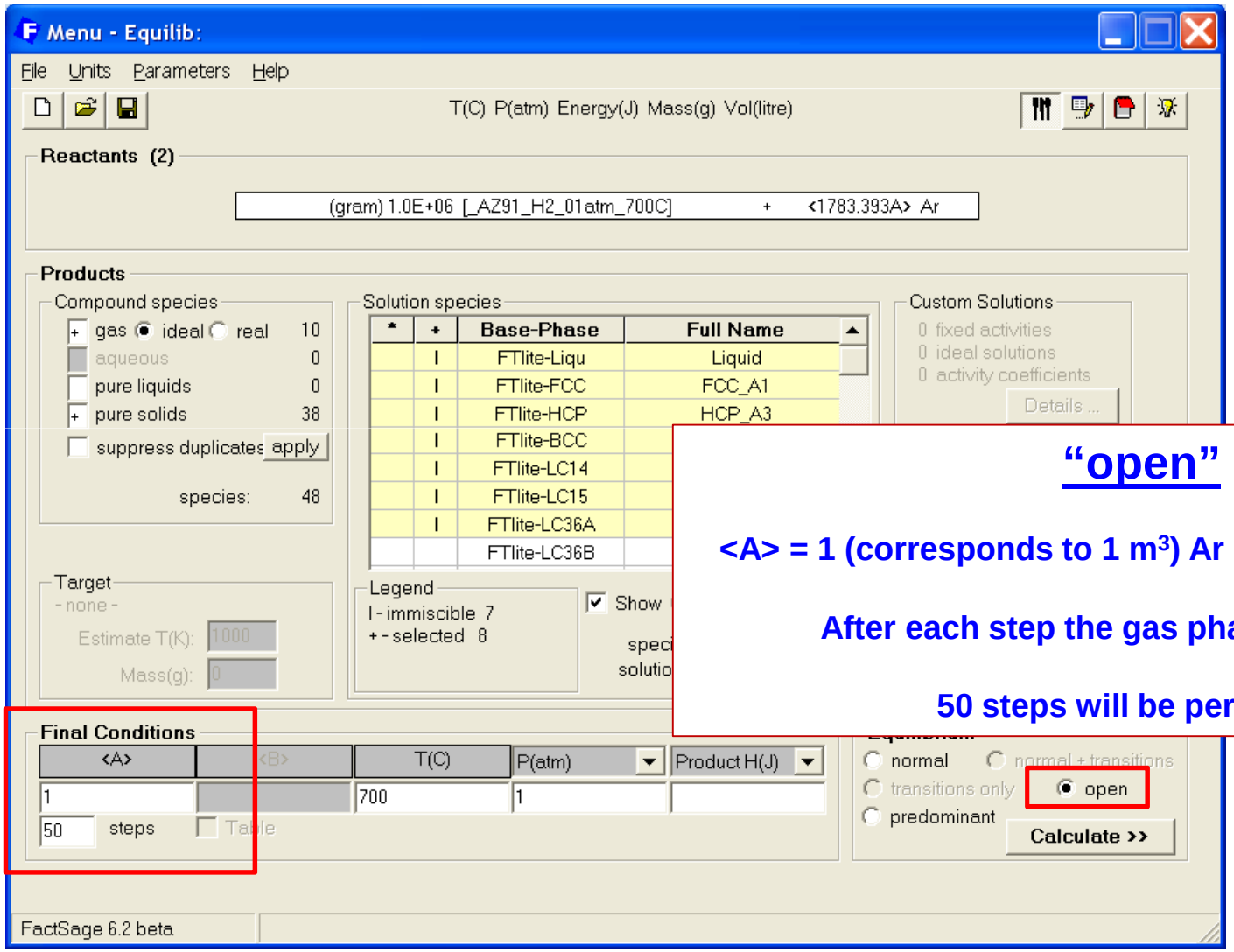


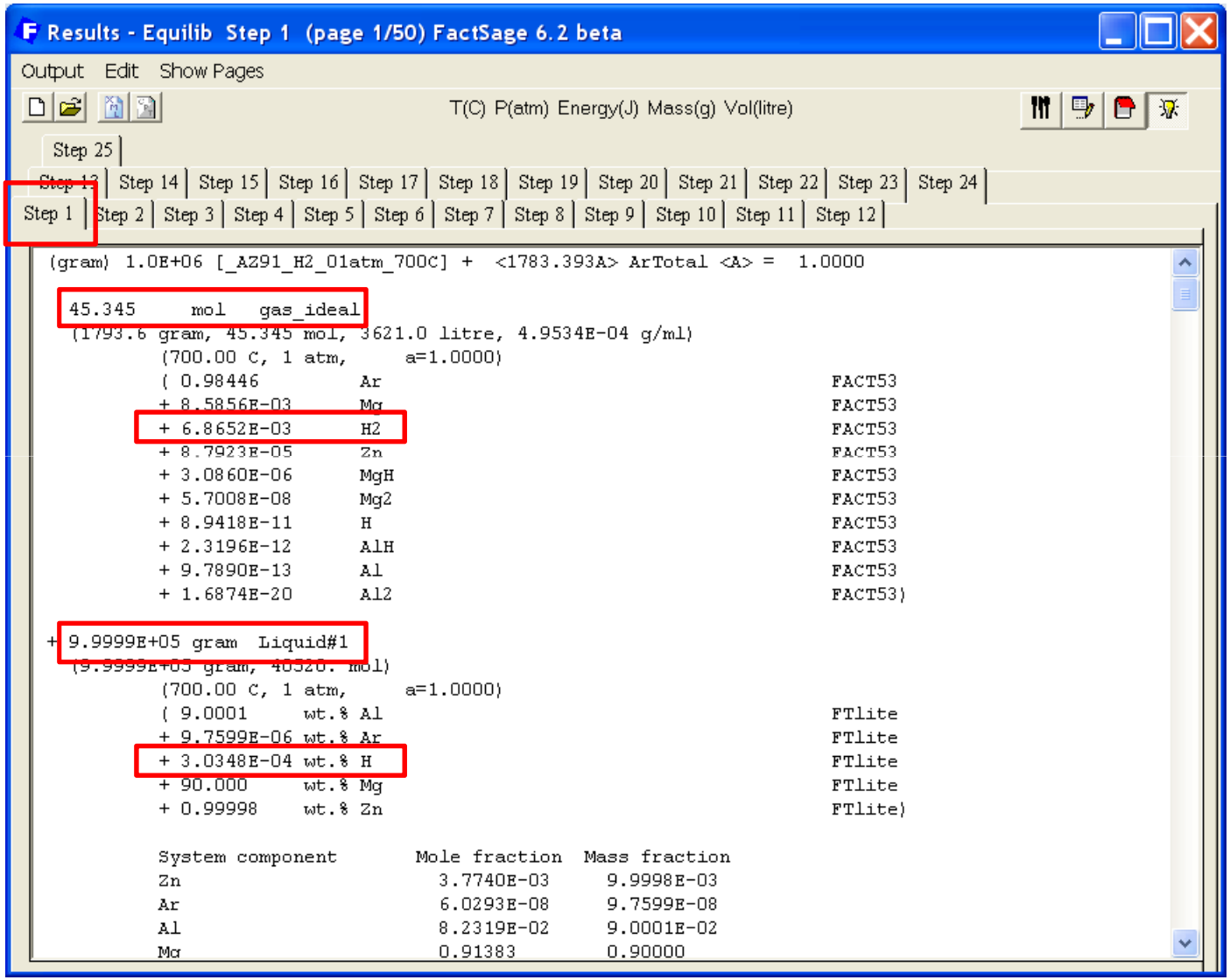
"open"

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

After each step the gas phase is removed

50 steps will be performed

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



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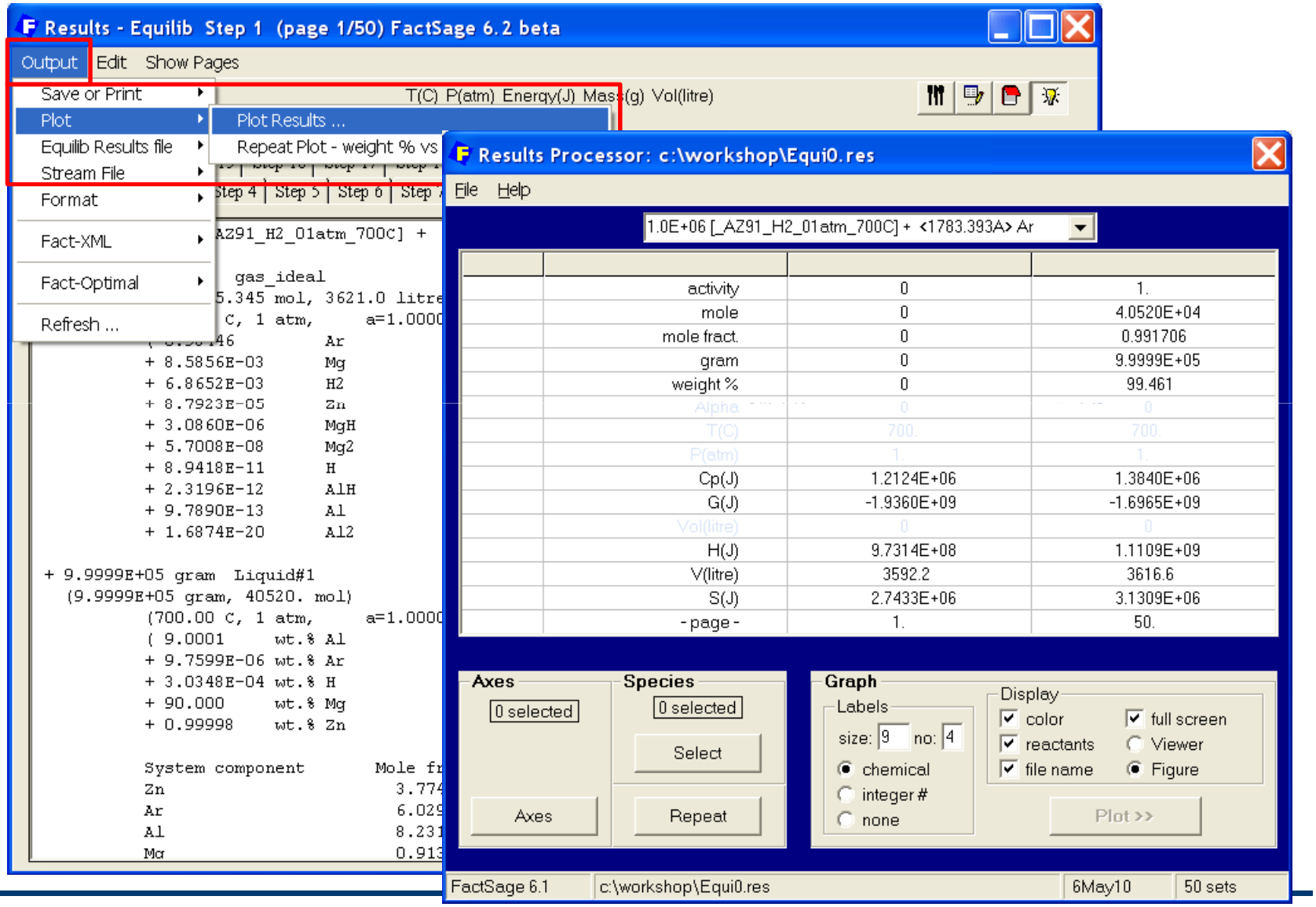

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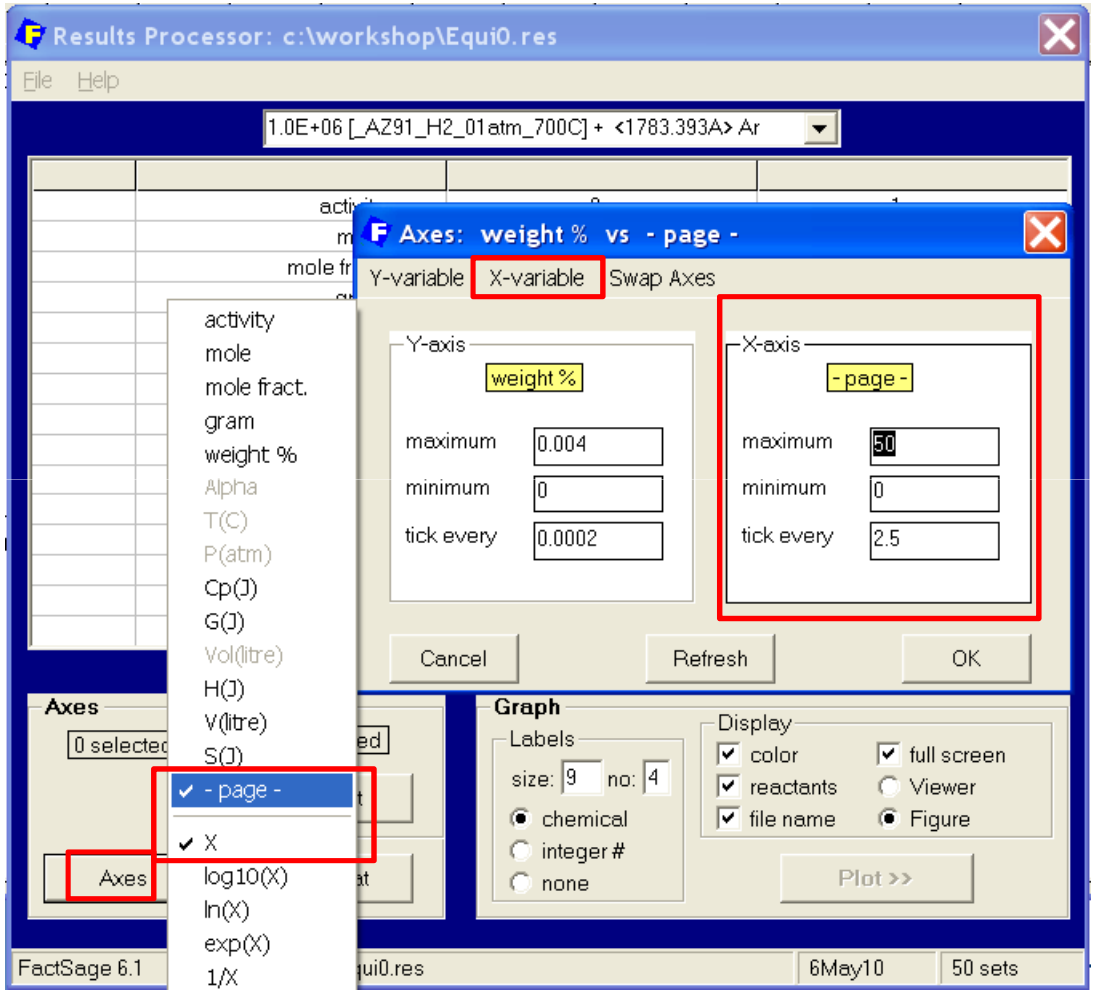

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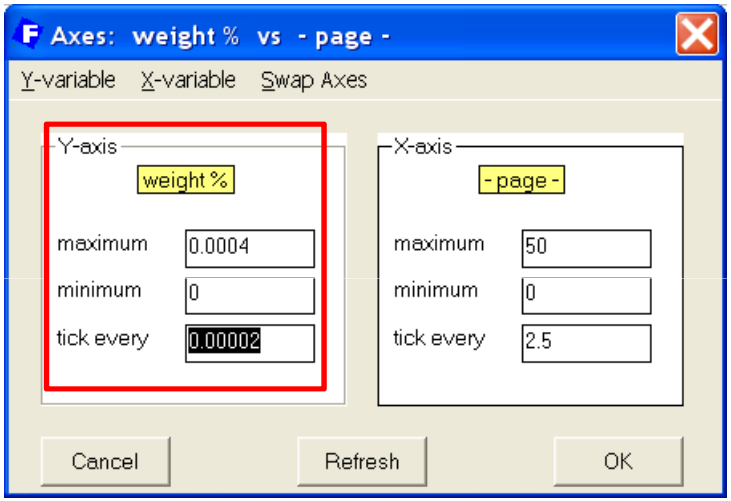

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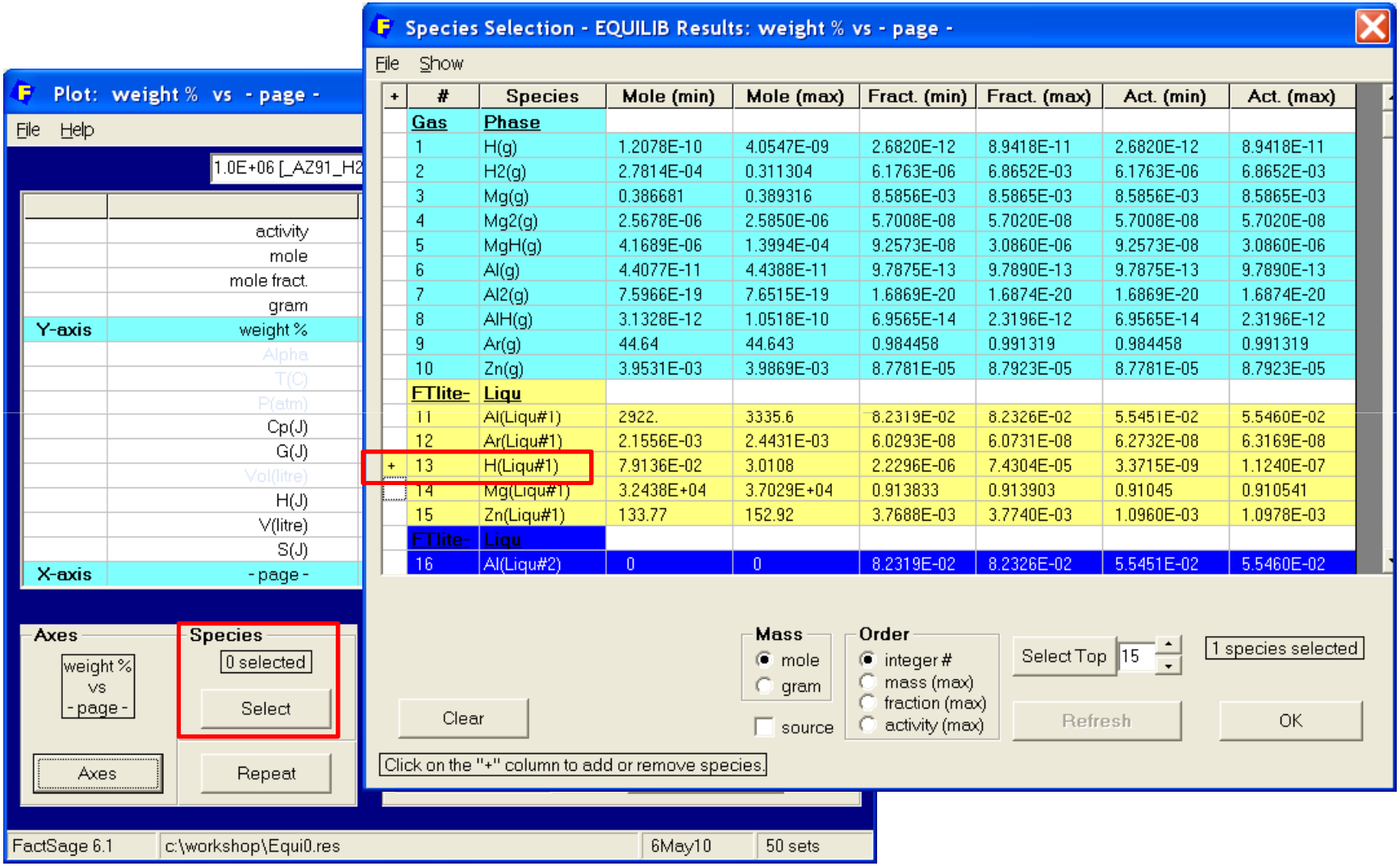

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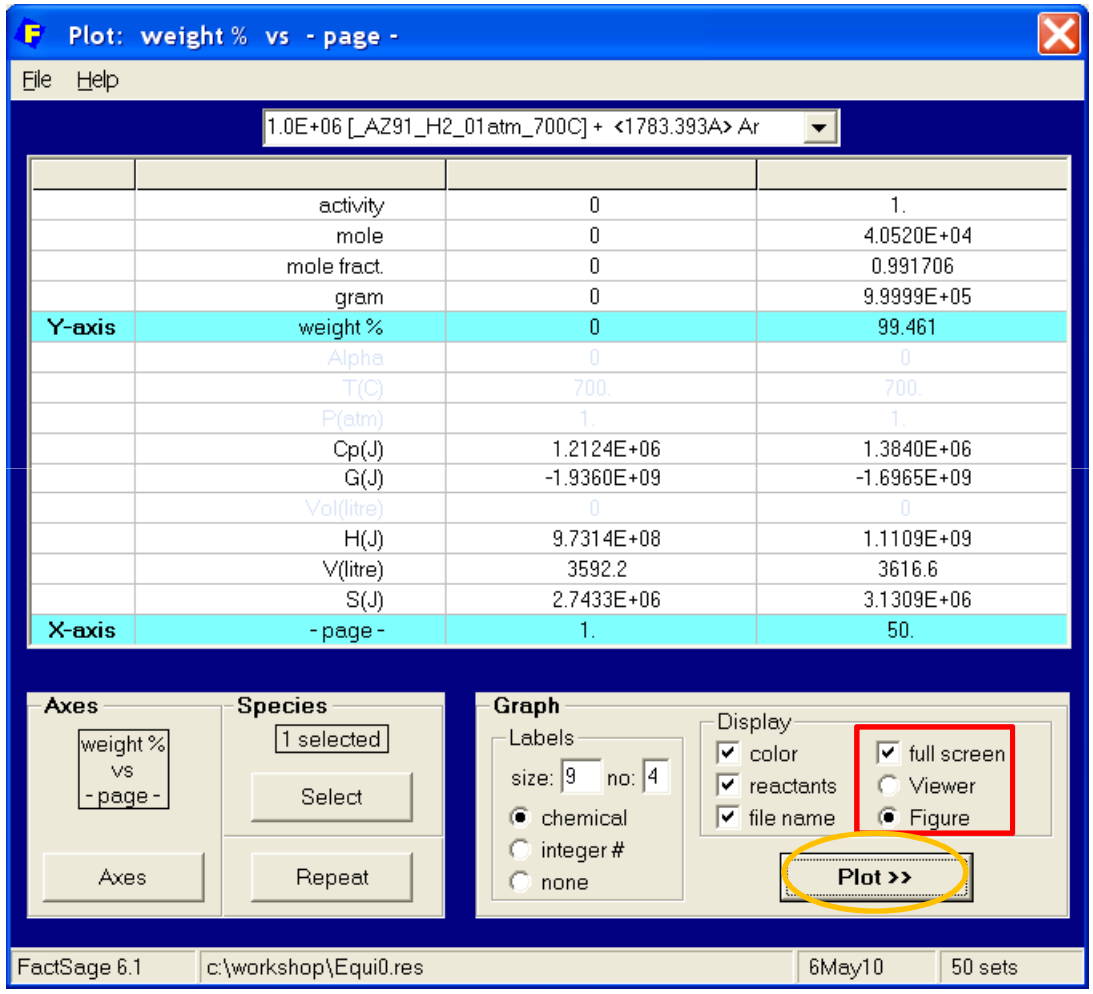

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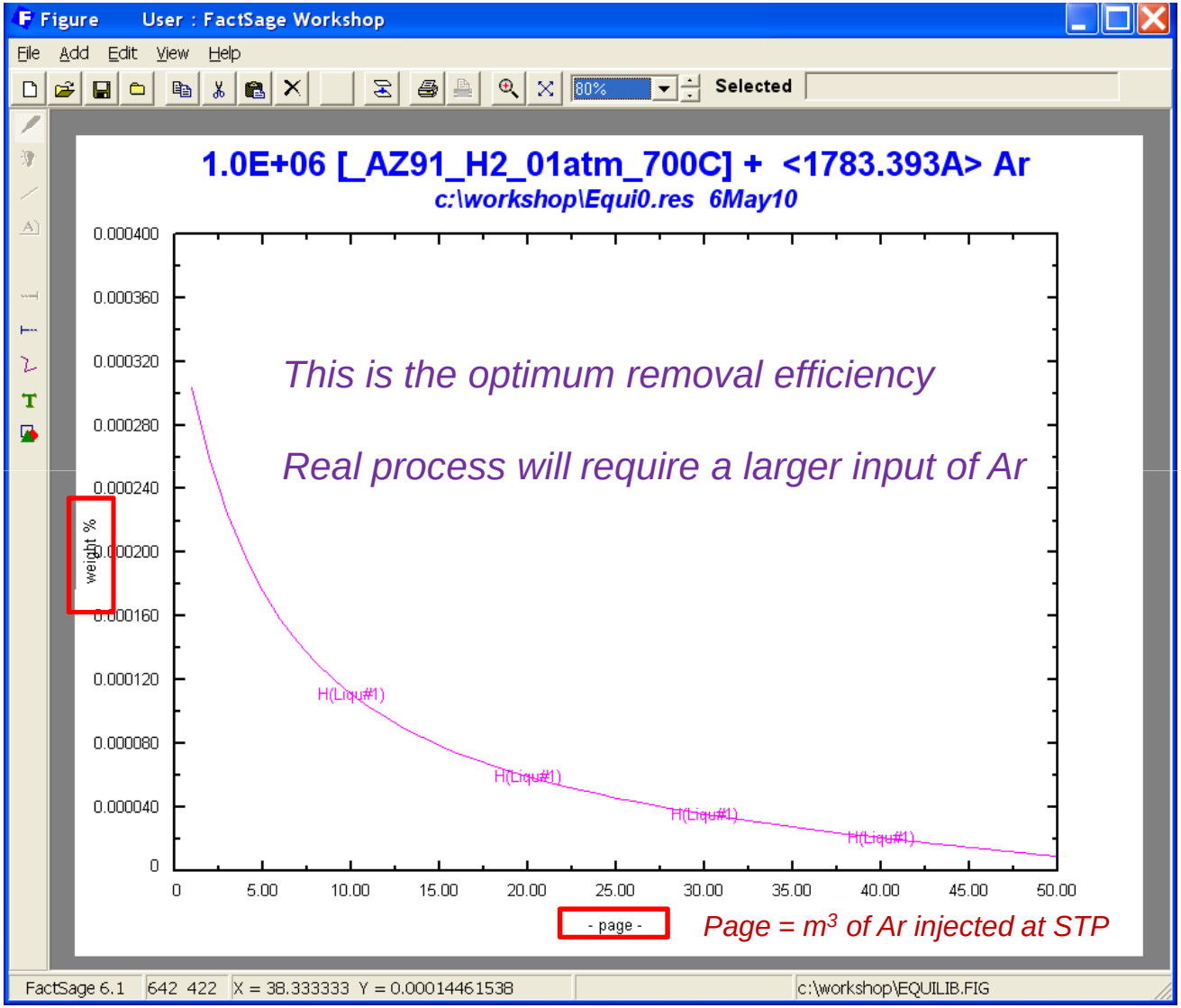

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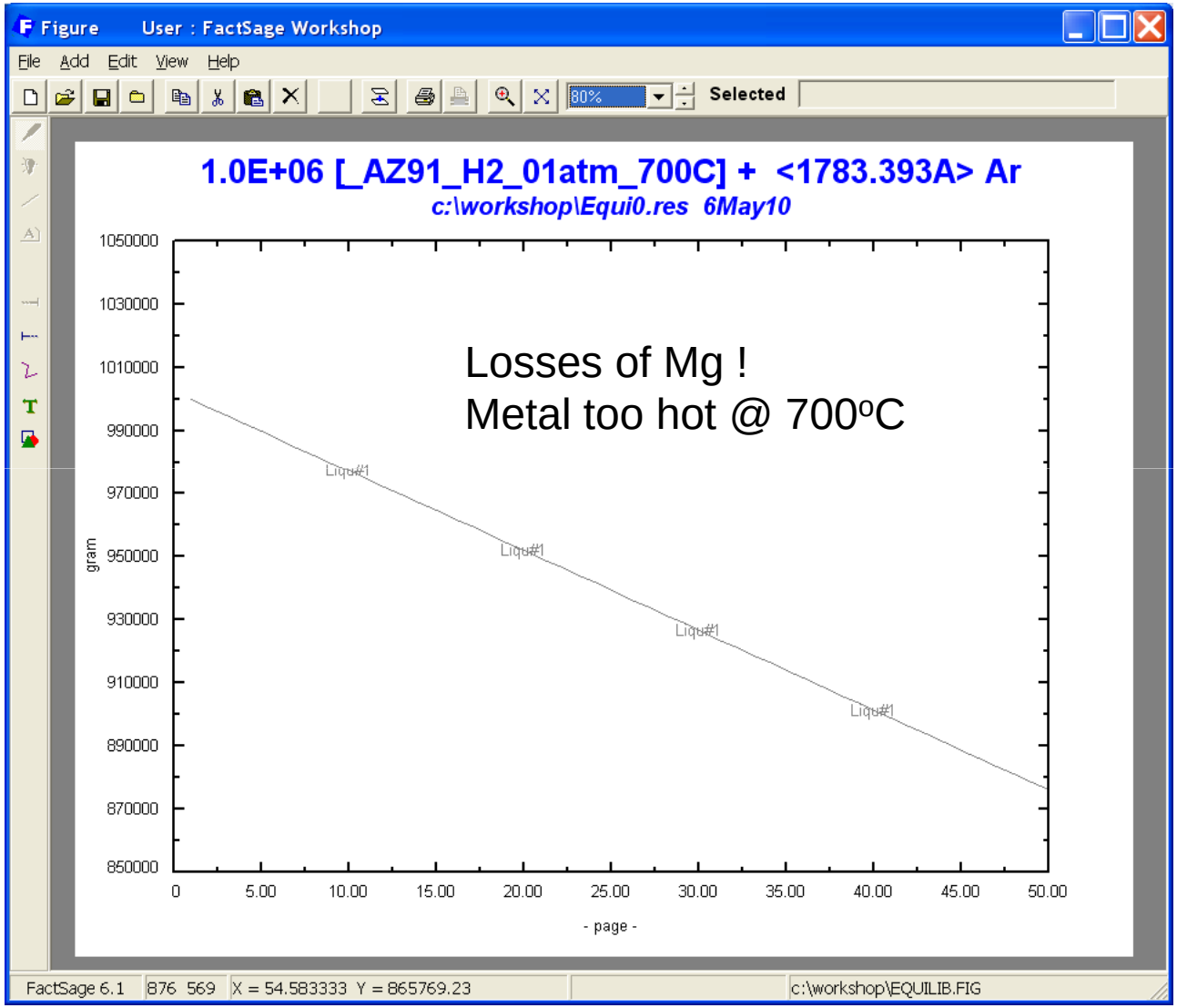

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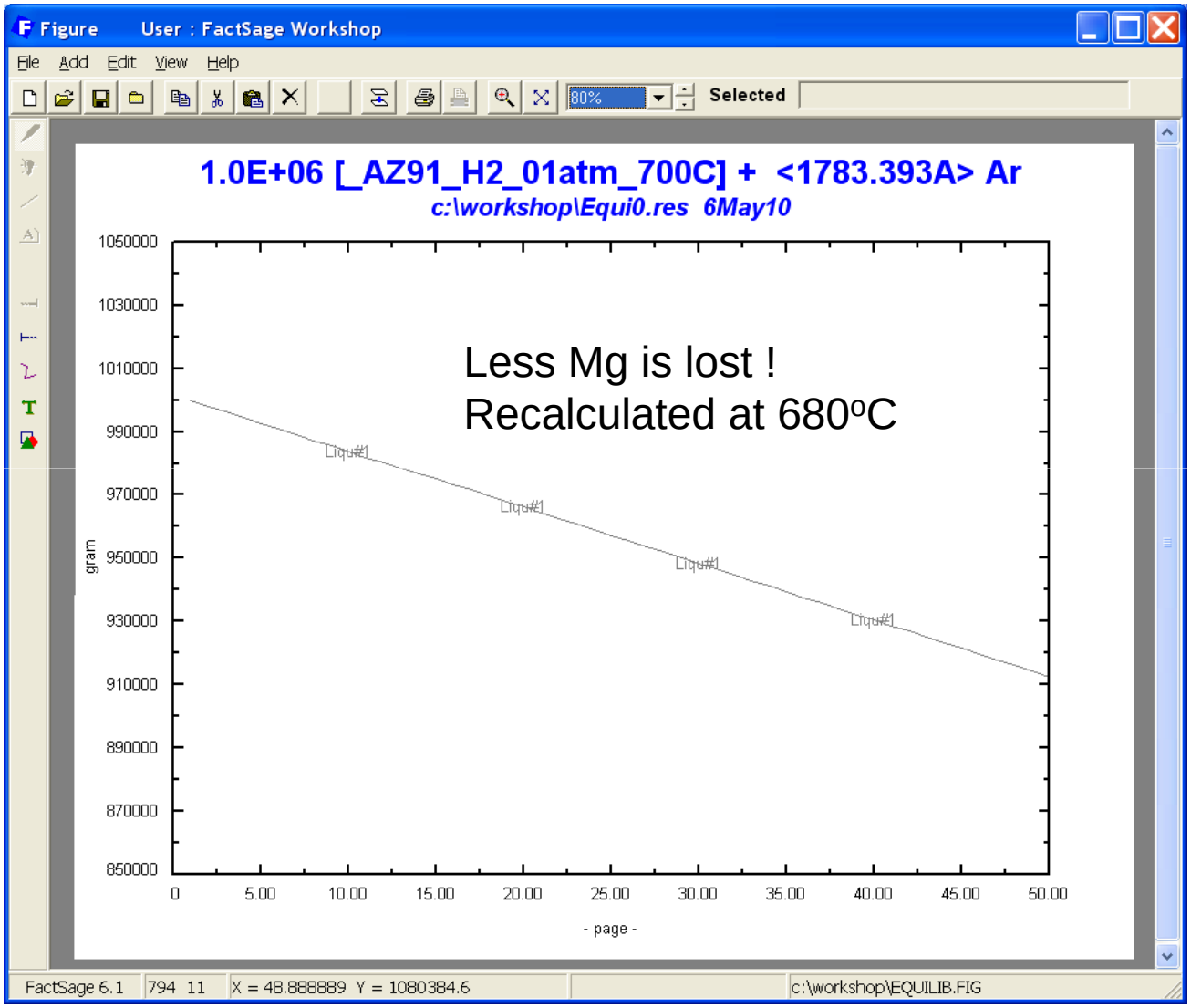

- Examples

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-$MnCl_2$

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

$KMgCl_3$ is used to remove Na & Ca from **liquid Al alloys**

$KMgCl_3 + 2\ \underline{Na} \rightarrow (KCl+2NaCl)_{liquid} + \underline{Mg}$

or $MgCl_2 + 2\ \underline{Na} \rightarrow (2NaCl)_{\text{ in liquid KCl}} + \underline{Mg}$

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 $KMgCl_3$ by a NaCl-KCl-$MnCl_2$ mixture** that will potentially melt faster but will keep its ability to remove Na and Ca ?

What would be a good composition ?

$MnCl_2 + 2\ \underline{Na} \rightarrow (2NaCl)_{\text{ in liquid KCl}} + \underline{Mn}$

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

Strategy:

1) **Liquidus projection → NaCl-KCl-$MnCl_2$:**

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

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EQUILIB

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

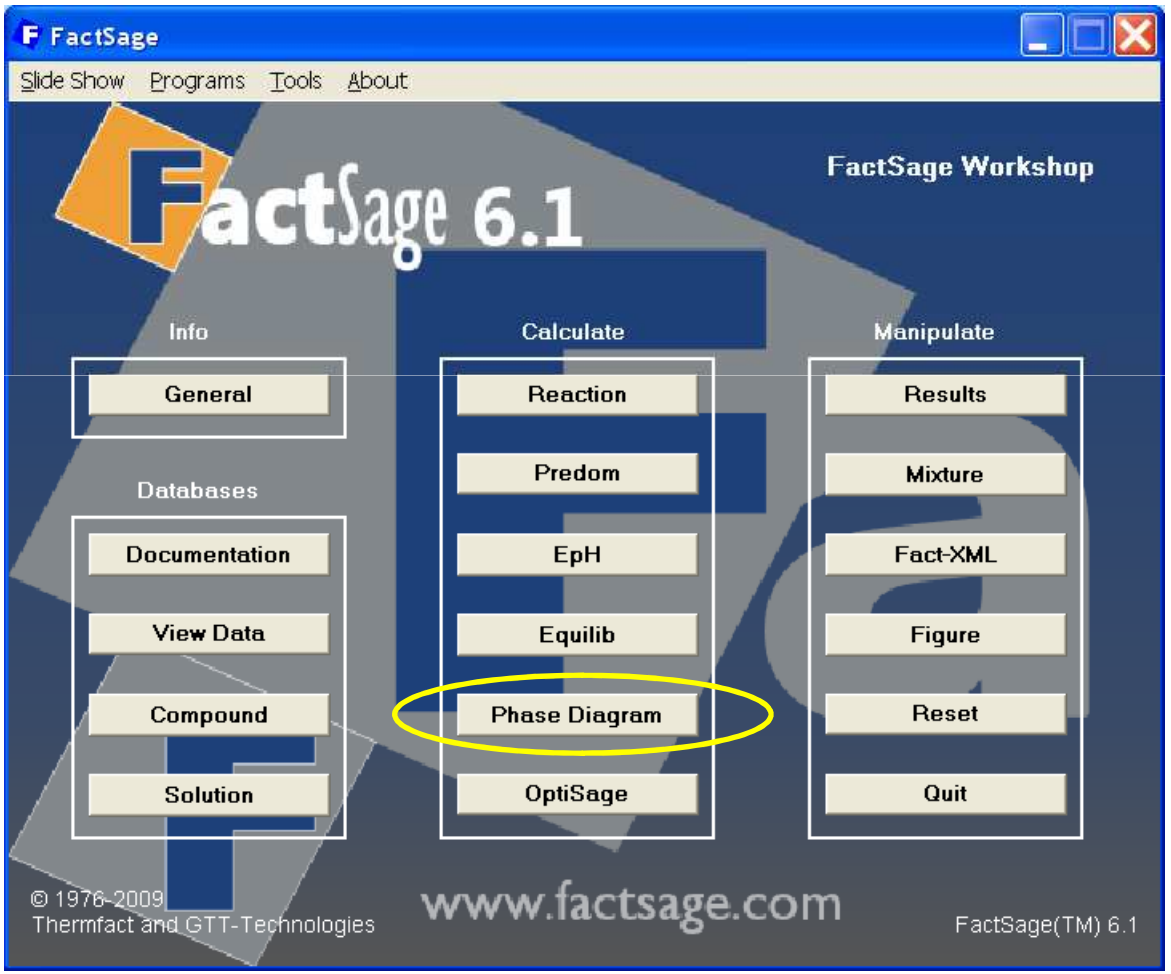
GOAL: check if the capability to remove Na and Ca is similar

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

Liquidus Projection

- NaCl
- KCl
- $MnCl_2$

FTsalt



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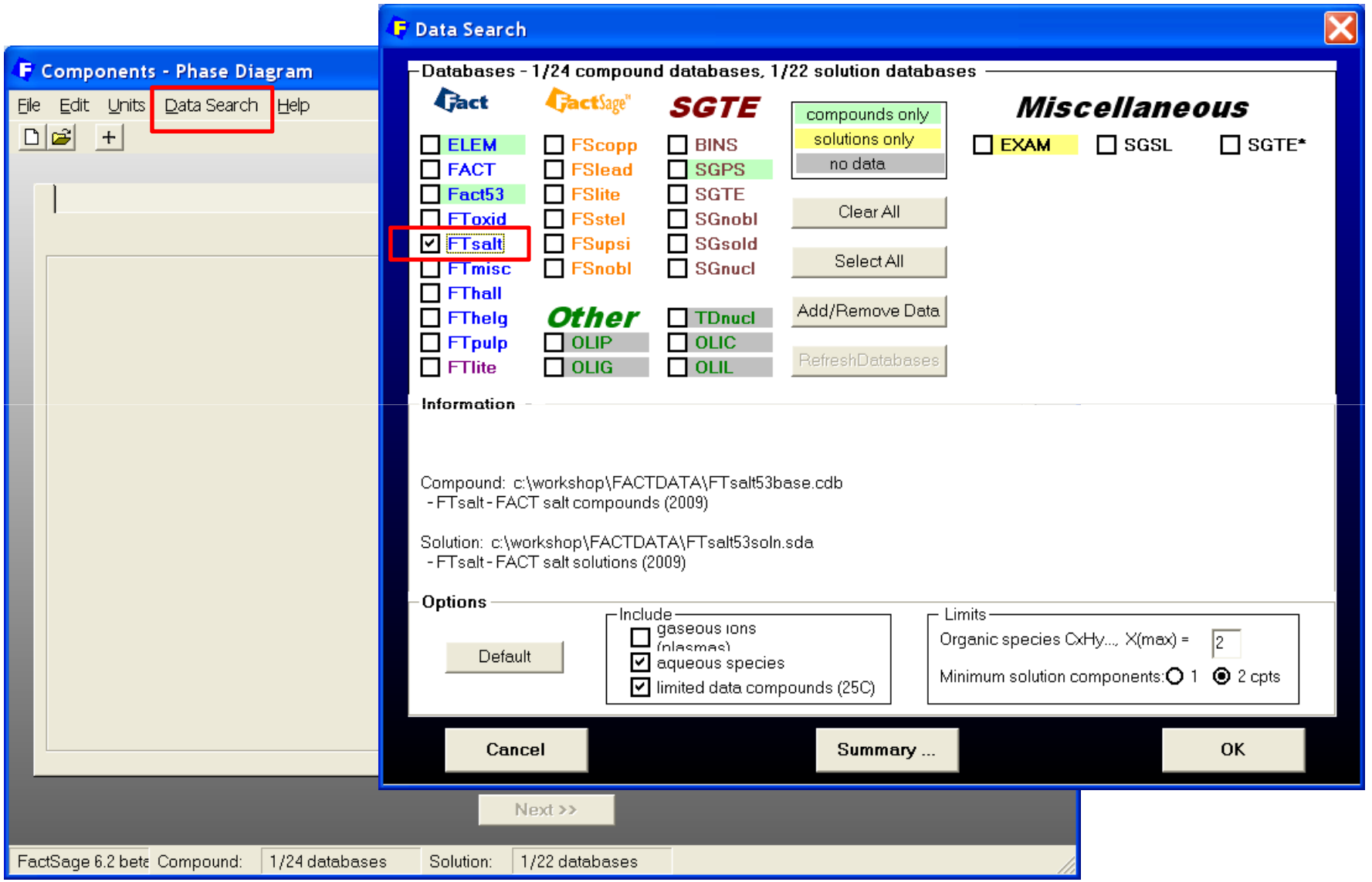

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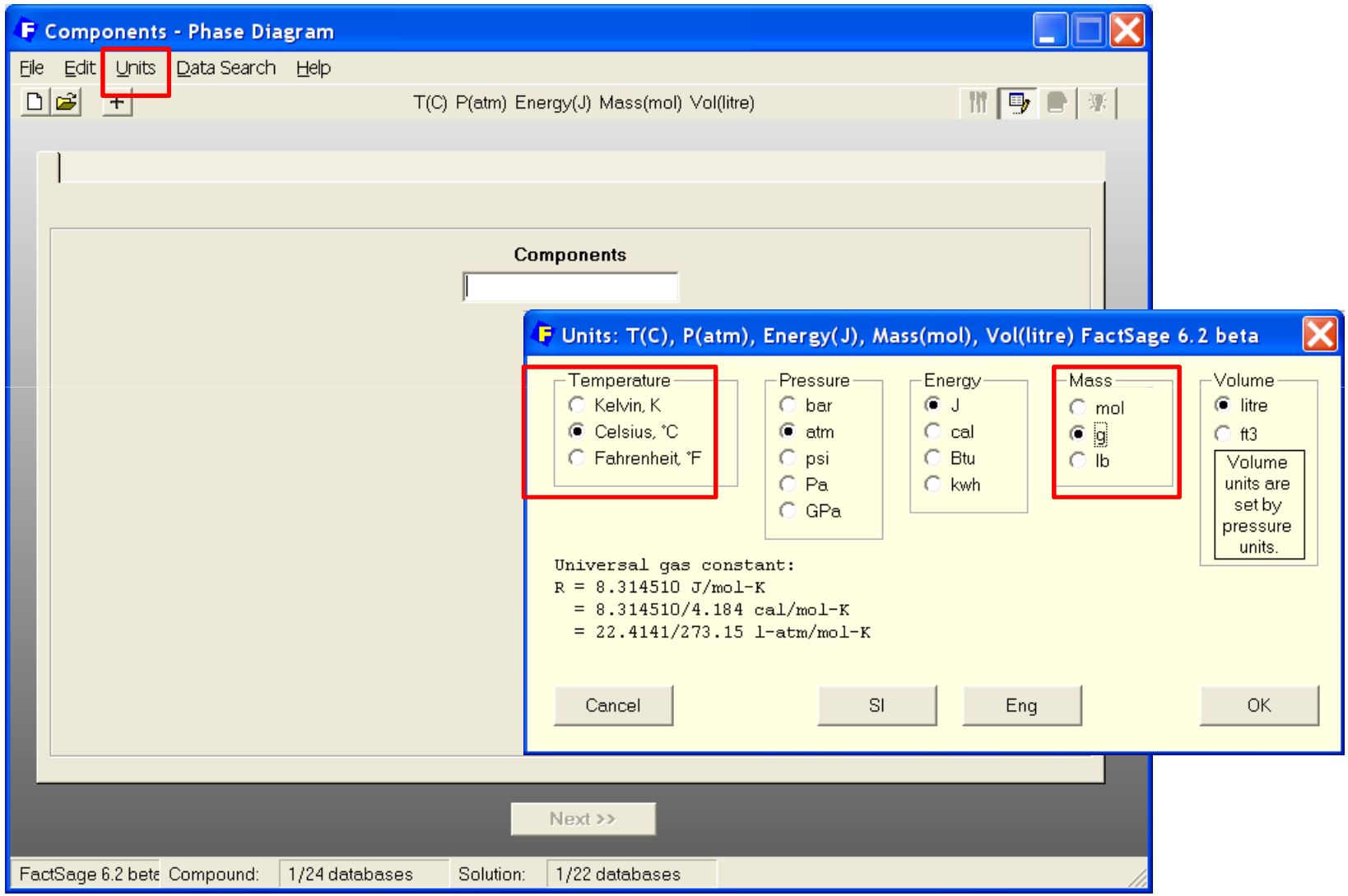

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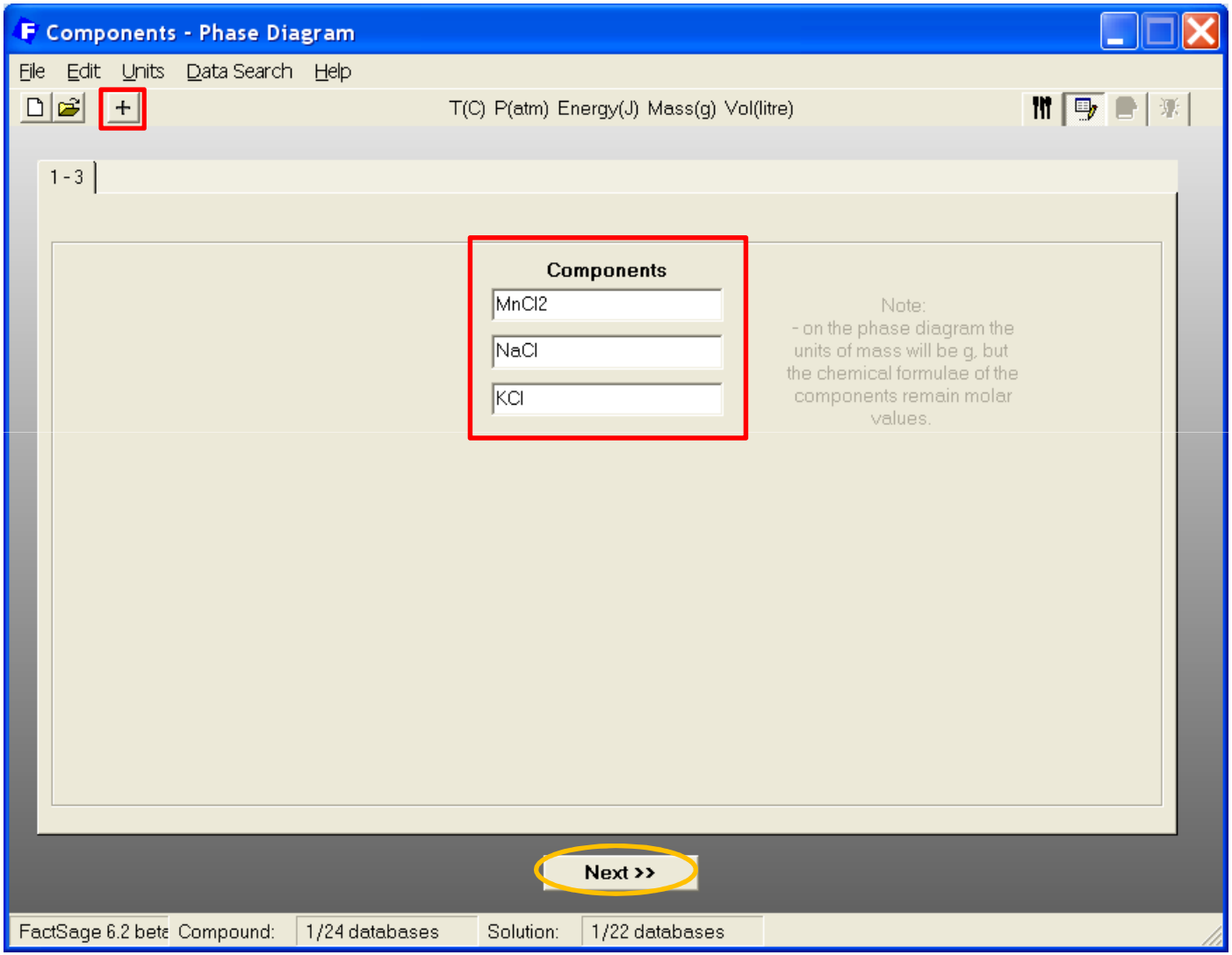

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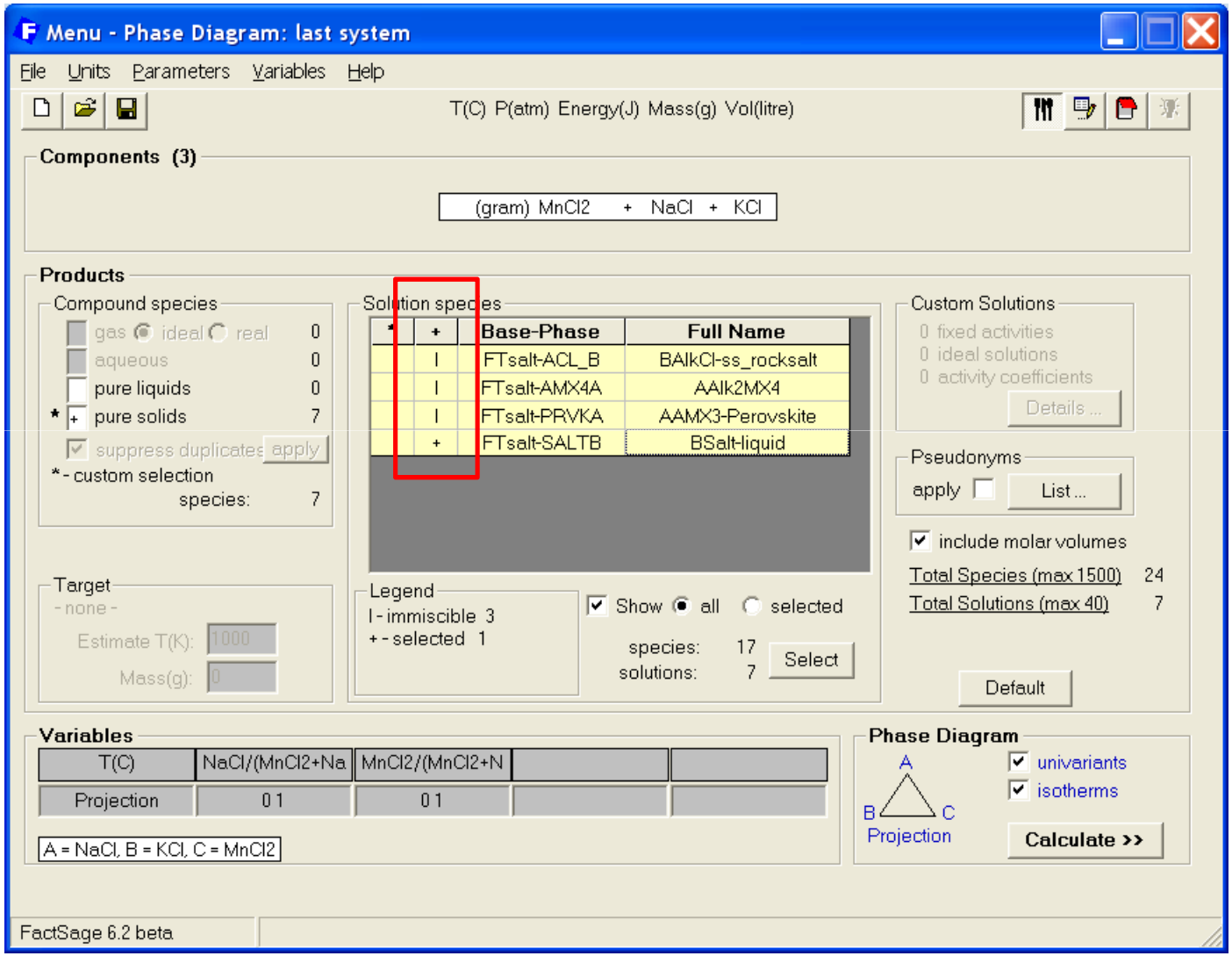

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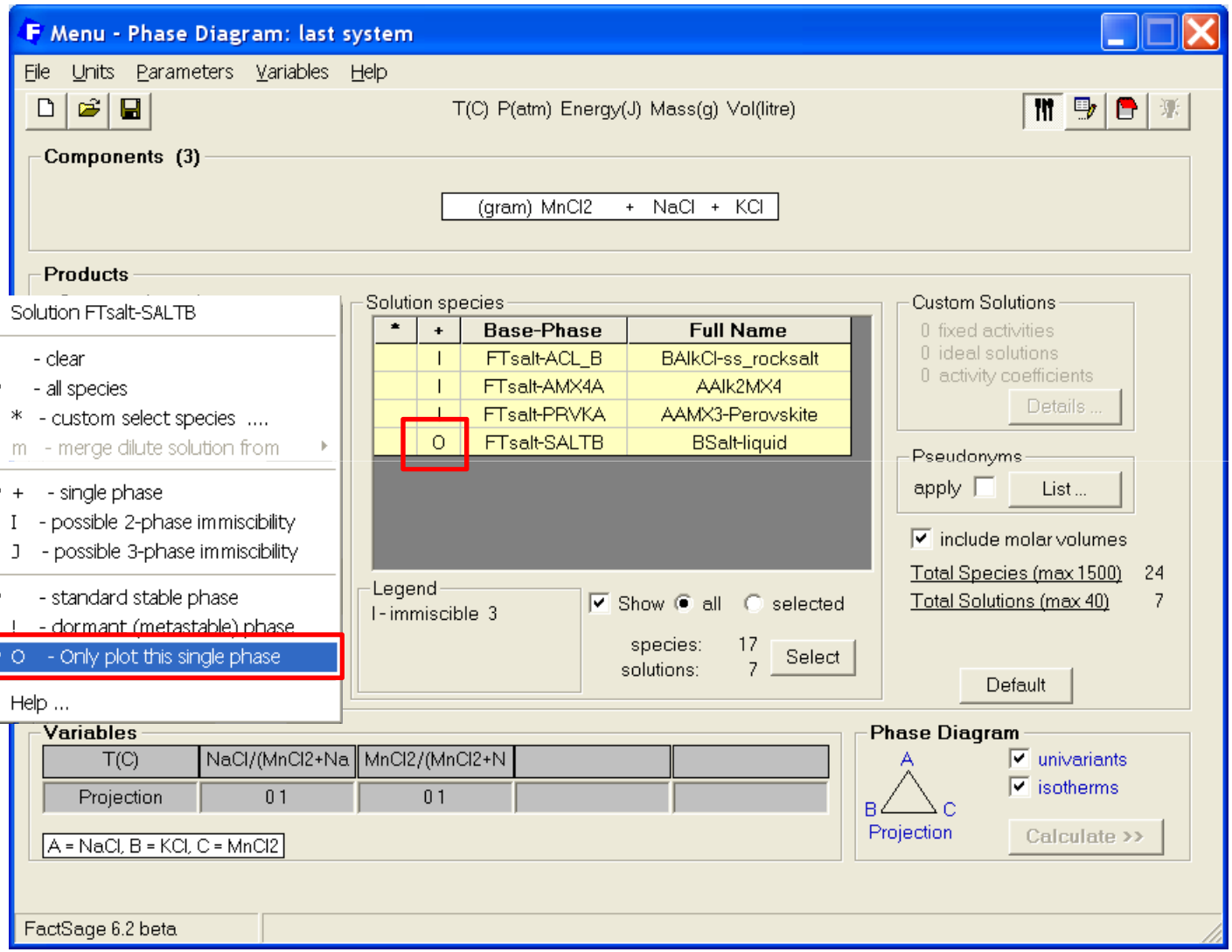

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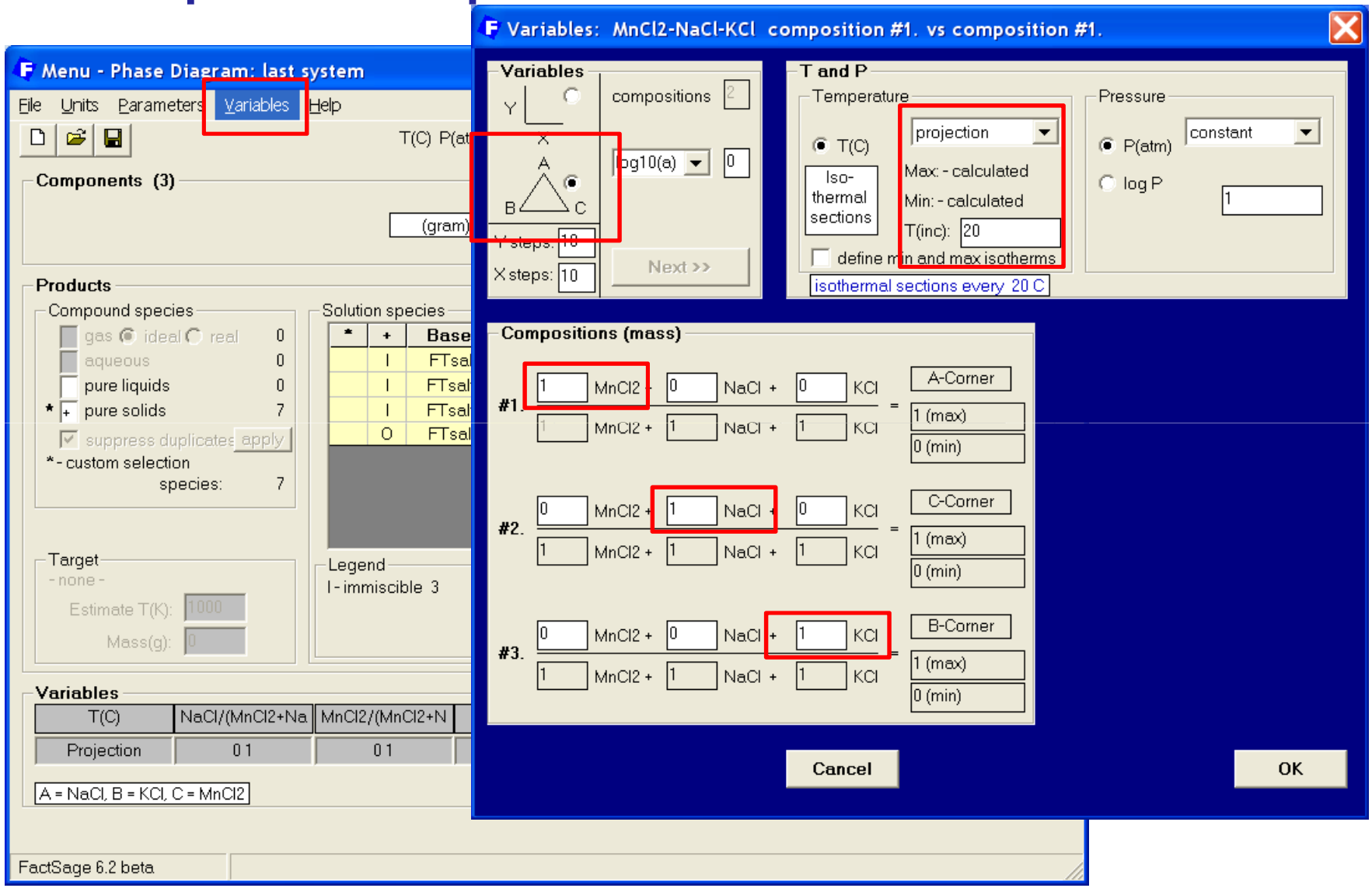

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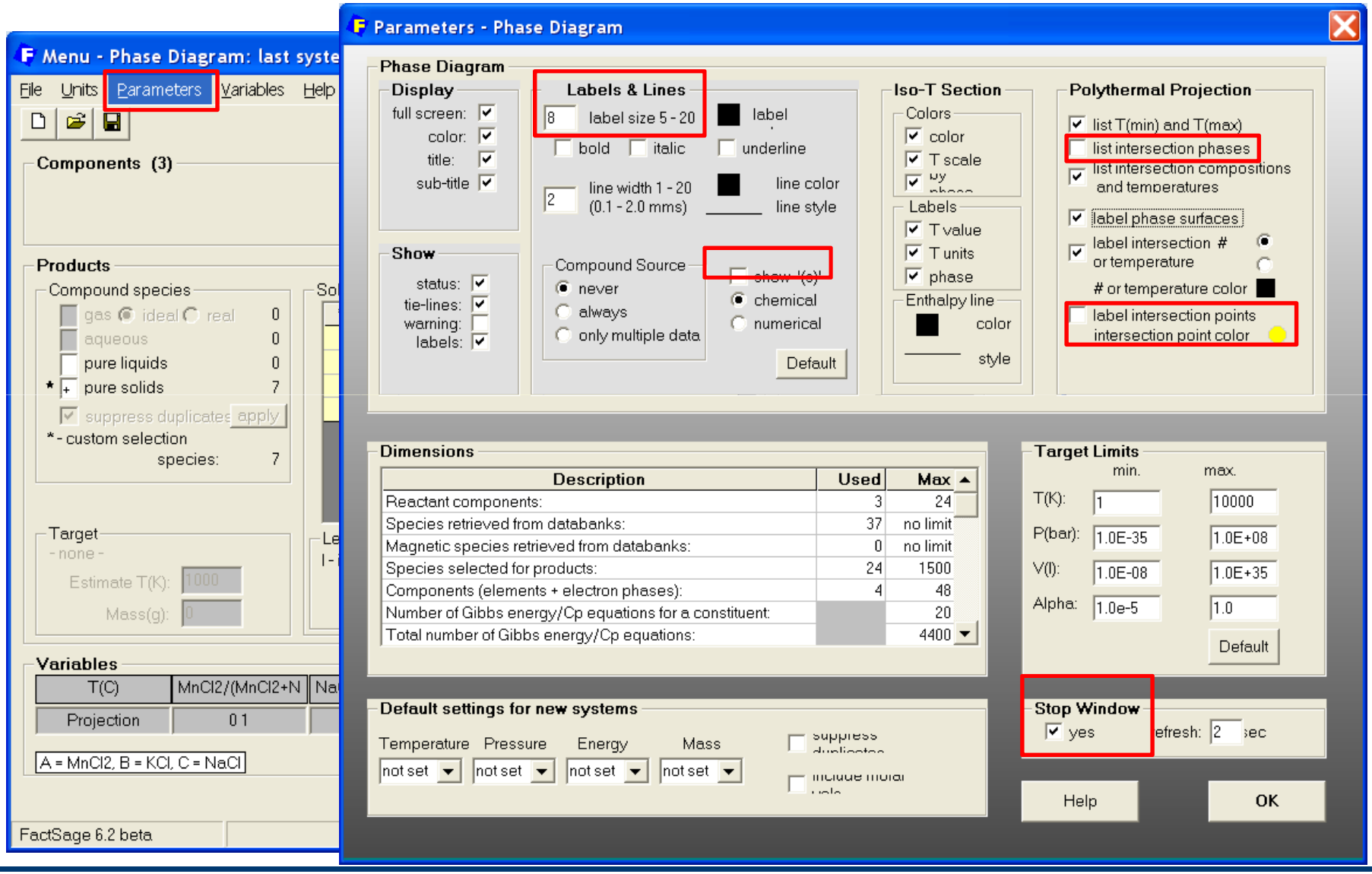

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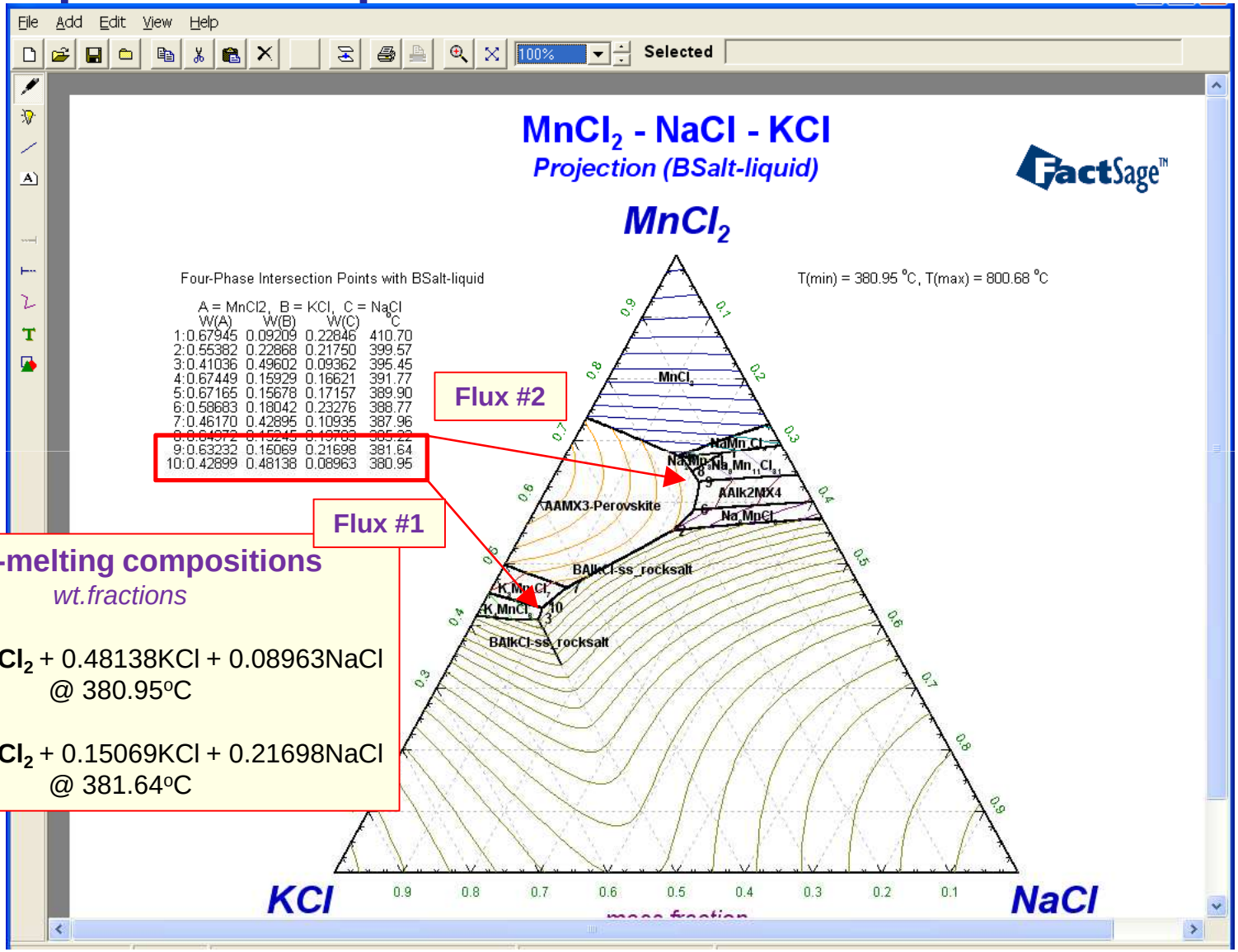

2 low-melting compositions
wt.fractions

0.42899 $MnCl_2$ + 0.48138KCl + 0.08963NaCl
@ 380.95°C

0.63232 $MnCl_2$ + 0.15069KCl + 0.21698NaCl
@ 381.64°C

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

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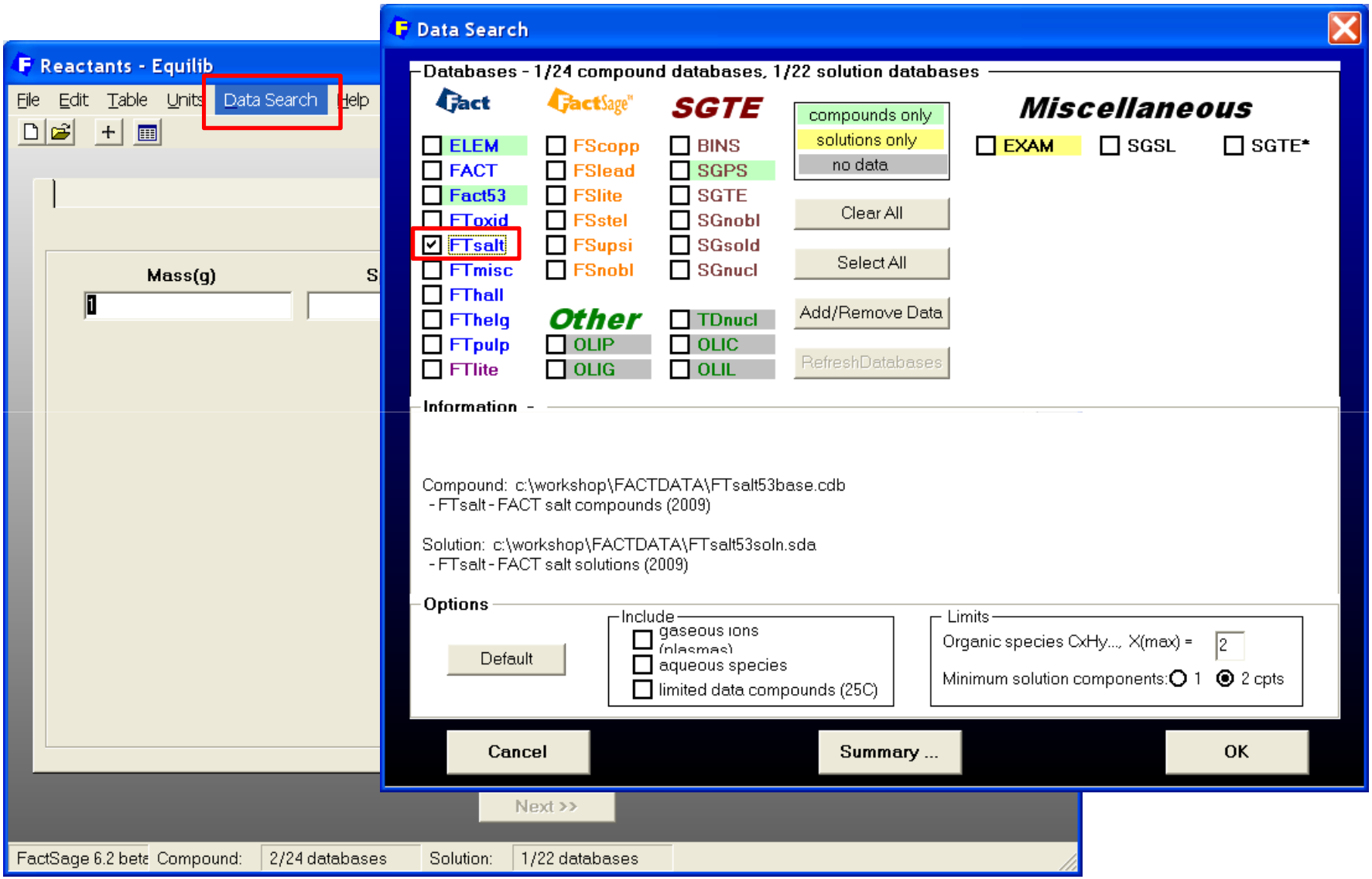

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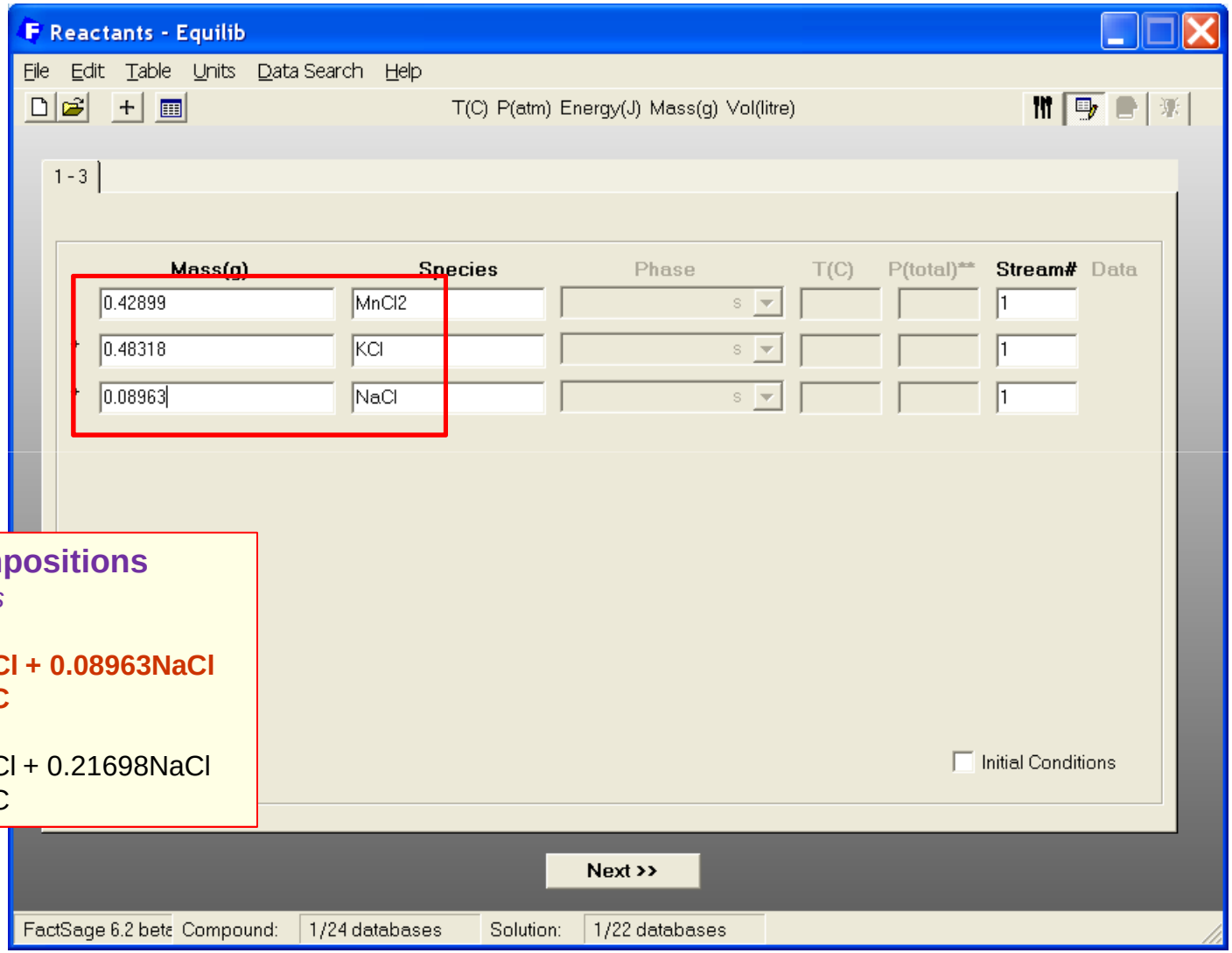

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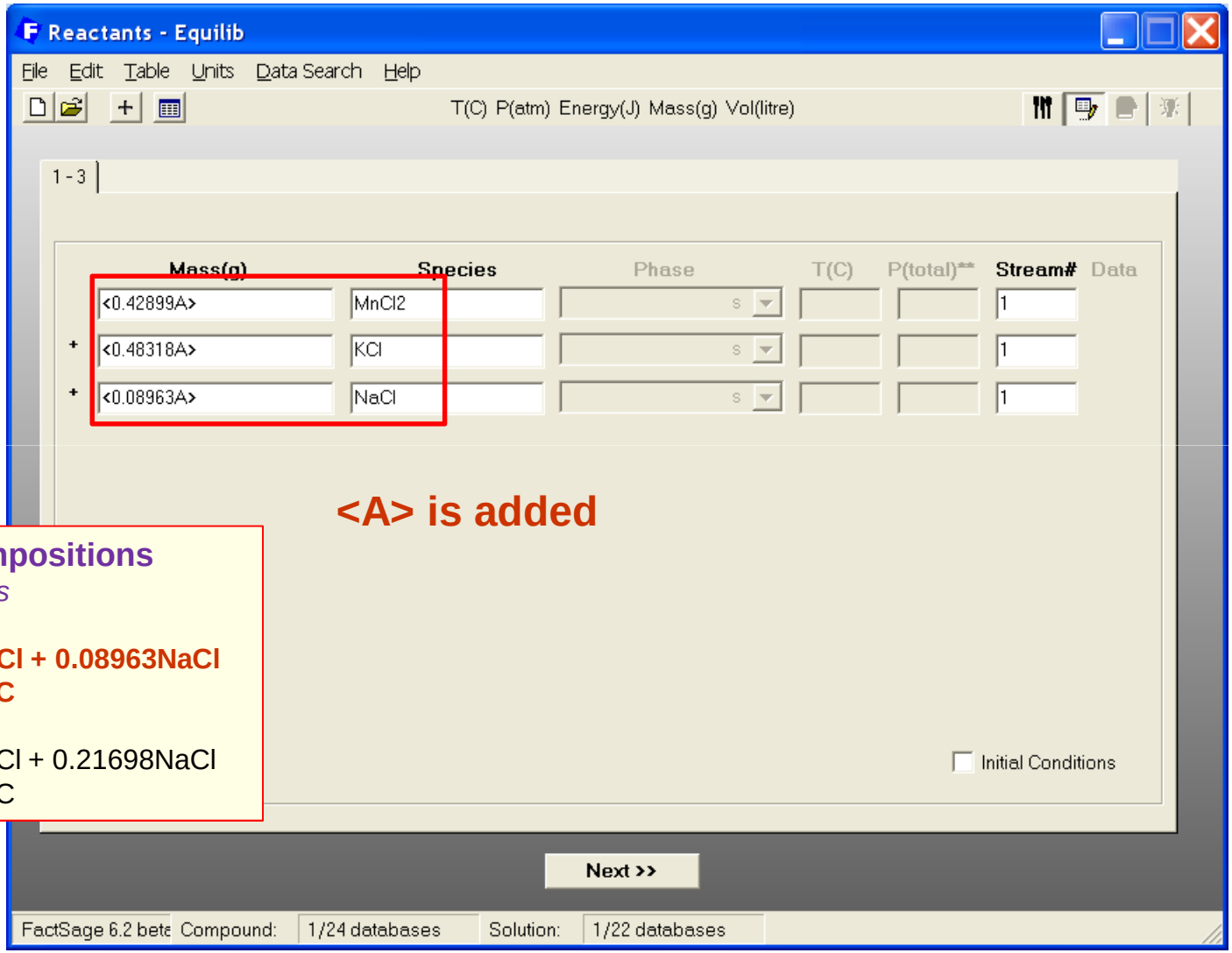

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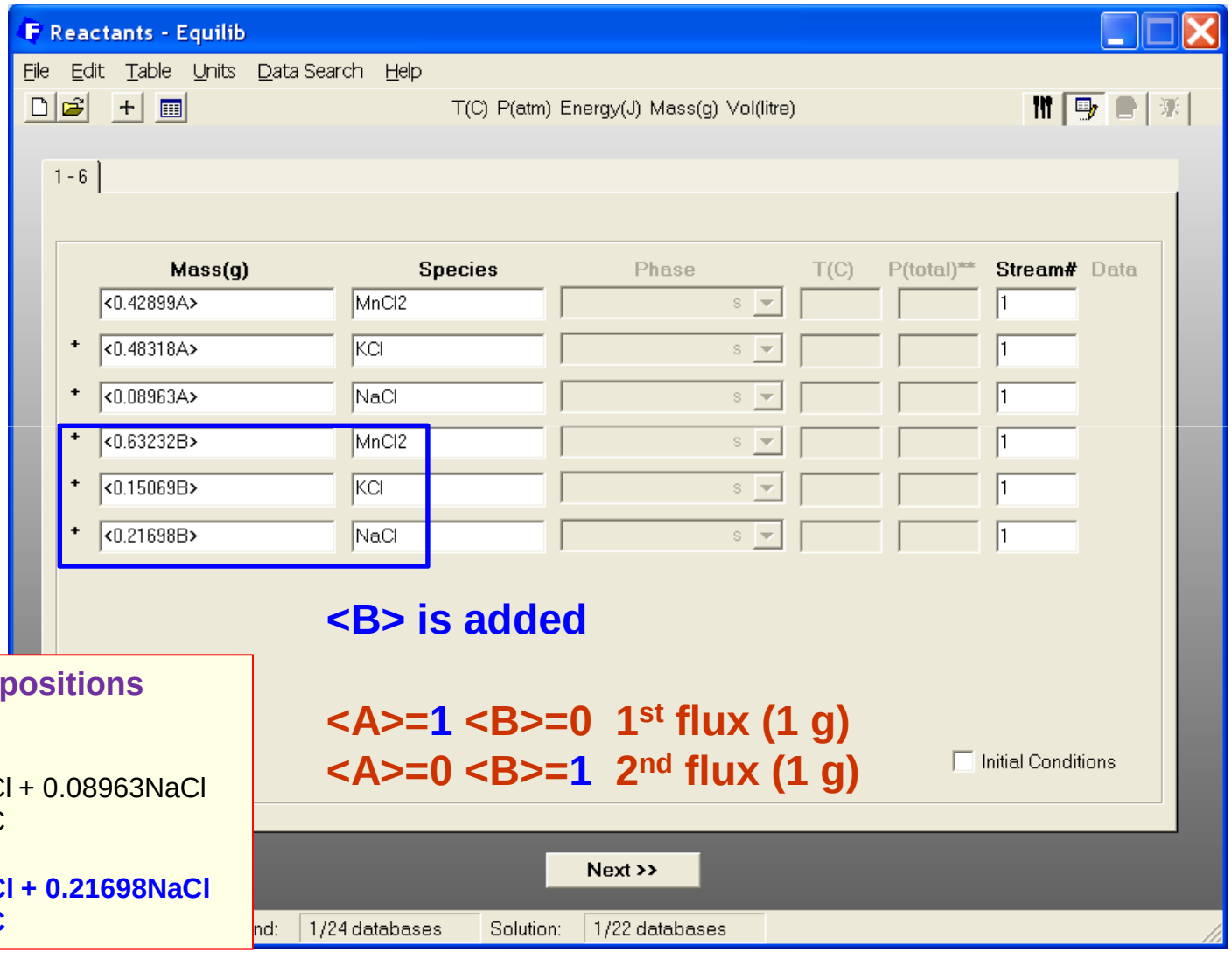

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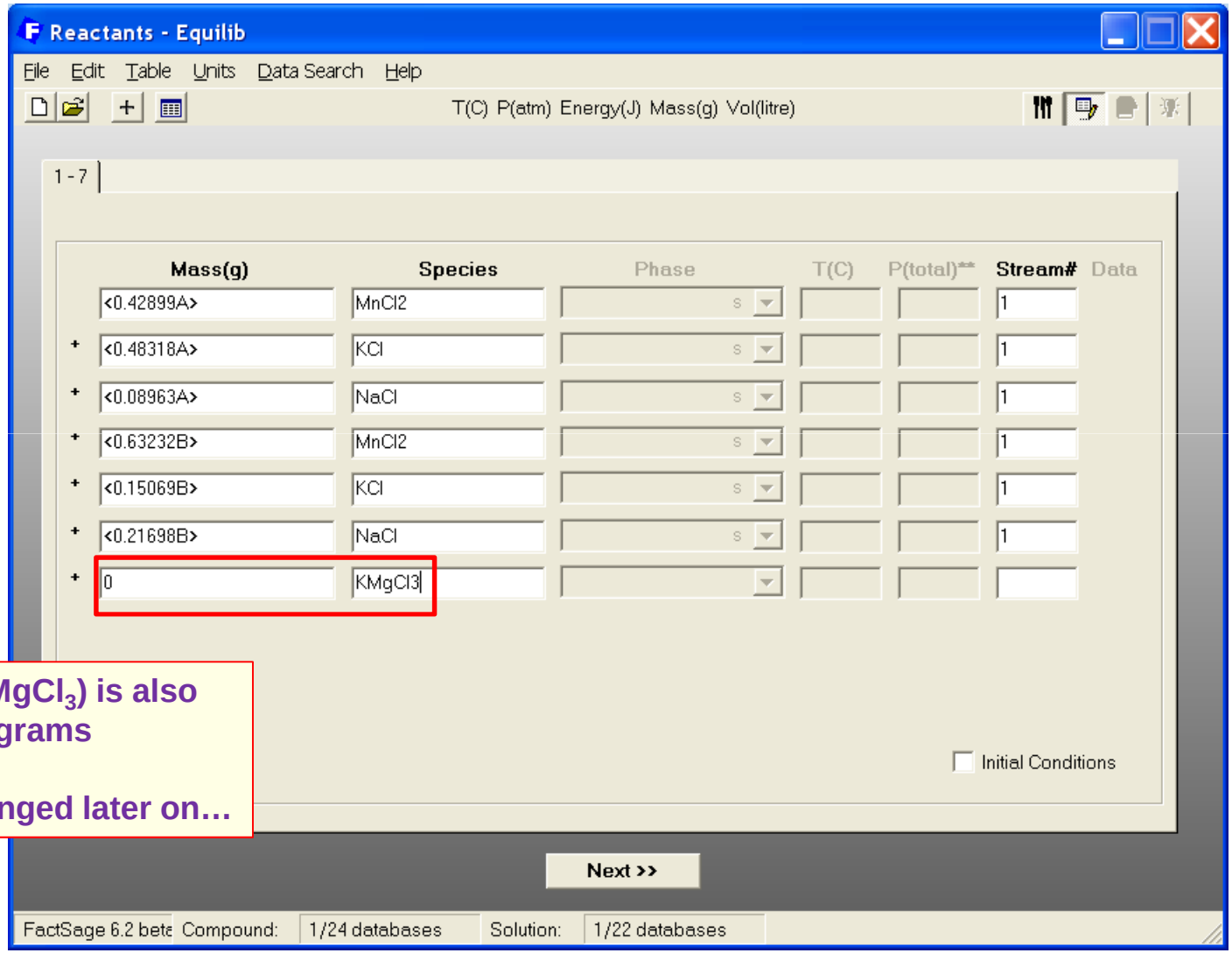


The reference flux ($KMgCl_3$) is also entered with 0 grams

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

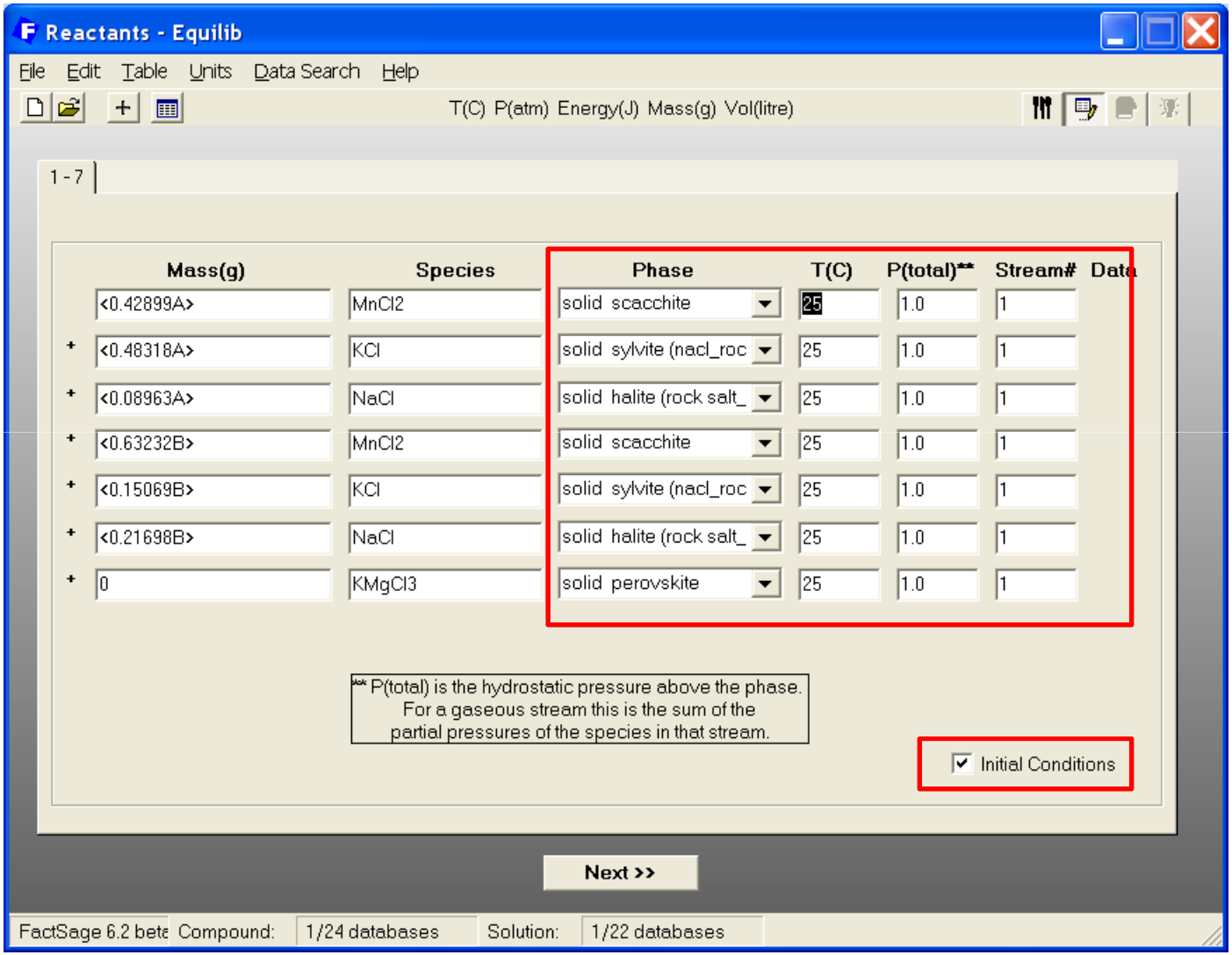
  GOAL : identify the lowest melting enthalpy

  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

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



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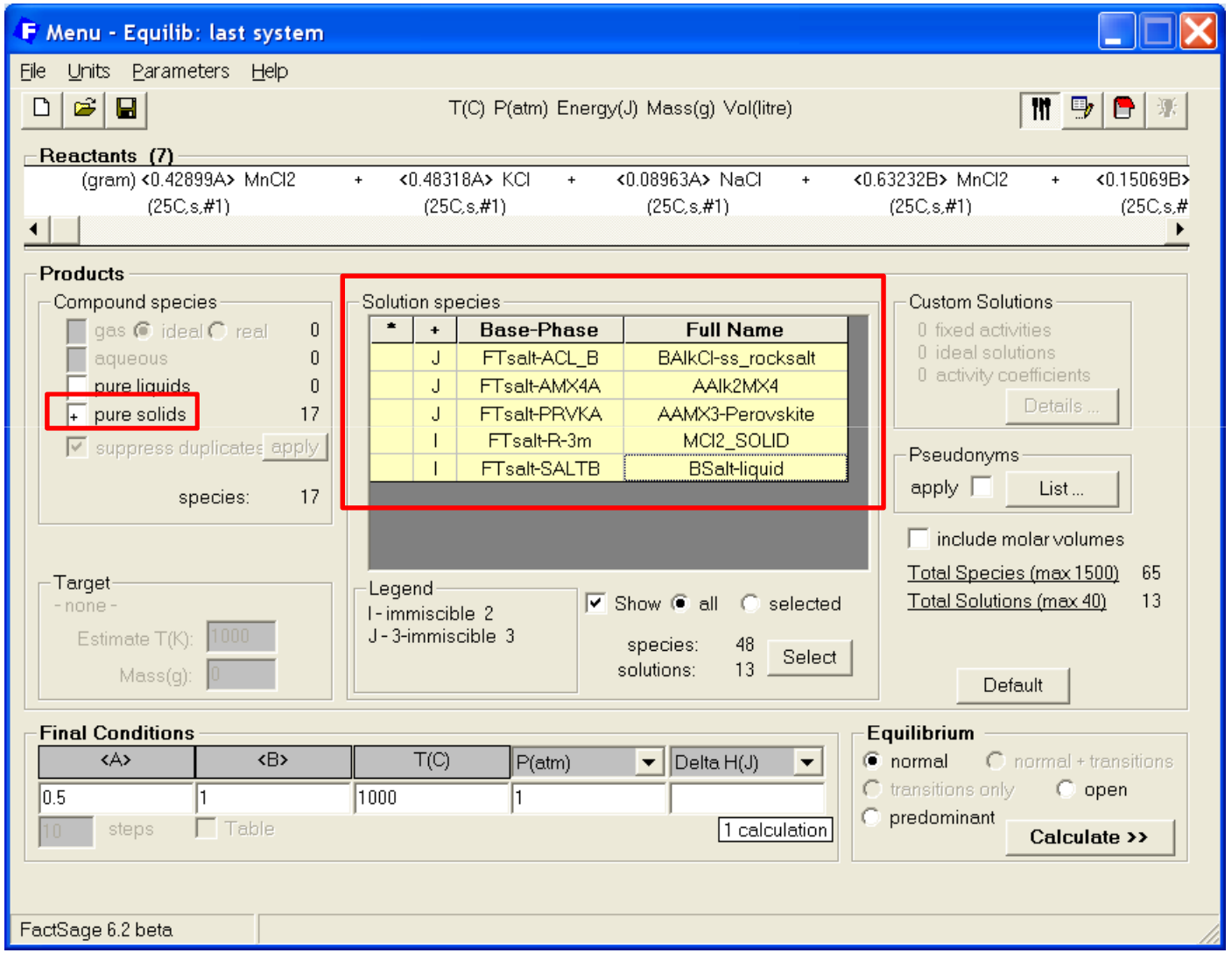

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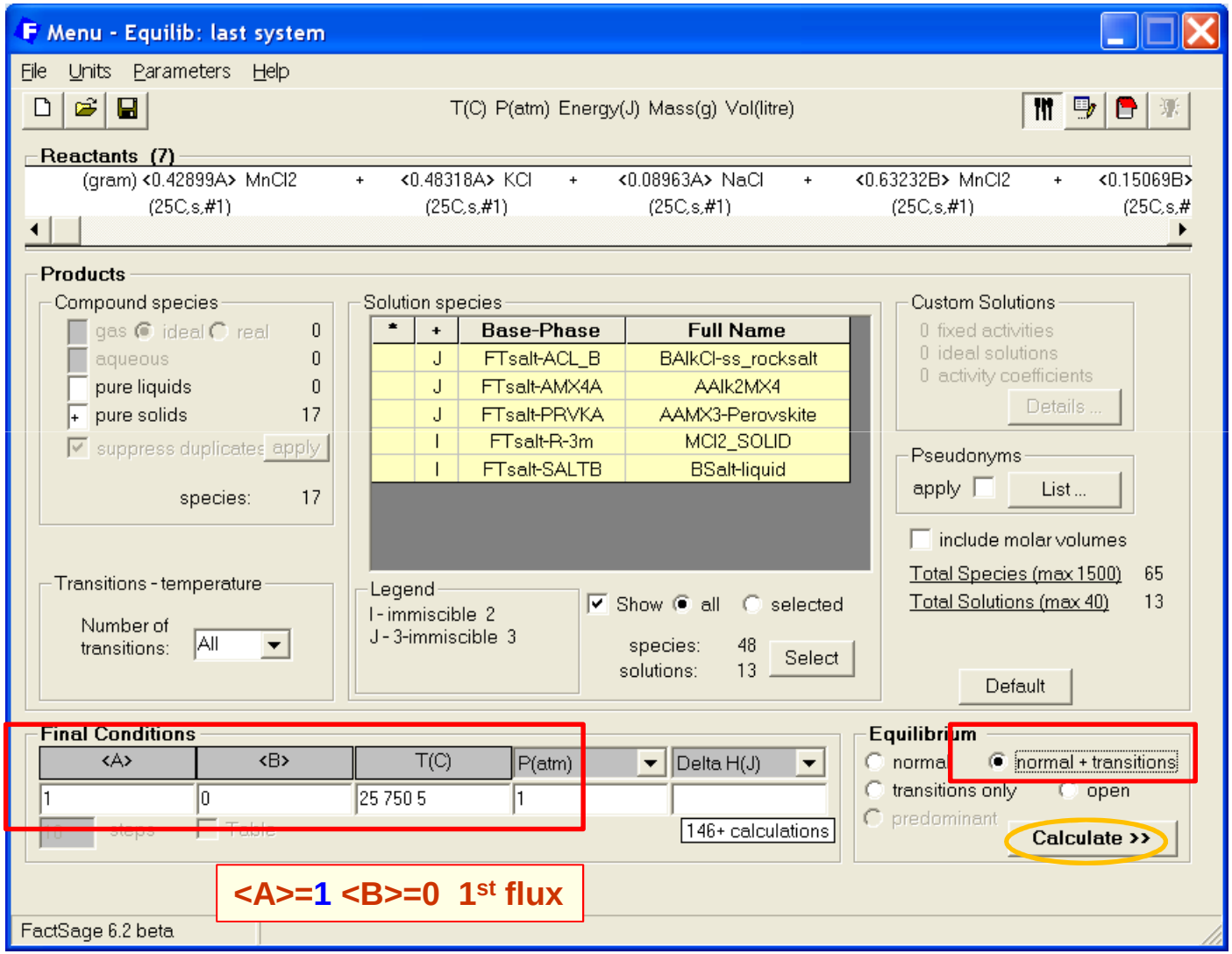

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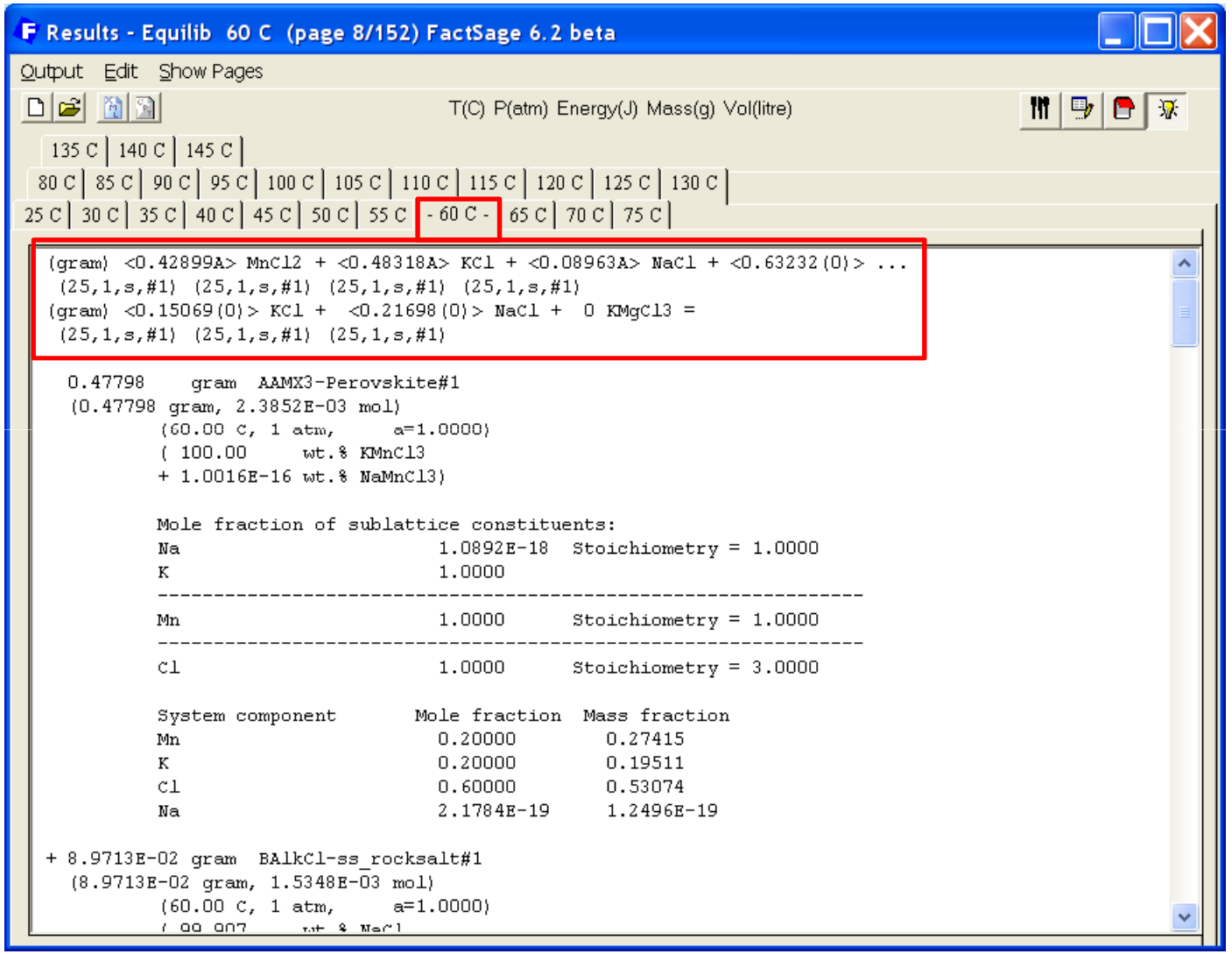

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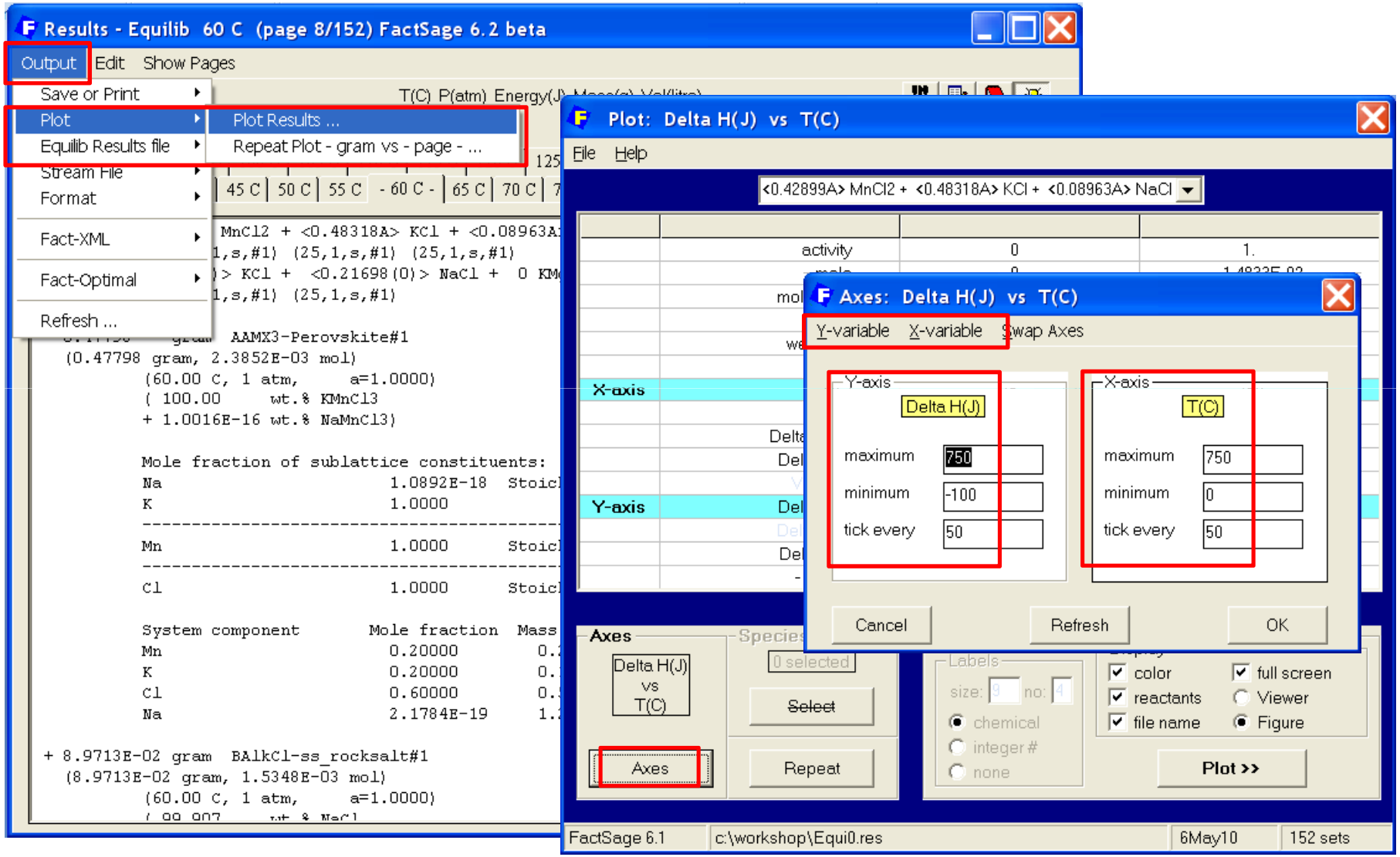
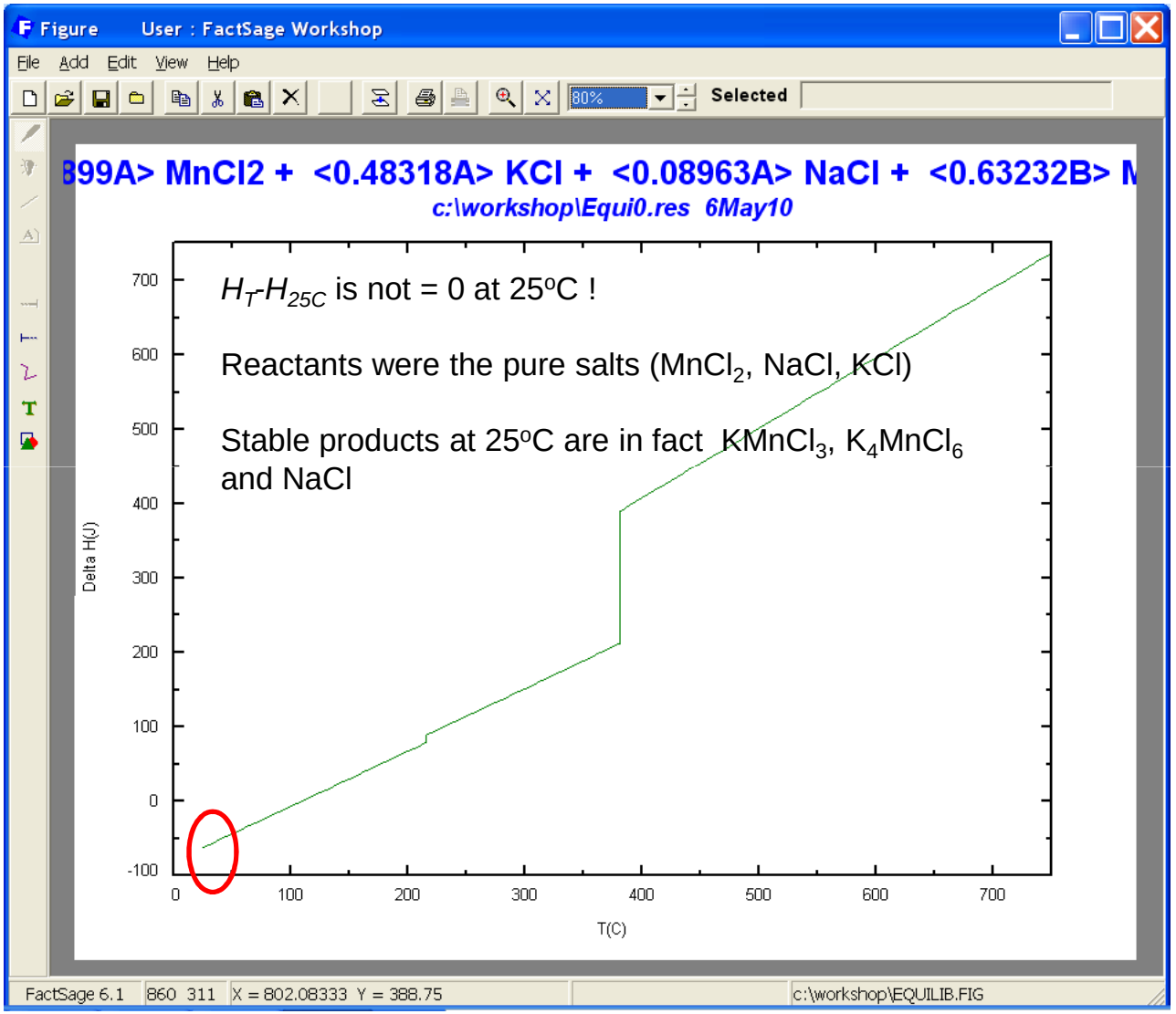


- **Example #2: Comparison of 2 salt fluxes for alkali removal**



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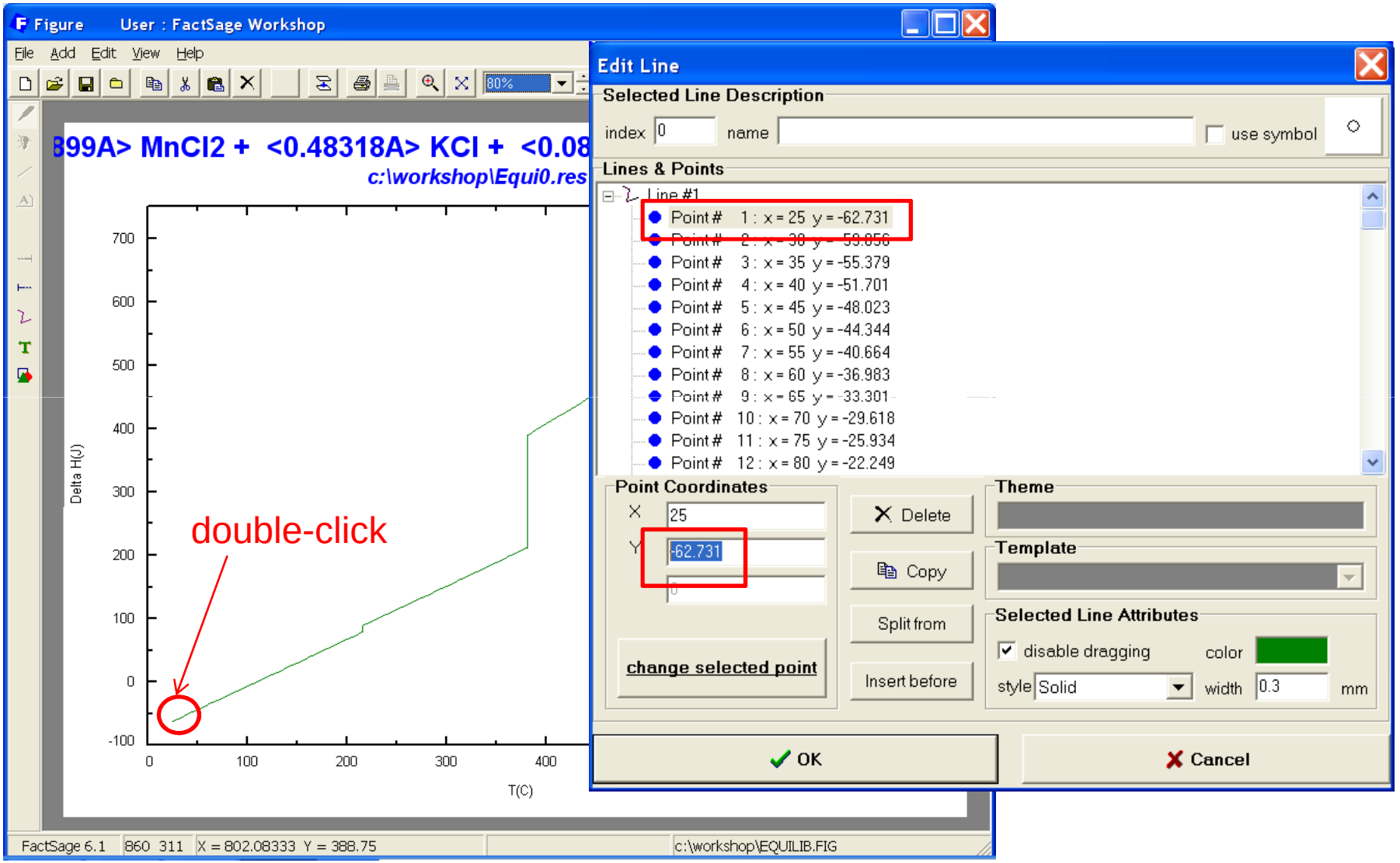

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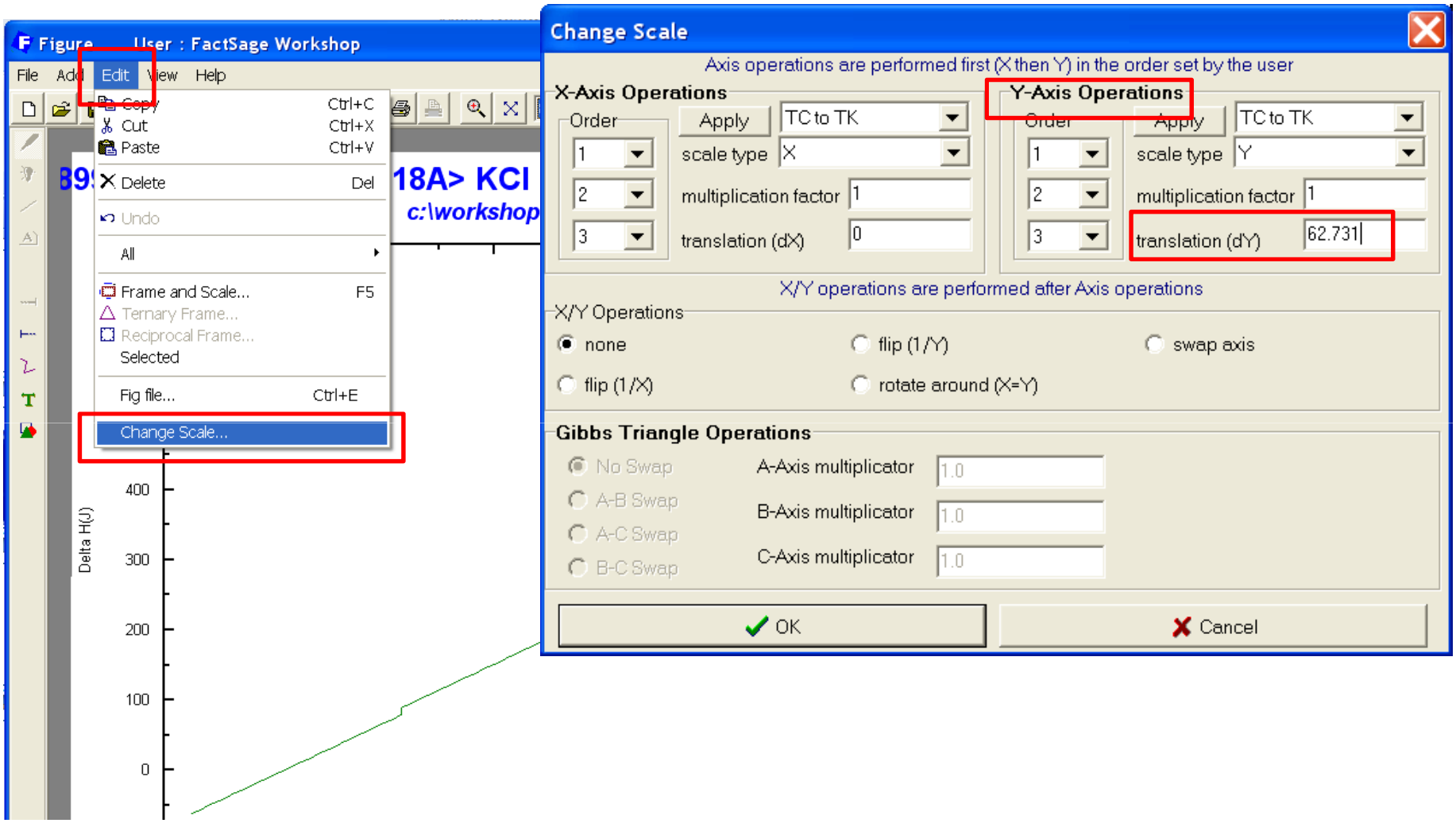

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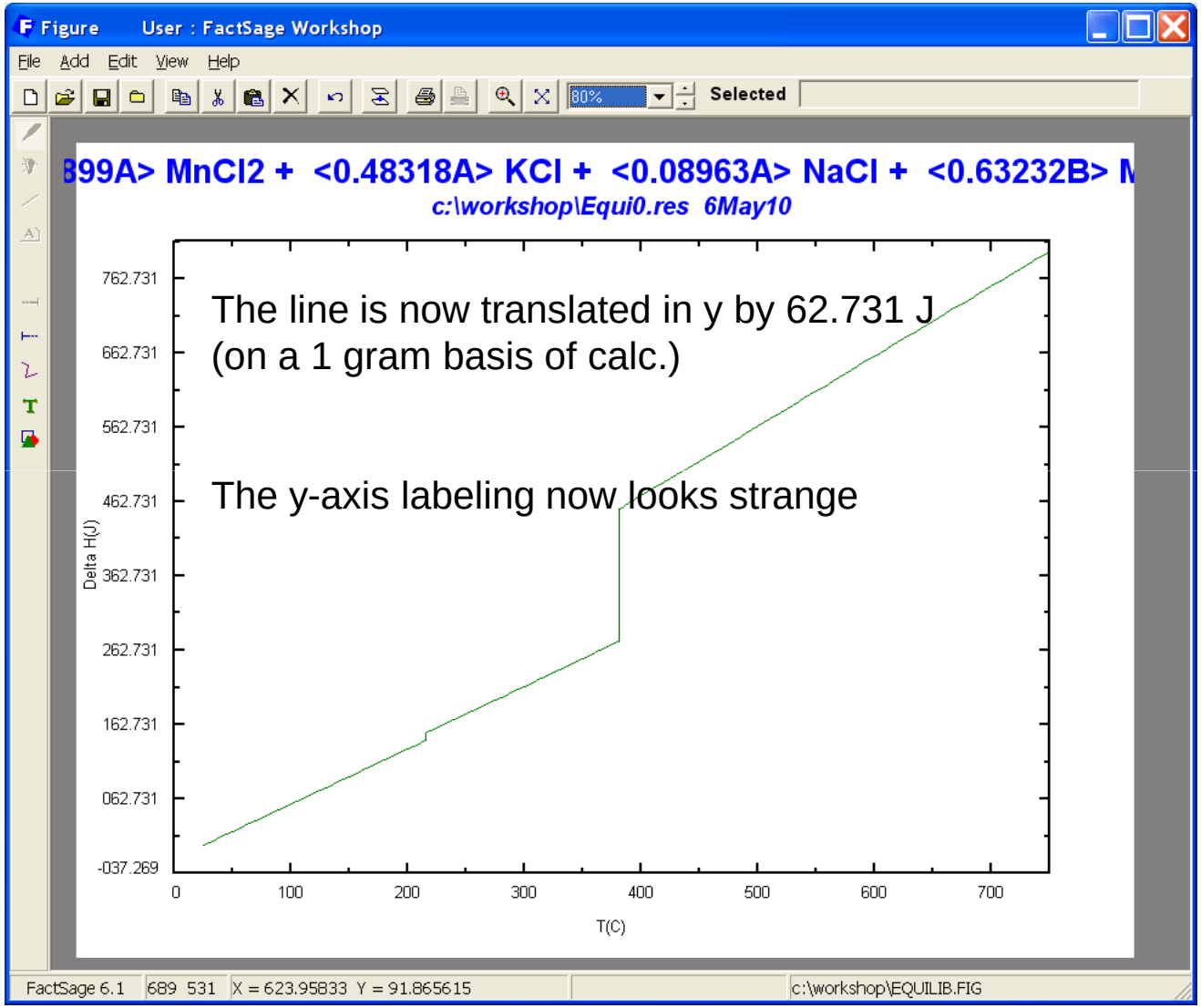

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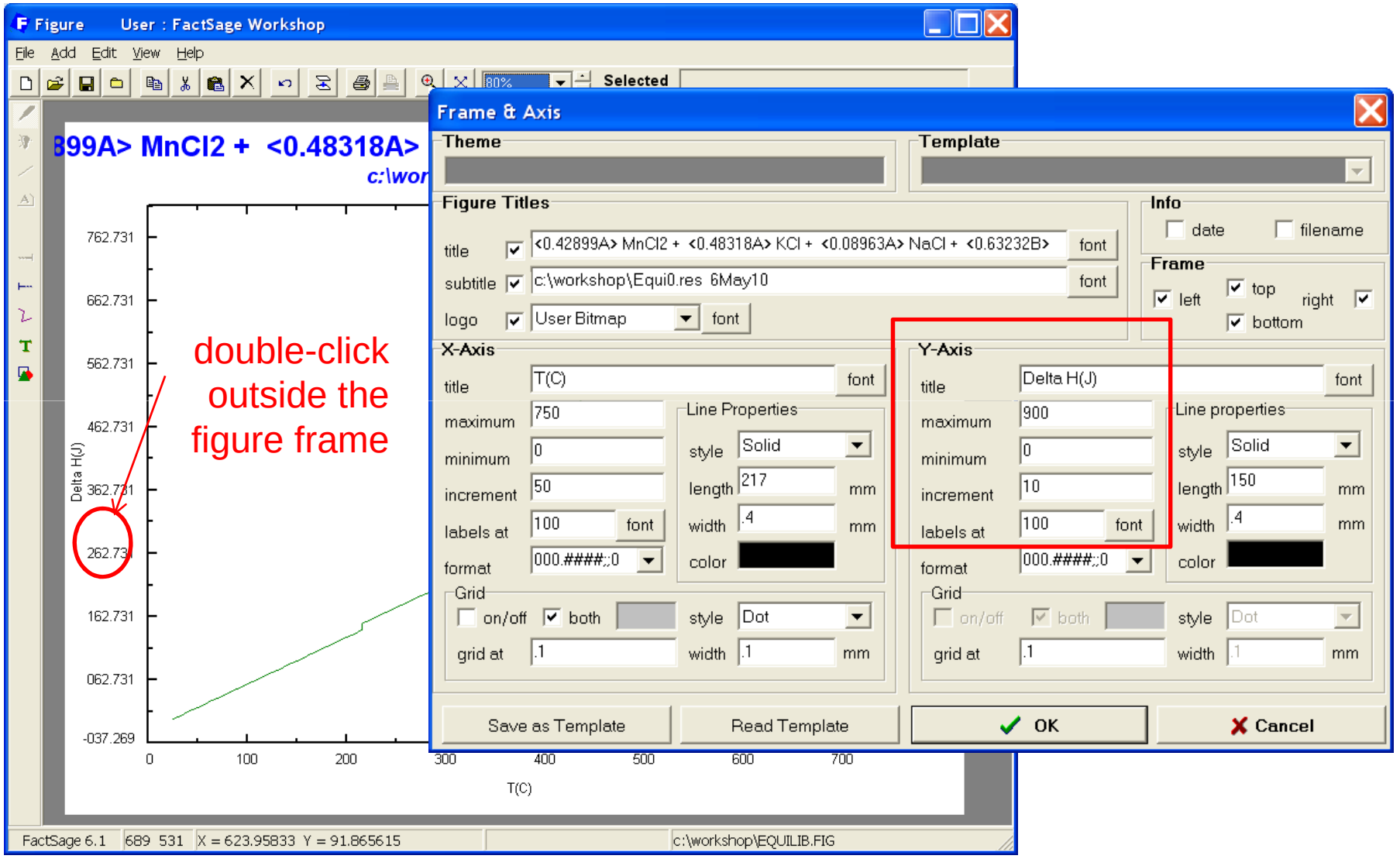

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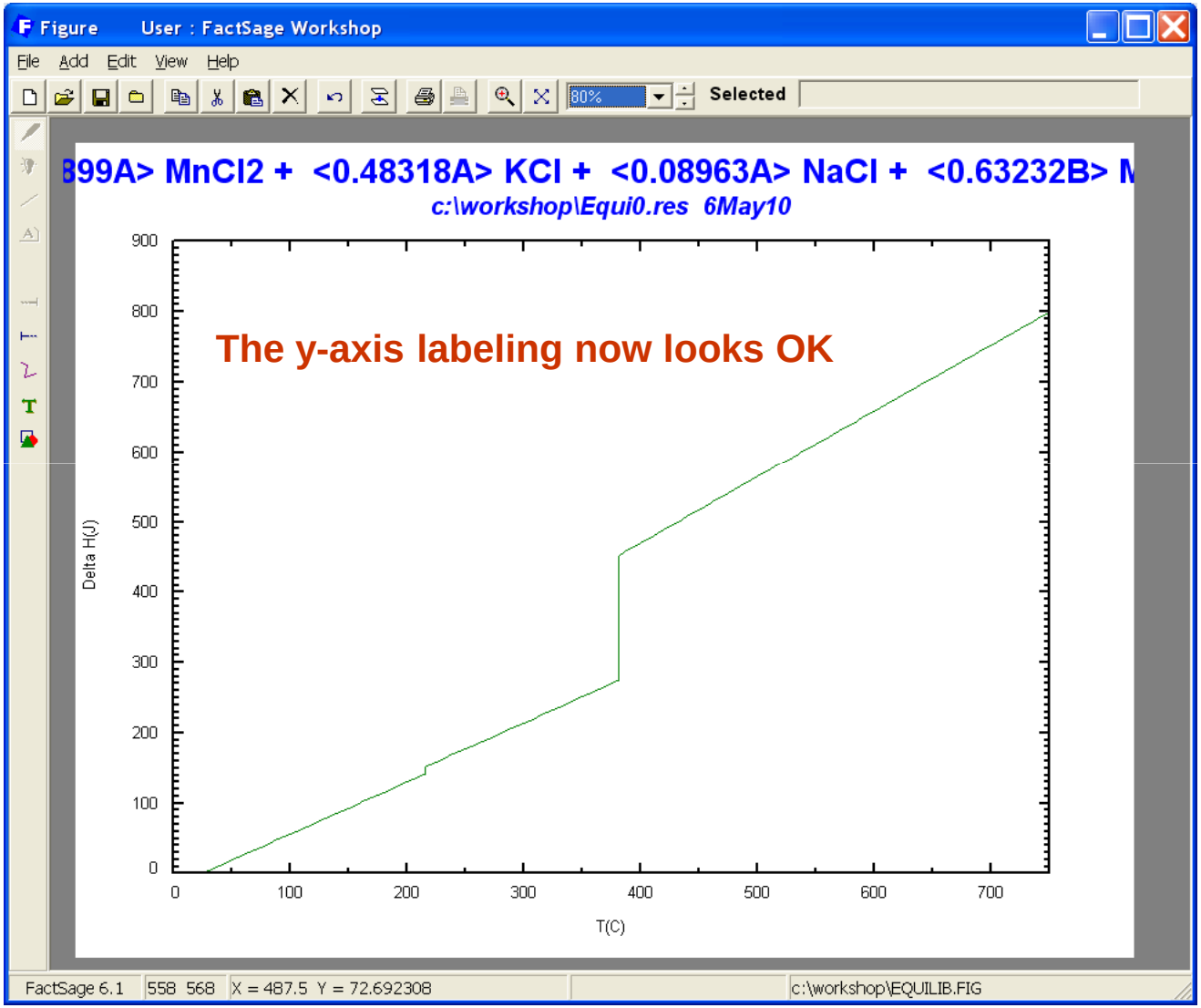

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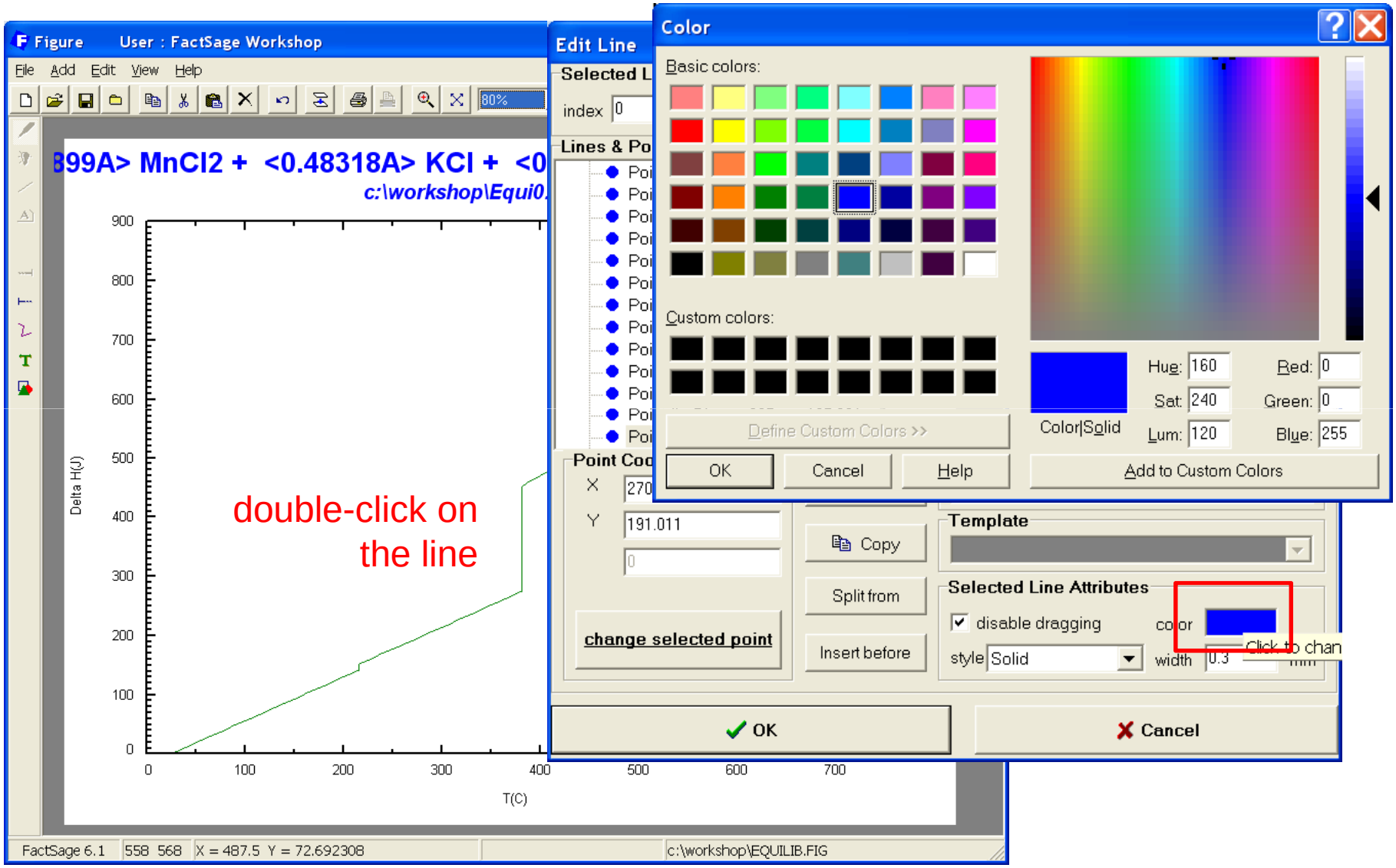

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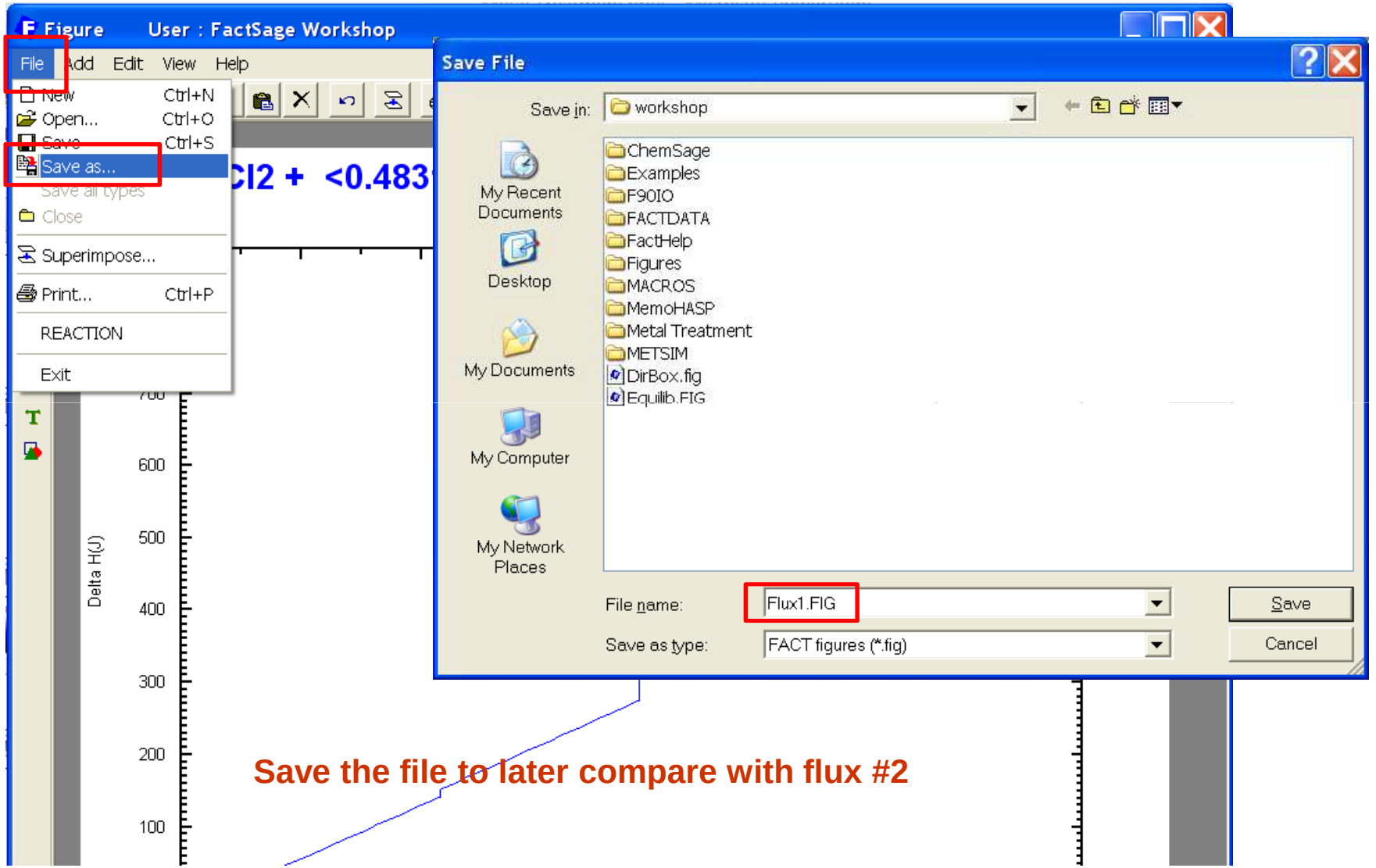

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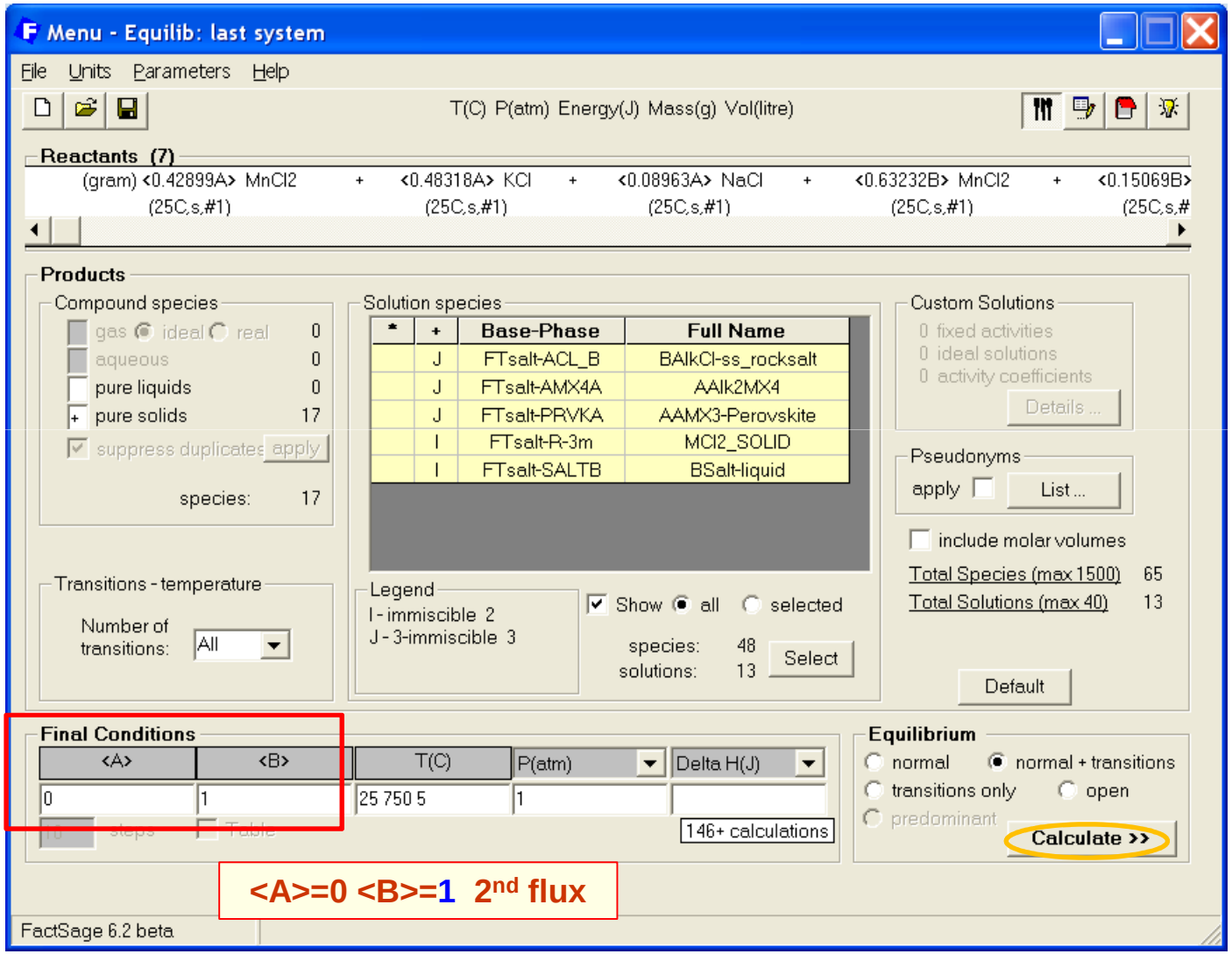

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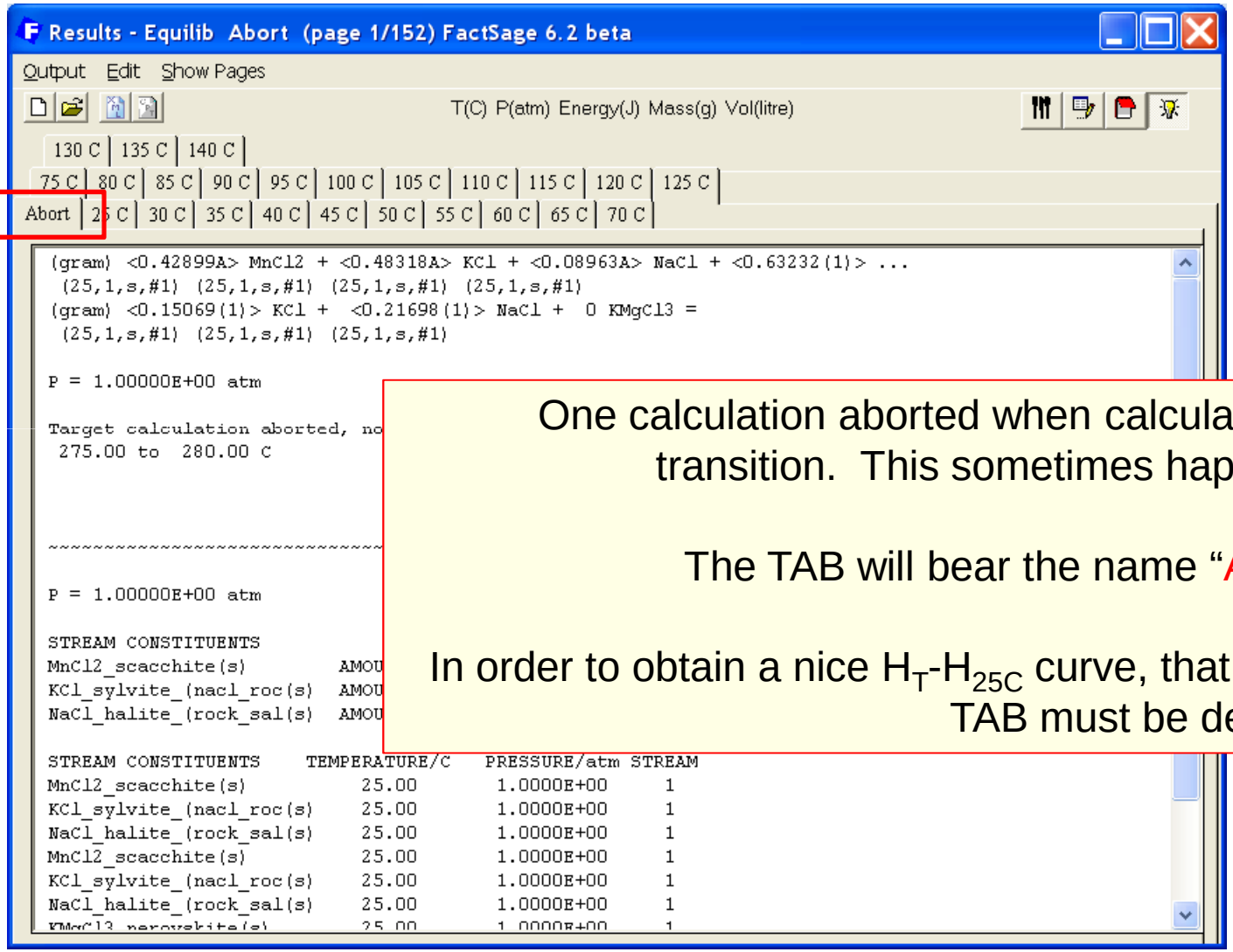
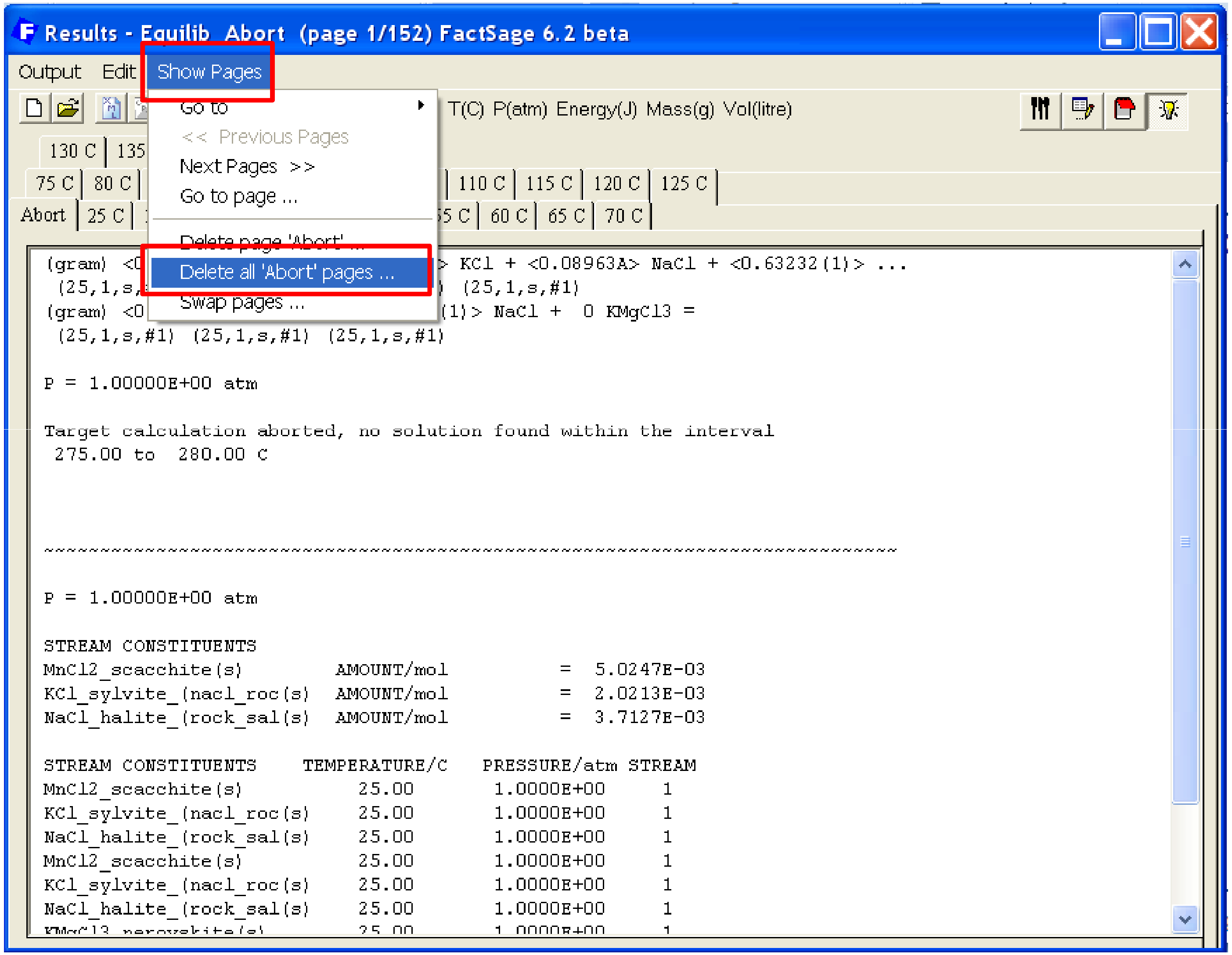


One calculation aborted when calculating a transition. This sometimes happens.

The TAB will bear the name "Abort"

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

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



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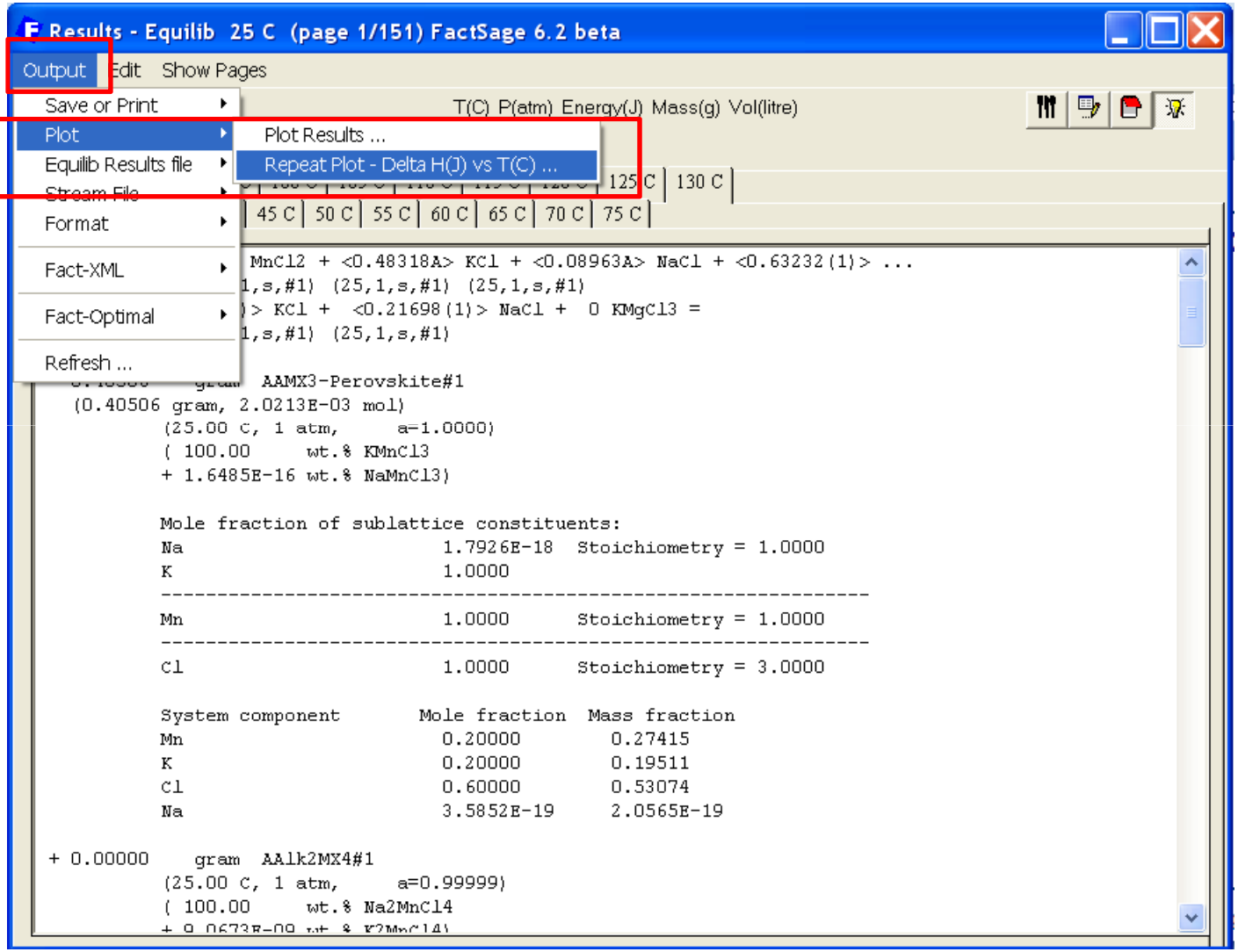

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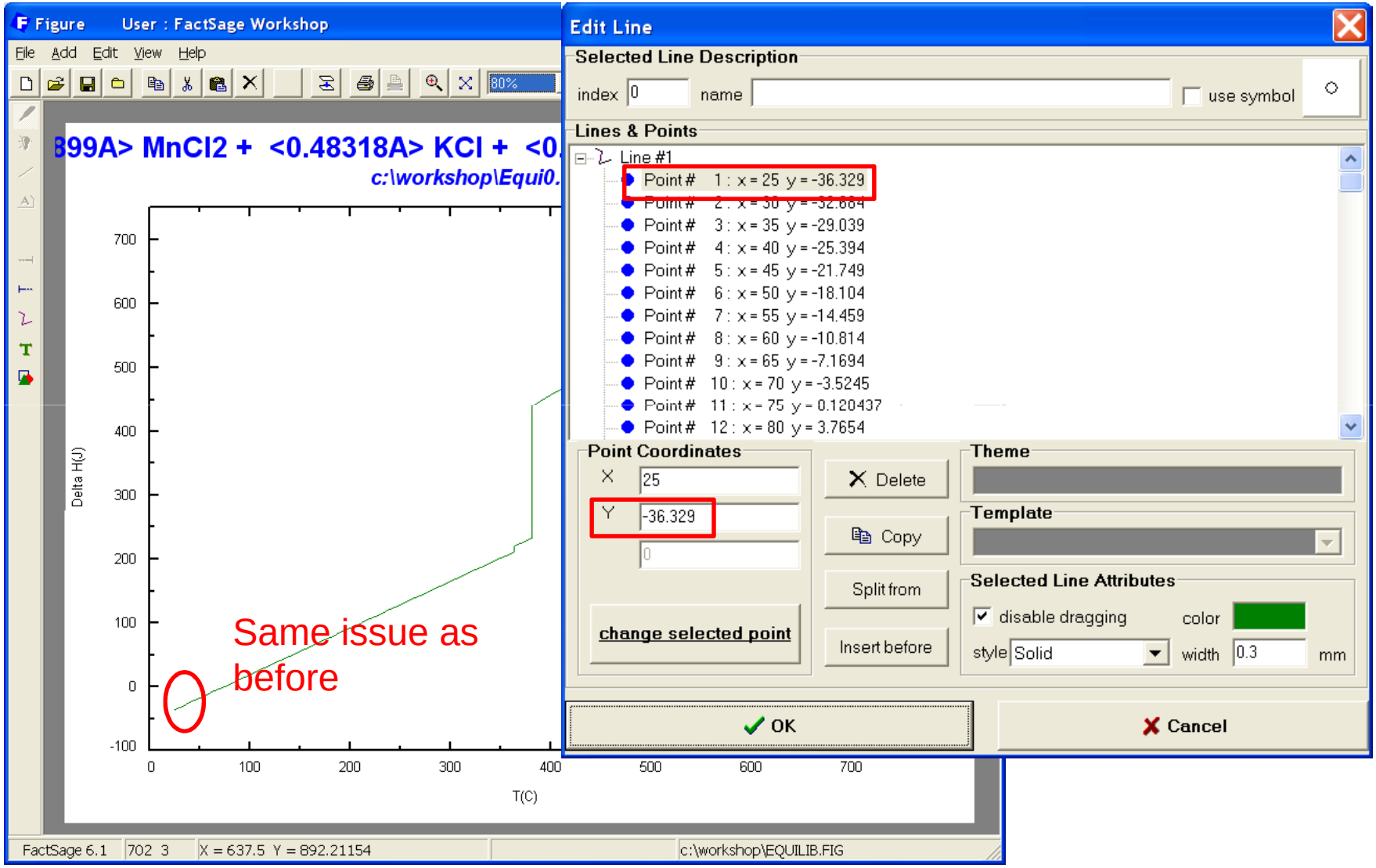
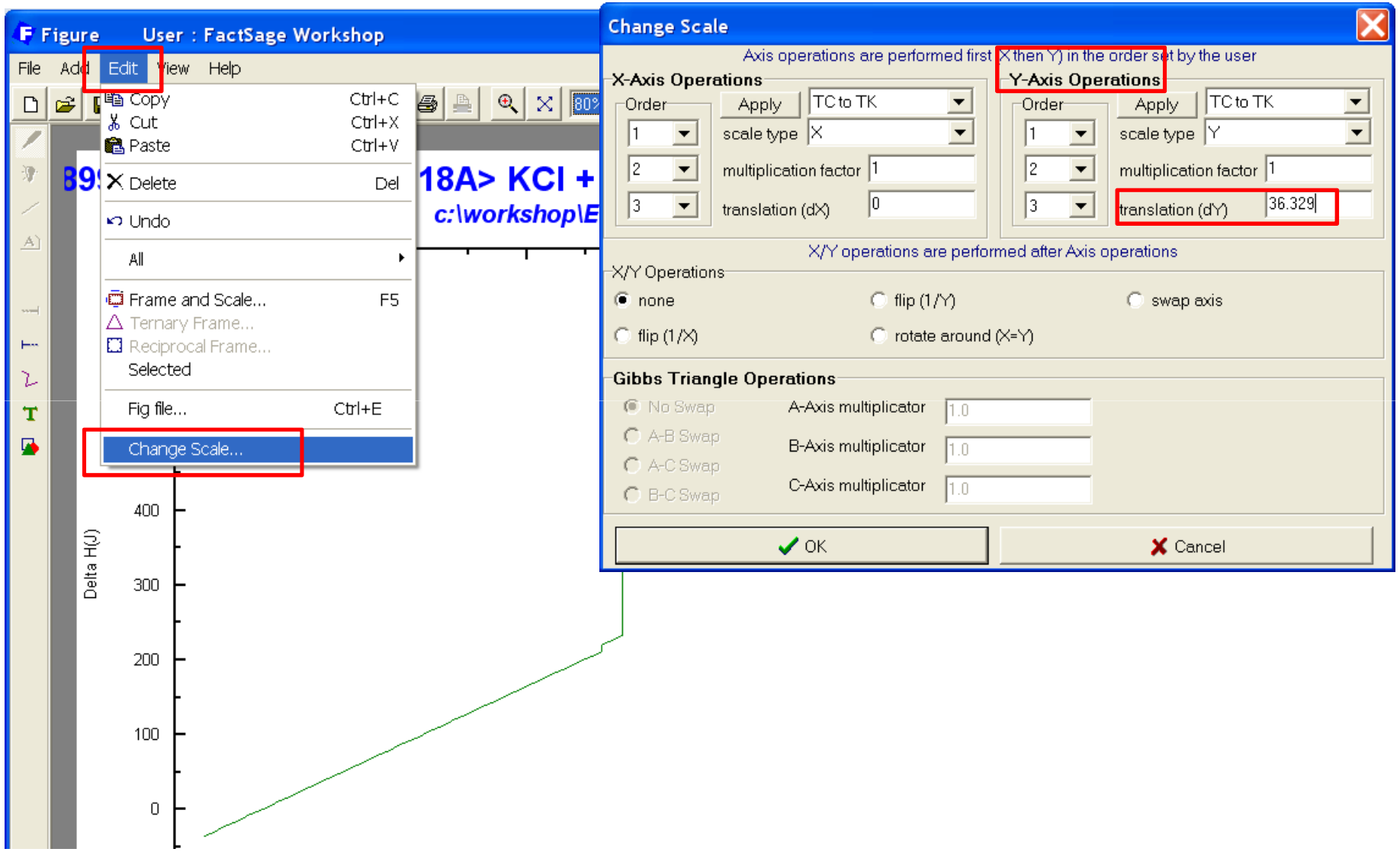


- **Example #2: Comparison of 2 salt fluxes for alkali removal**



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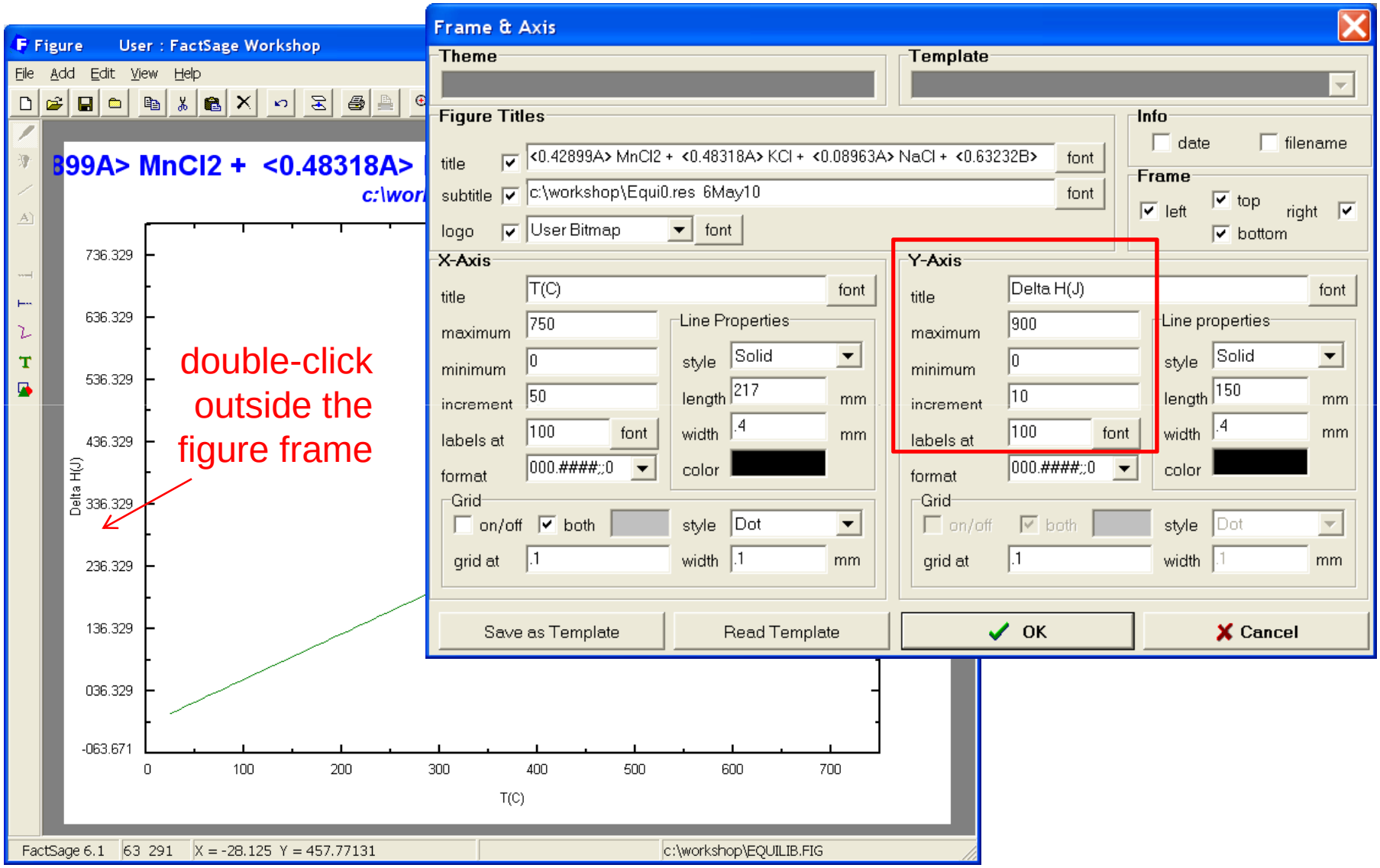
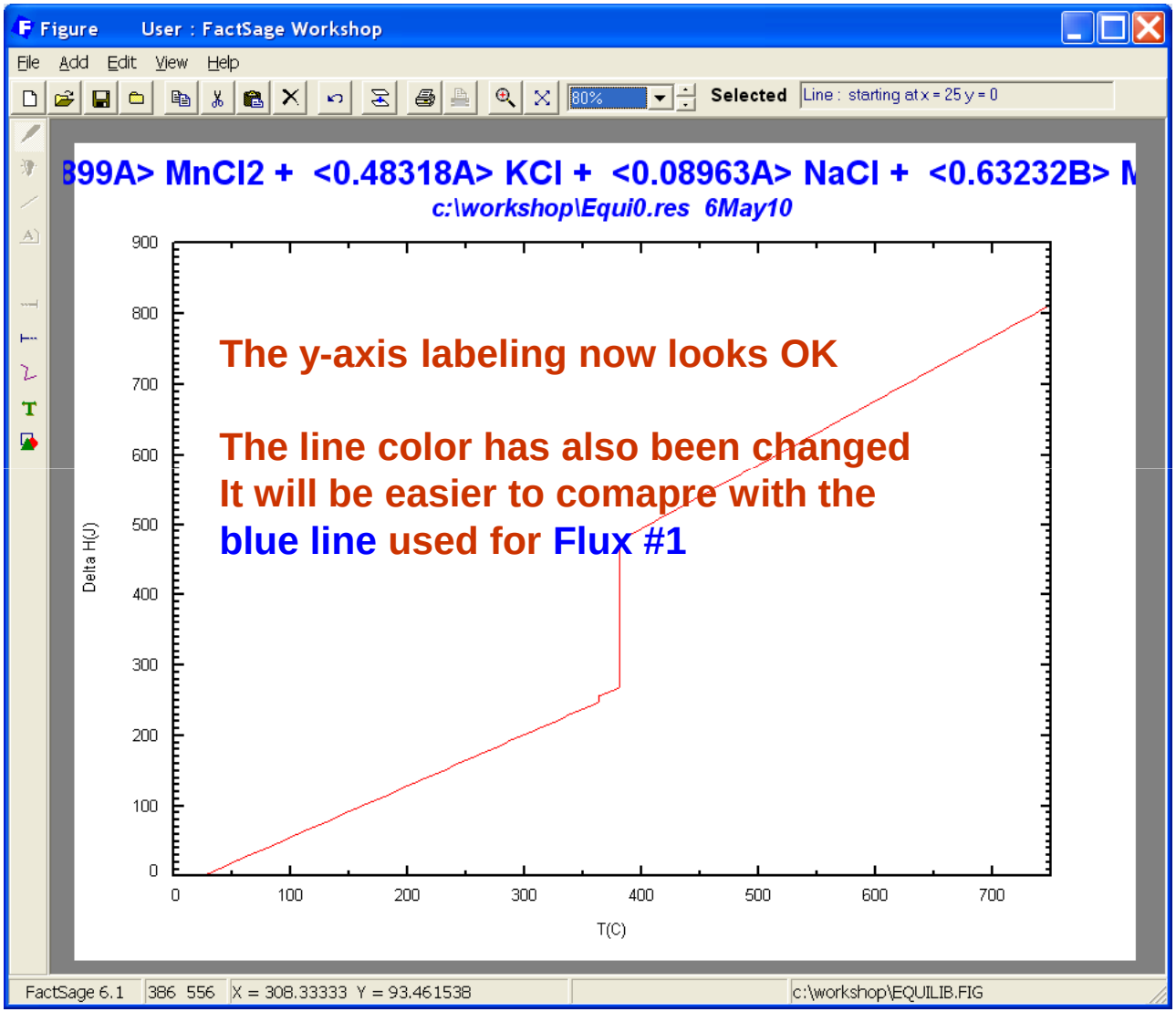
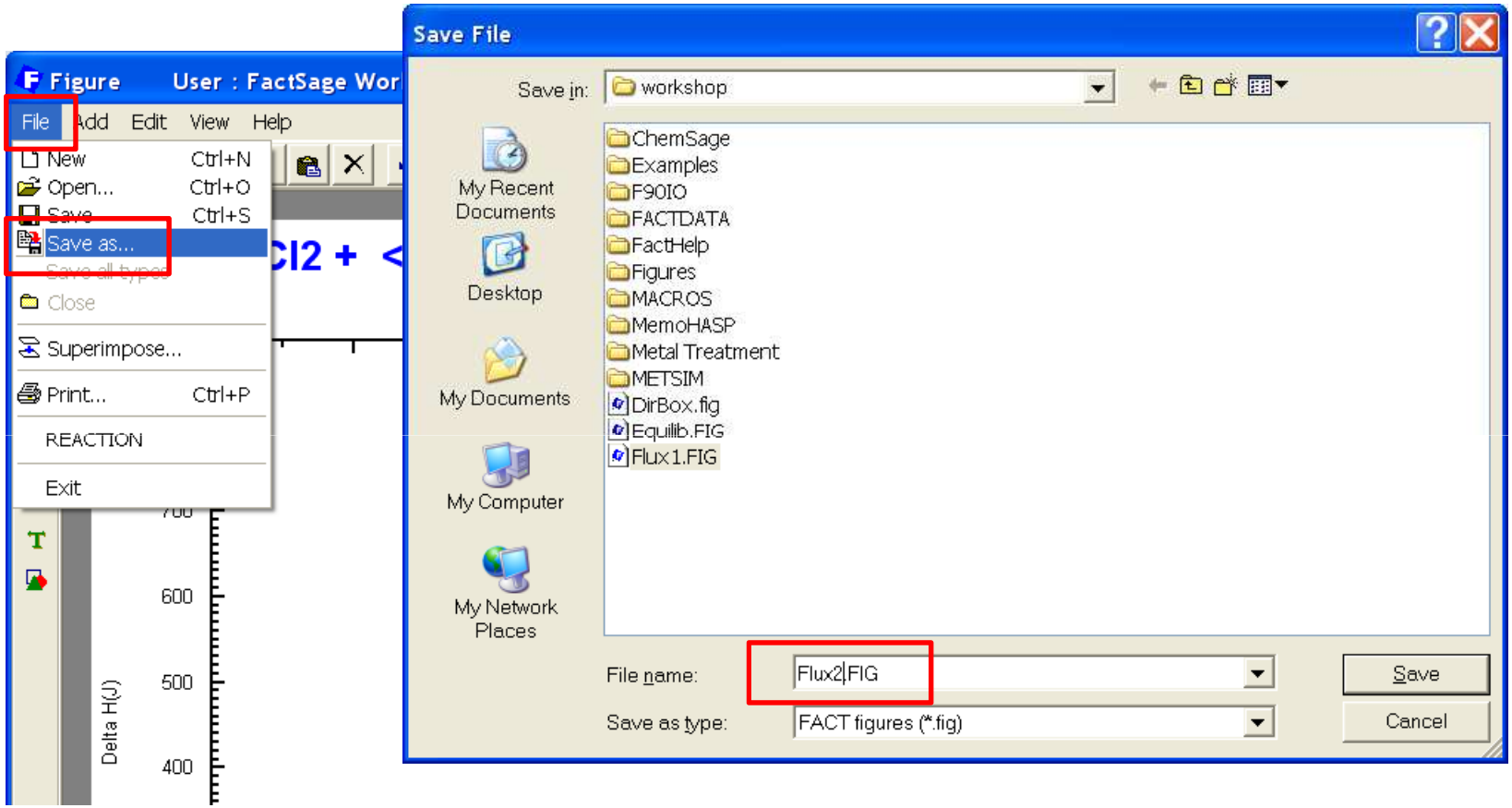


- **Example #2: Comparison of 2 salt fluxes for alkali removal**



- **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 → NaCl-KCl-$MnCl_2$:

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

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

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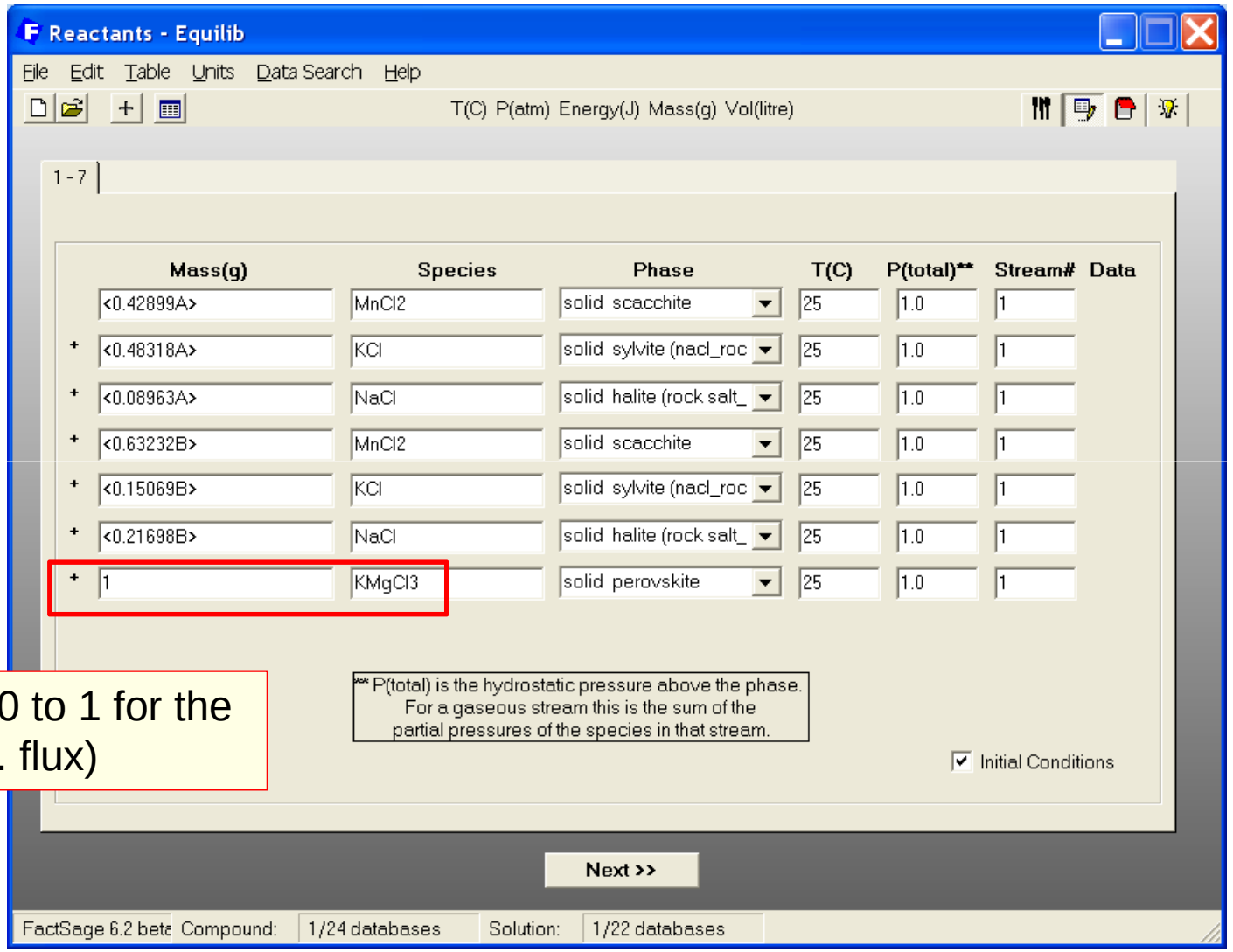
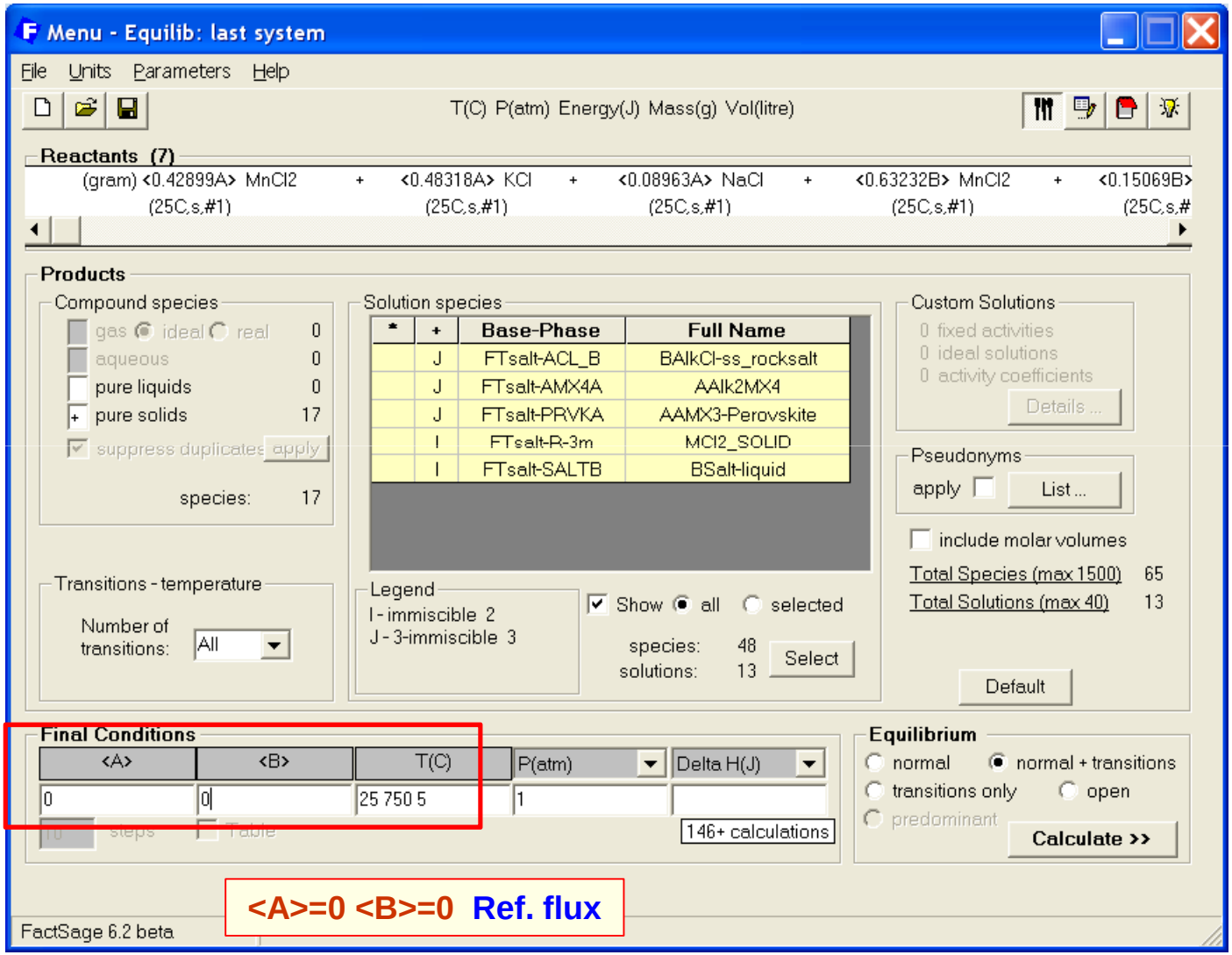
- **Example #2: Comparison of 2 salt fluxes for alkali removal**



Change value from 0 to 1 for the input of $KMgCl_3$ (ref. flux)

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



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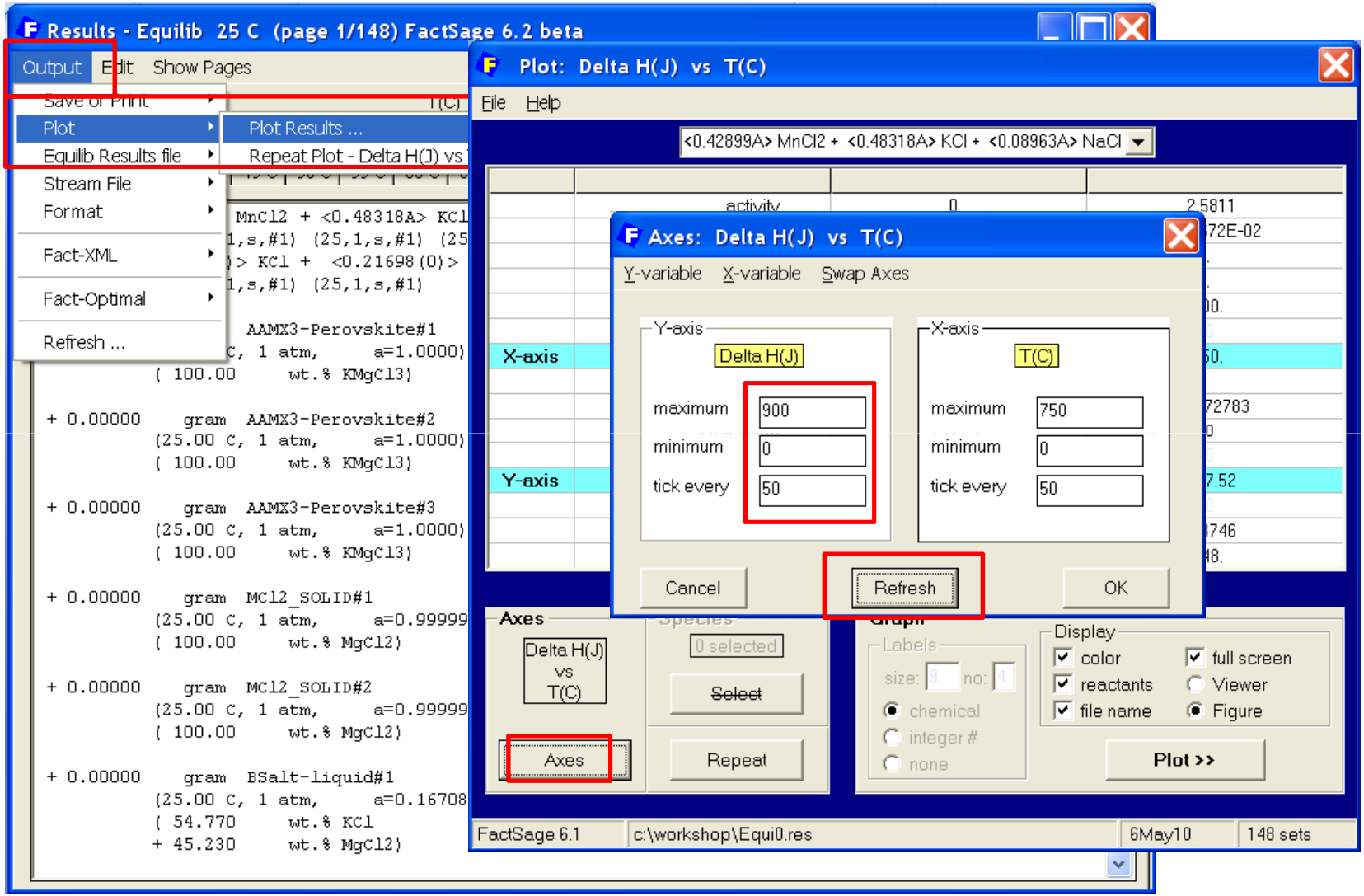

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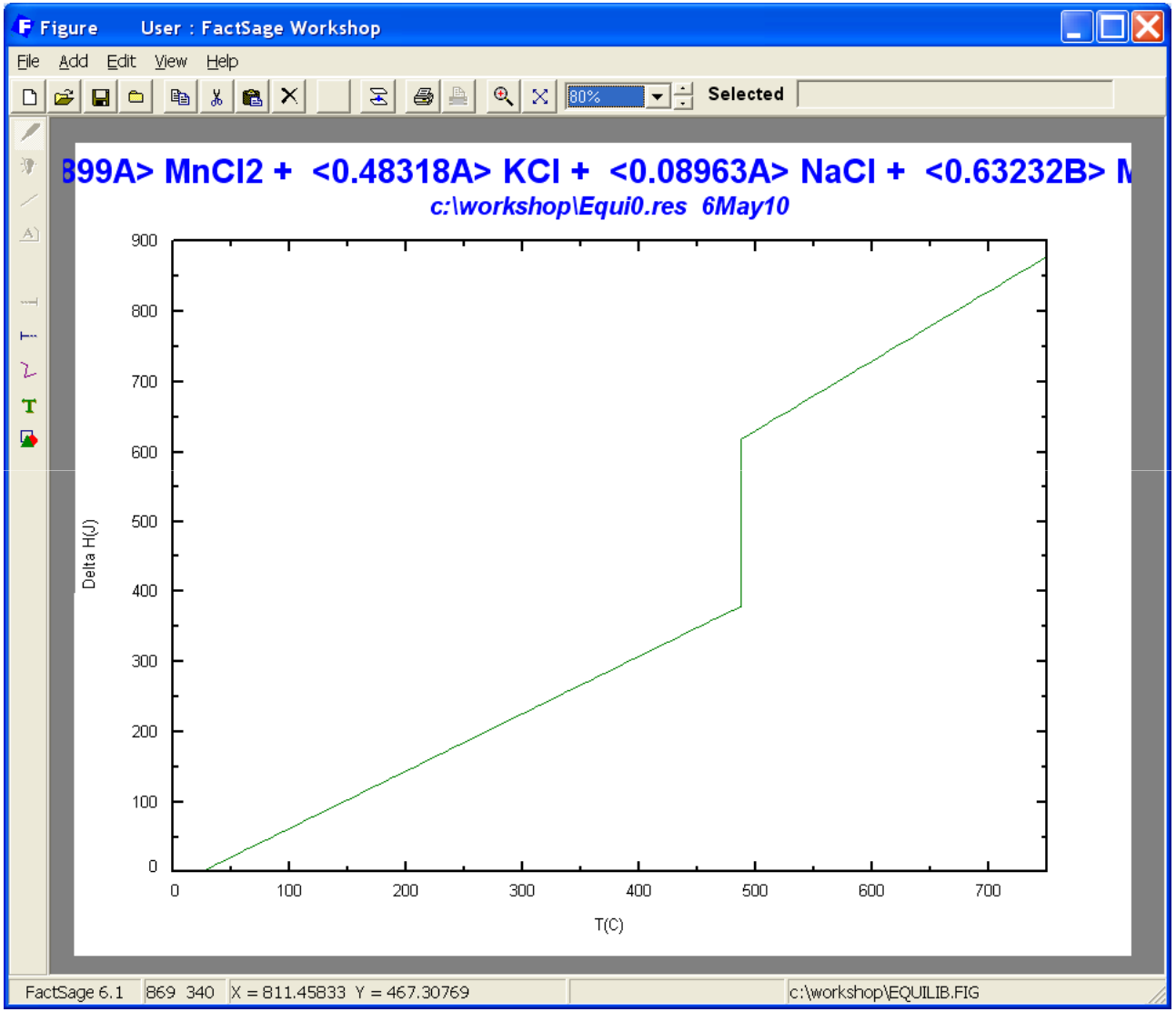

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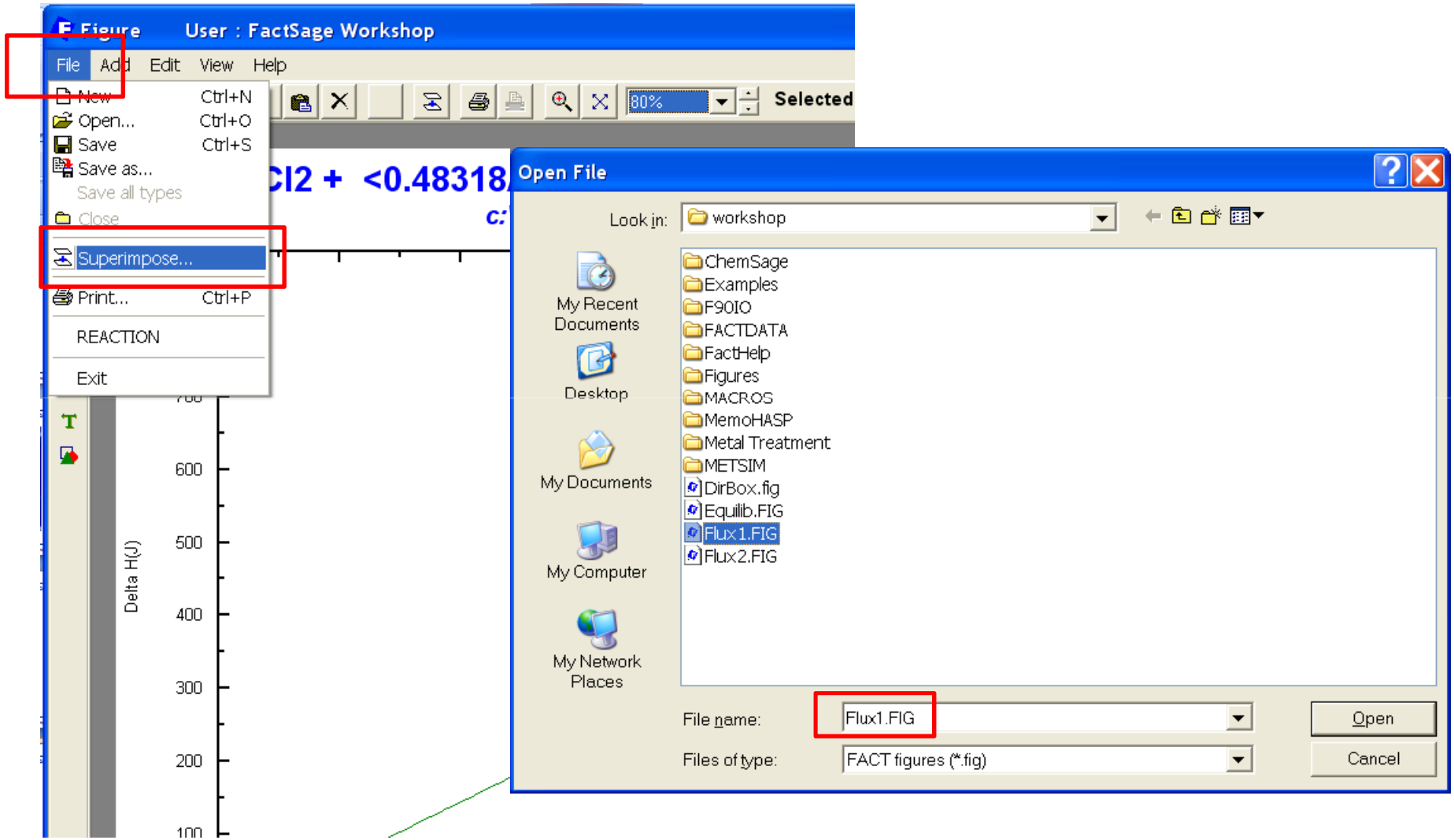

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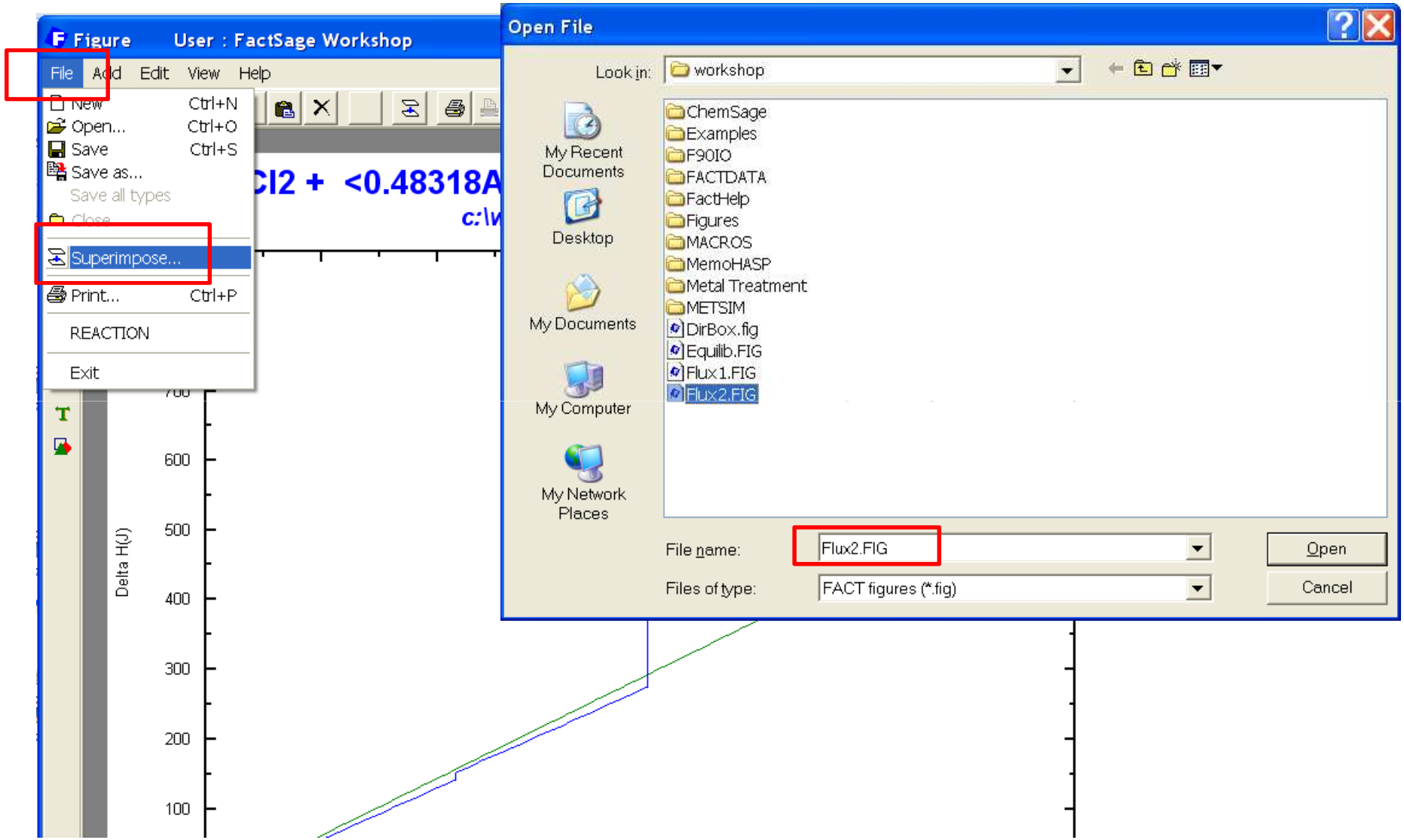


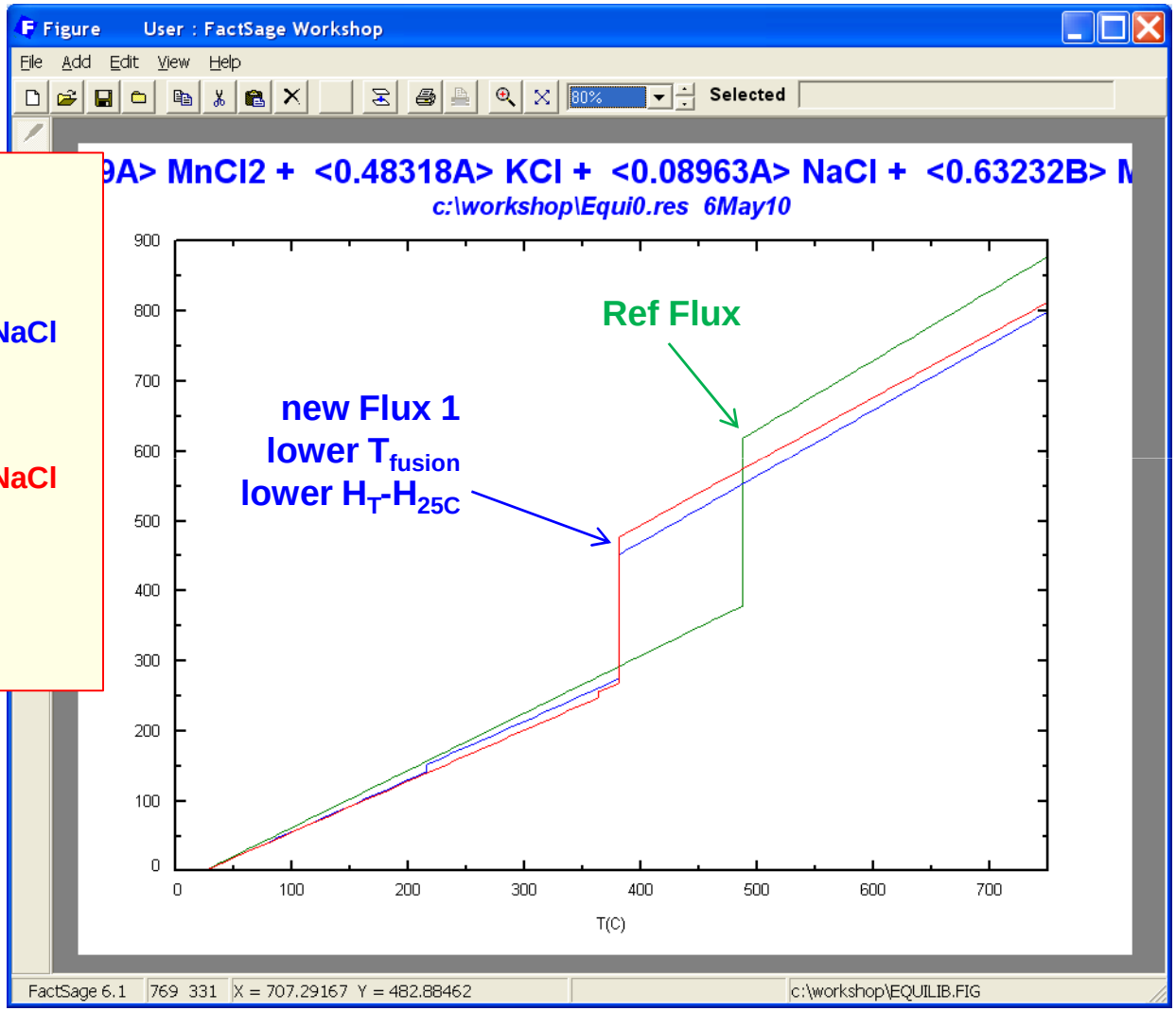
- **Example #2: Comparison of 2 salt fluxes for alkali removal**

2 low-melting compositions
wt.fractions

Flux 1
0.42899 $MnCl_2$ + 0.48138KCl + 0.08963NaCl
@ 380.95°C

Flux 2
0.63232 $MnCl_2$ + 0.15069KCl + 0.21698NaCl
@ 381.64°C

Ref. Flux
$KMgCl_3$
@ 487°C



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

Strategy :

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

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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

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

Strategy :

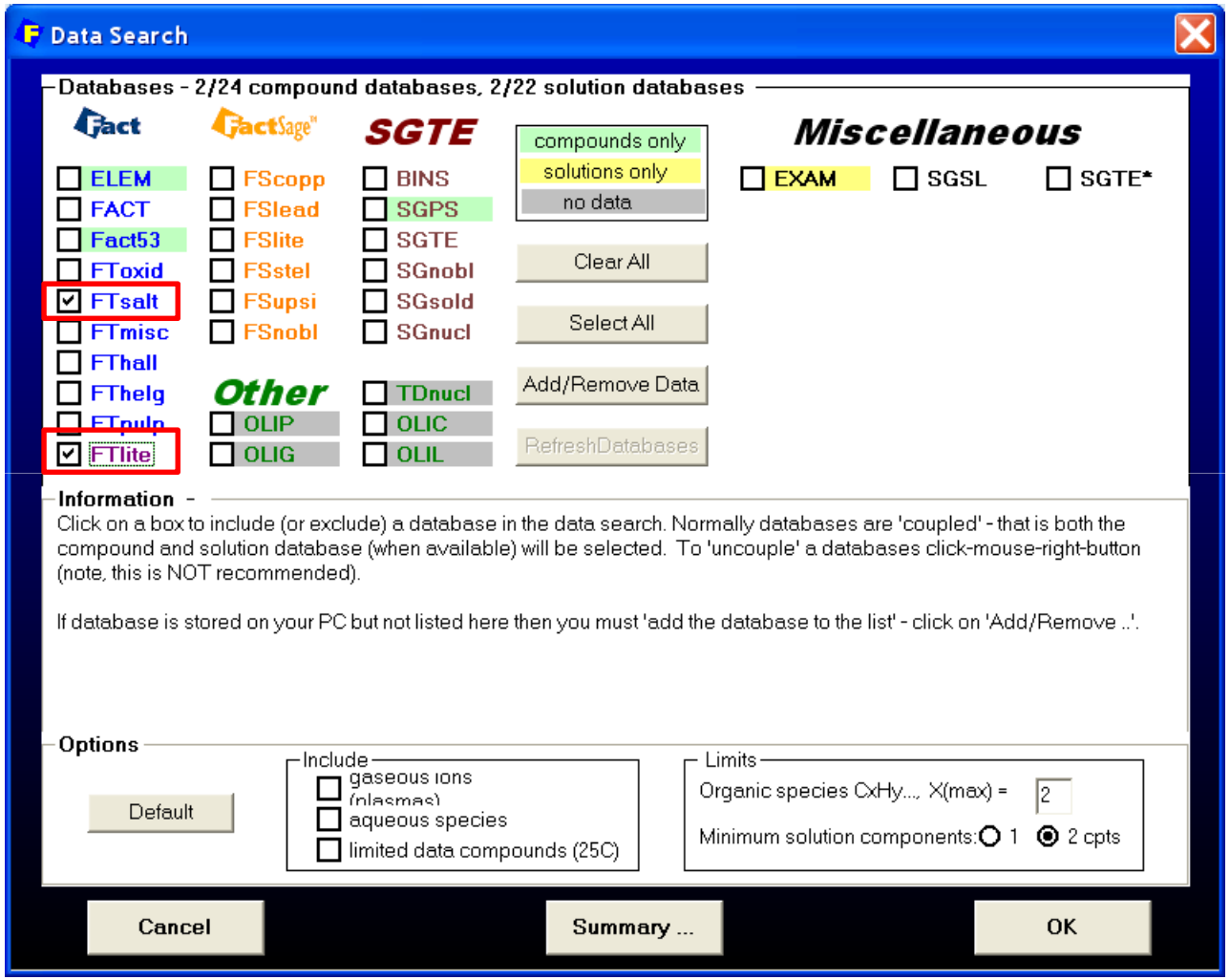
4) Calculate the alkali removal from a Al-5%Mg alloy with the fluxes

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

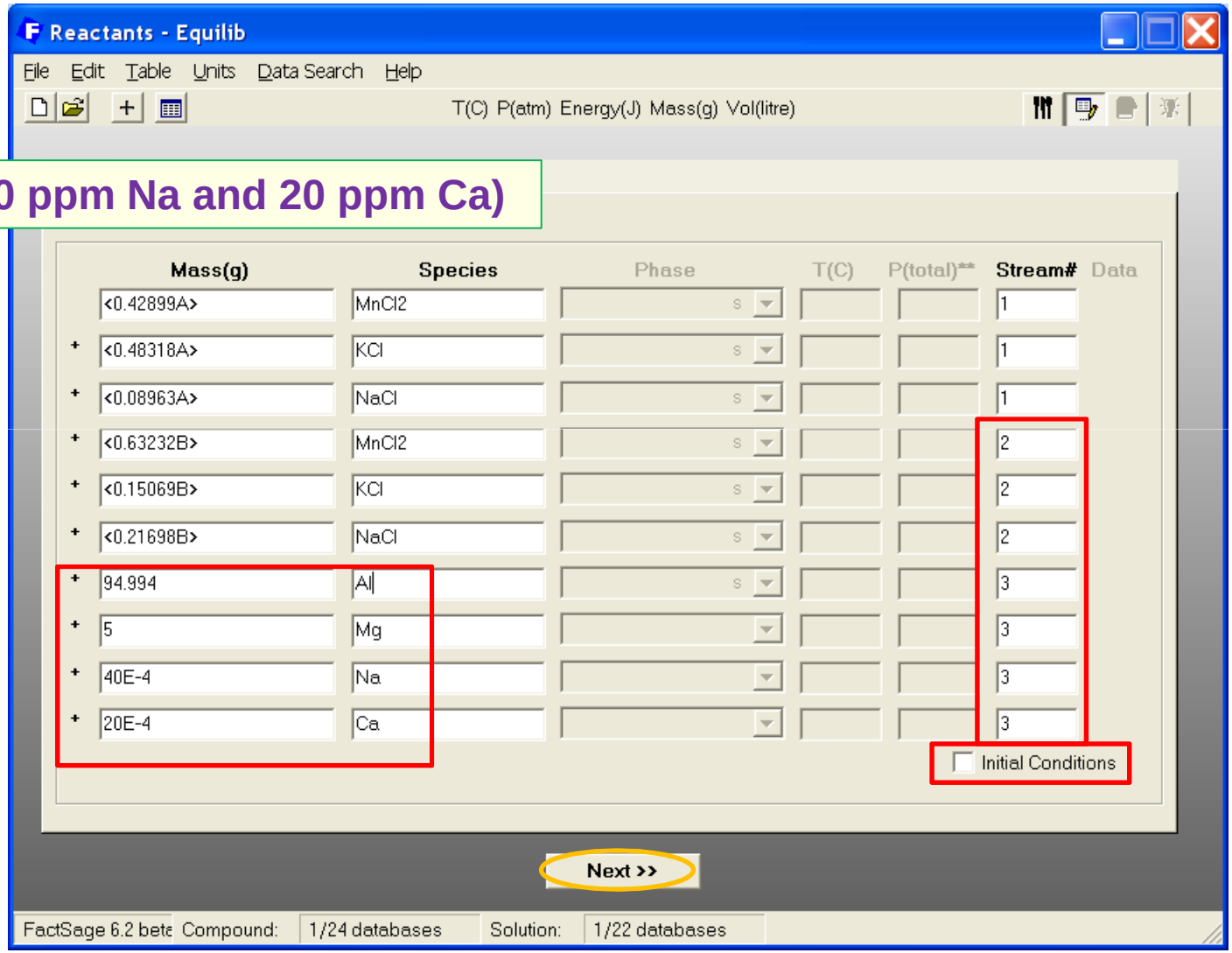
As a light metal alloy is used, the FTlite database must be now activated

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



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

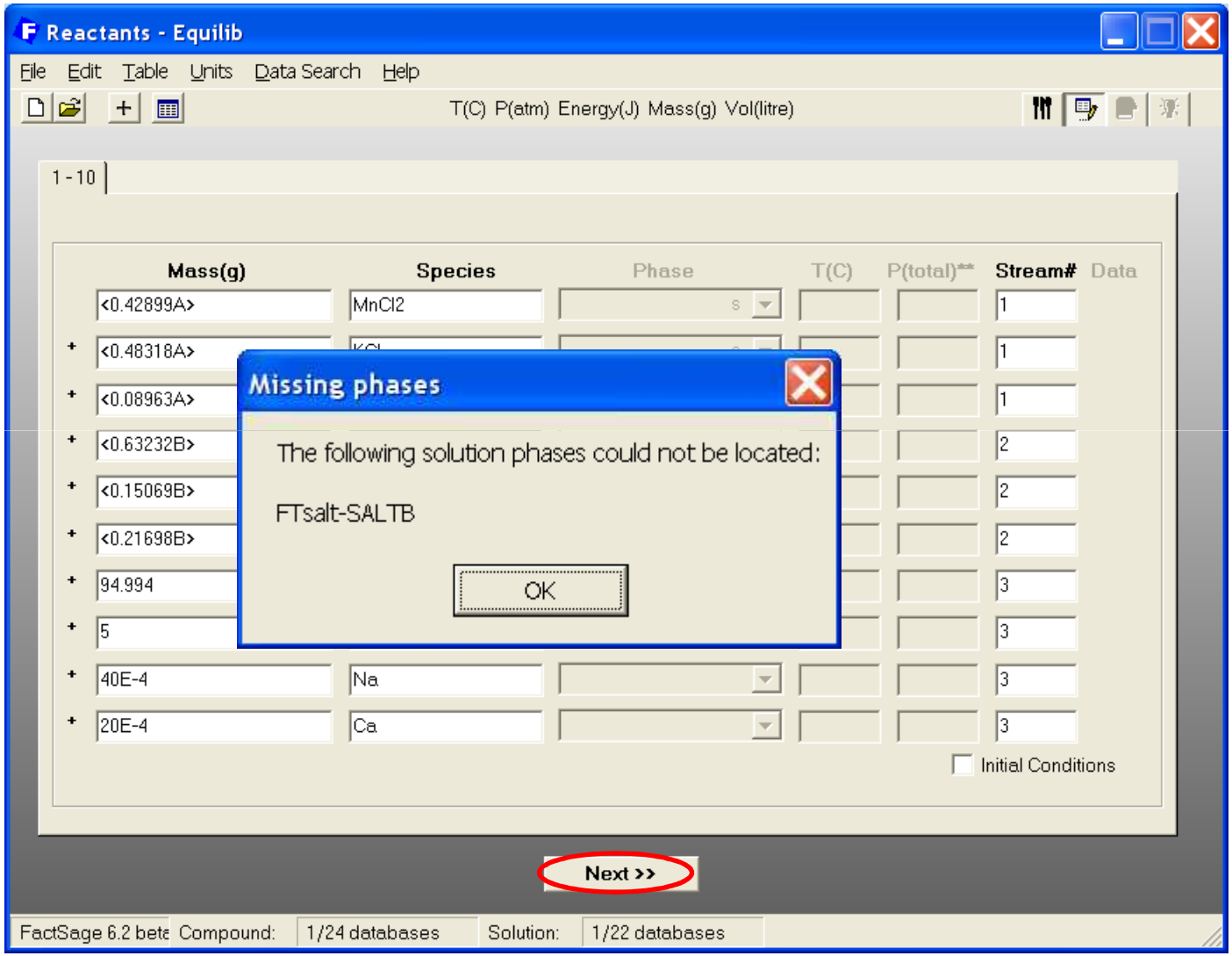
Al-5%Mg with (40 ppm Na and 20 ppm Ca)



- **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



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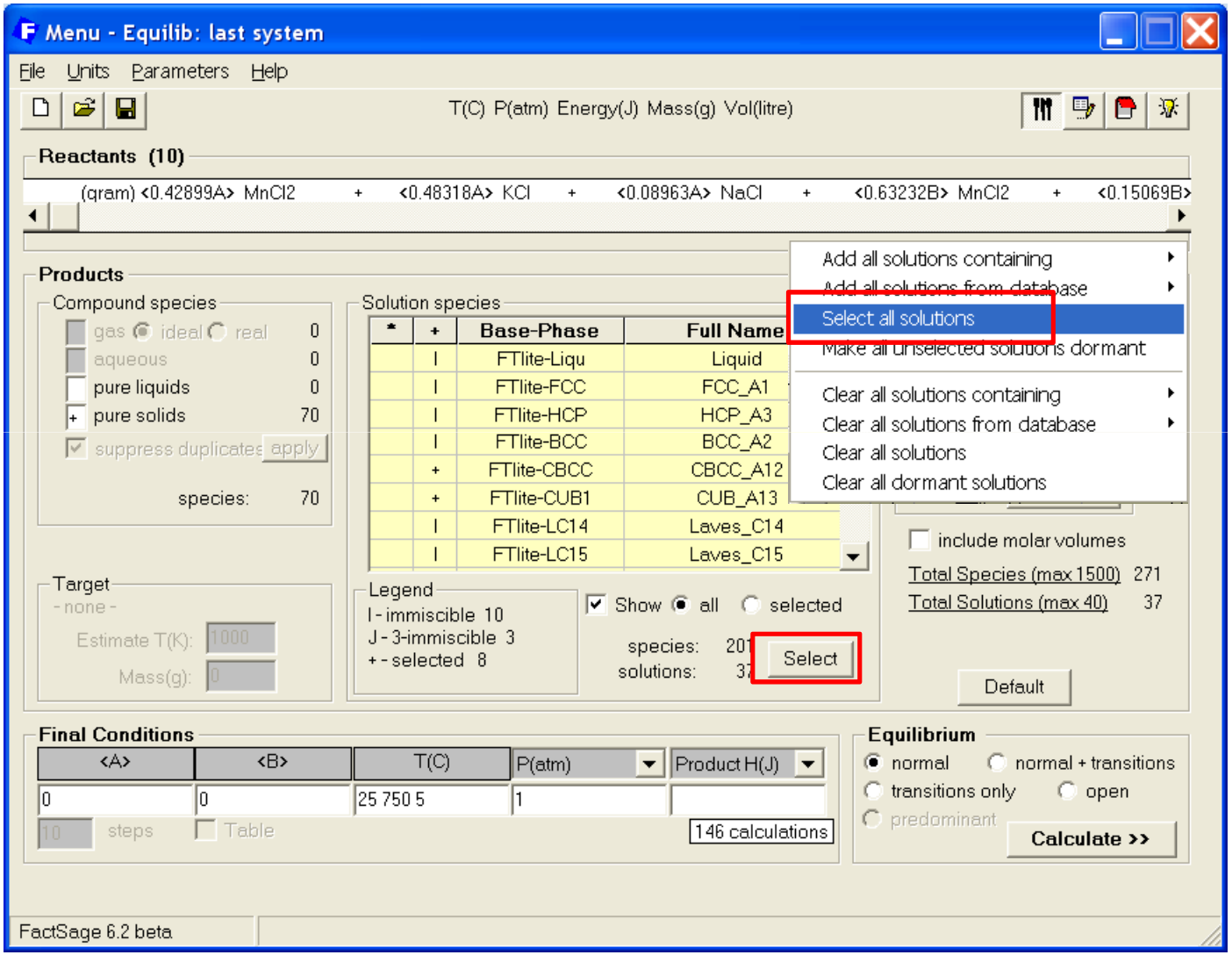

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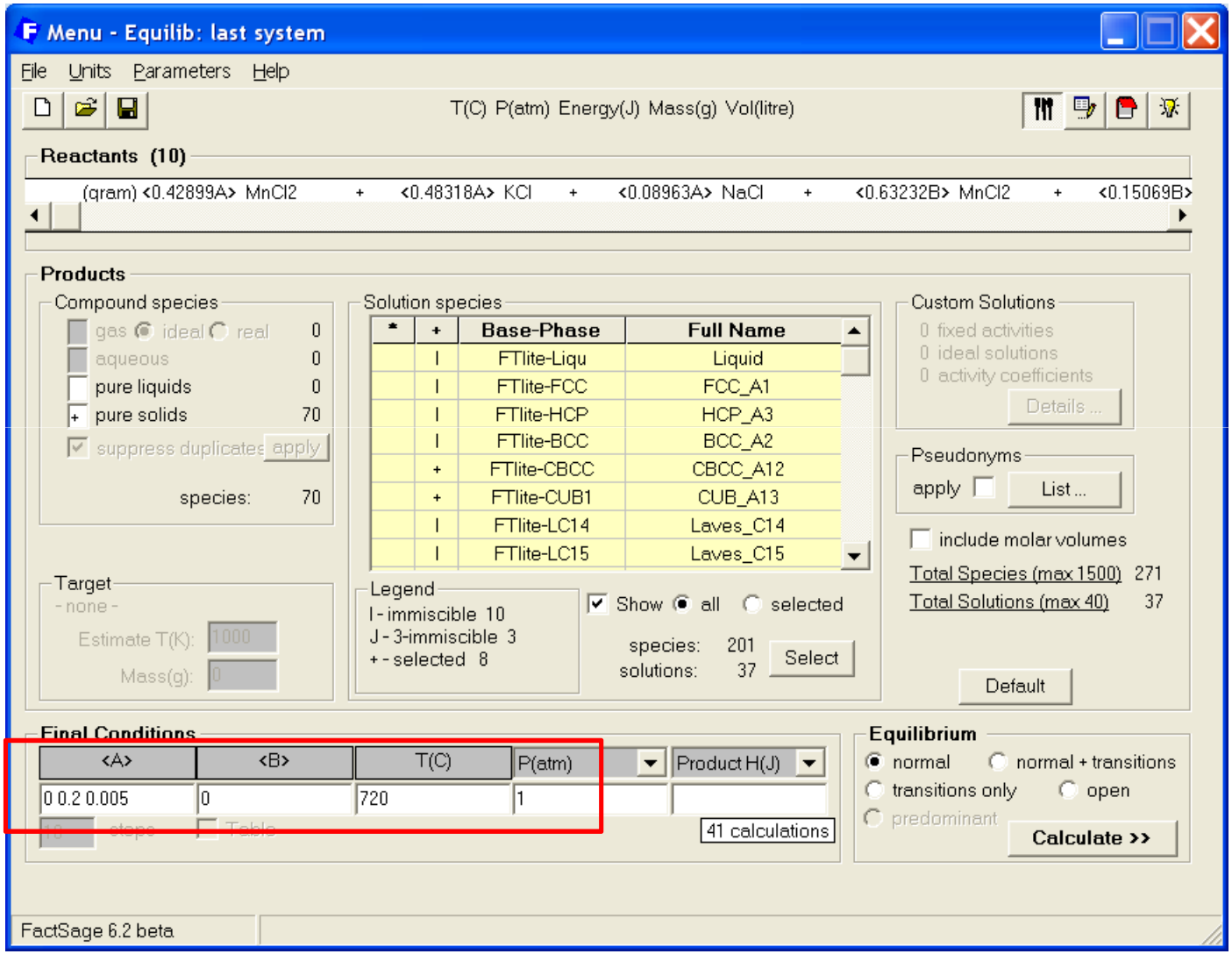
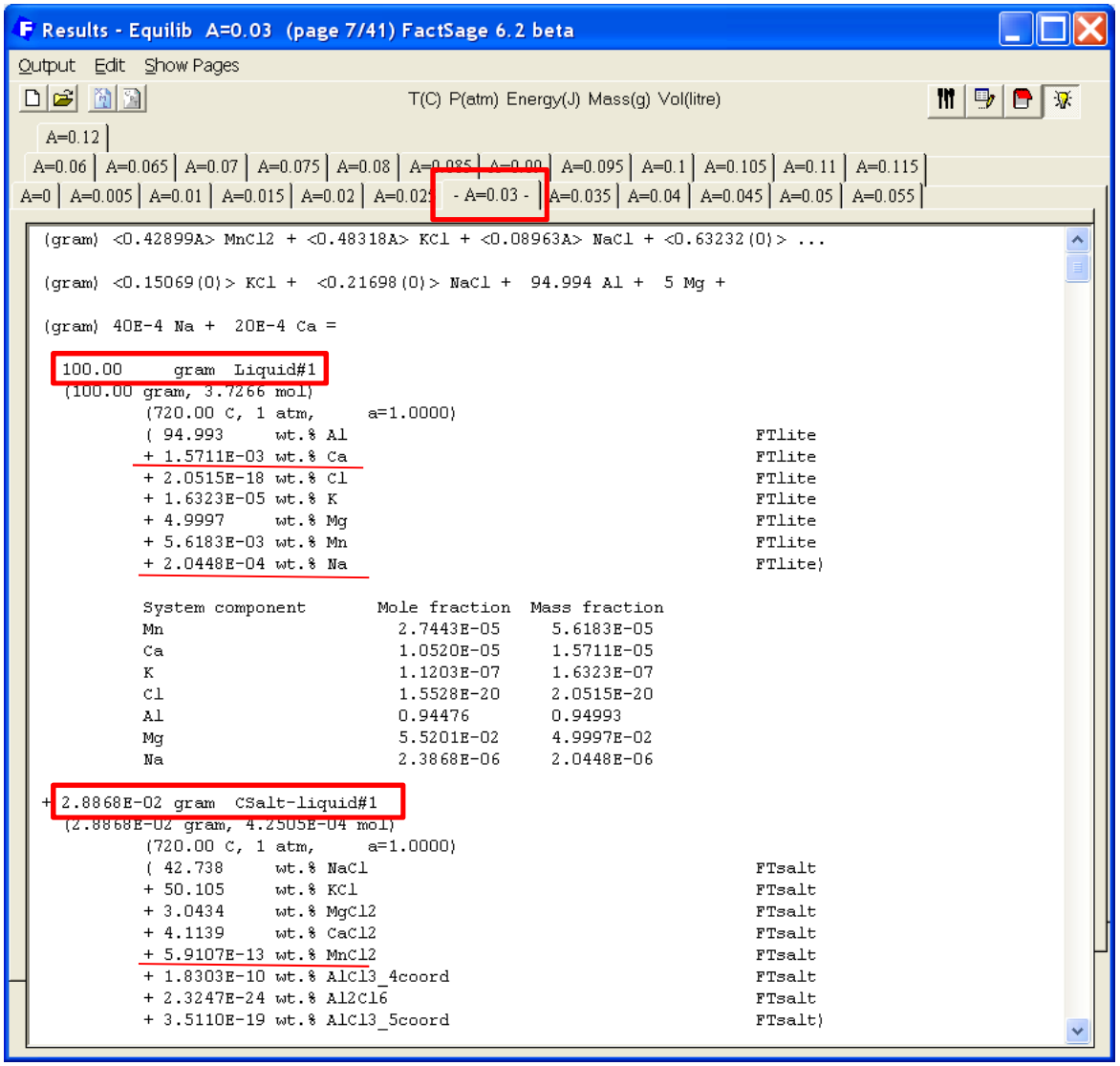


- **Example #2: Comparison of 2 salt fluxes for alkali removal**

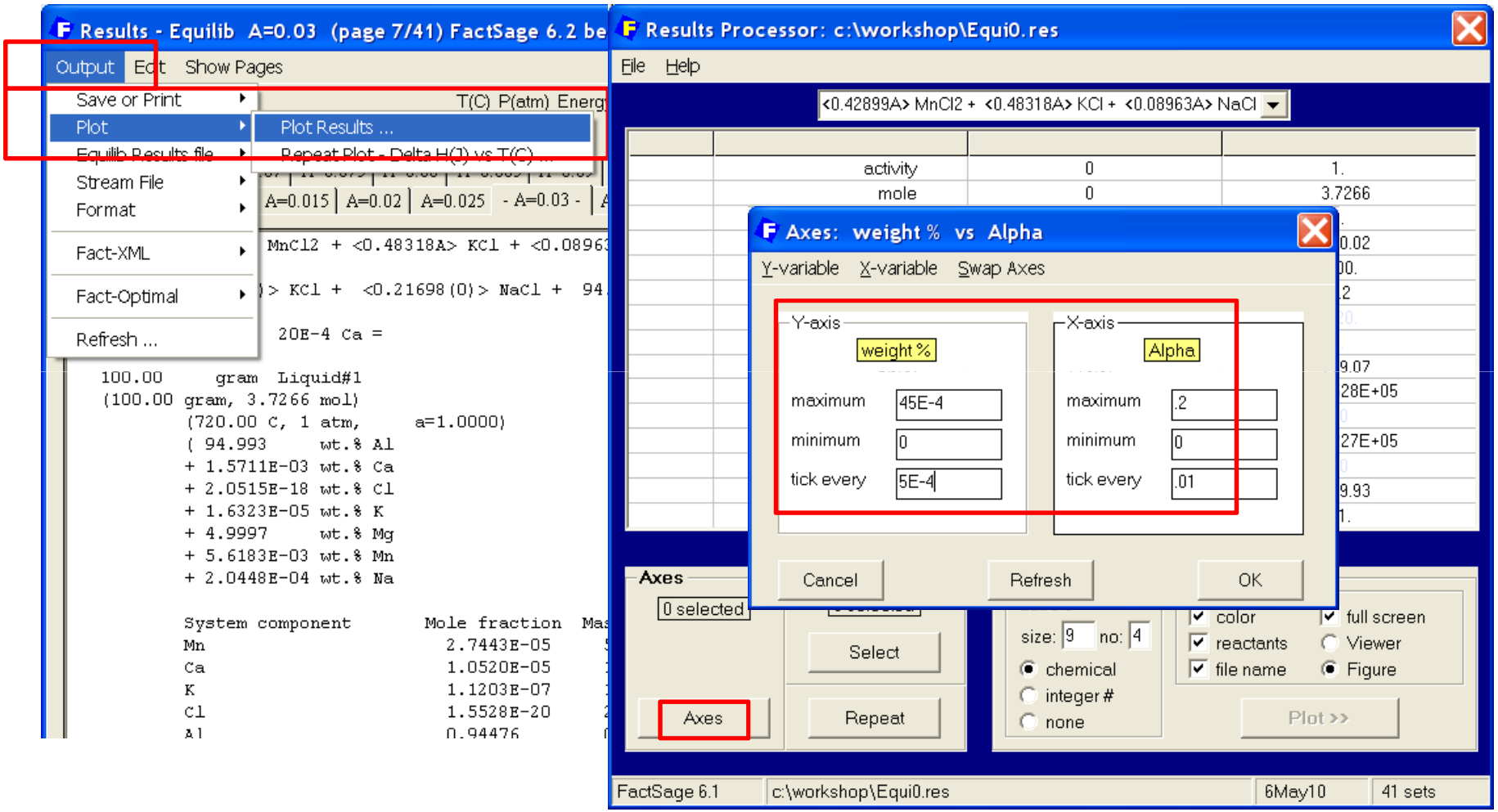
$MnCl_2 + 2\ \underline{Na} \rightarrow (2NaCl)_{\ in\ liquid\ KCl} + \underline{Mn}$

Liquid Alloy
100 grams

Molten Salt
0.0288 grams



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



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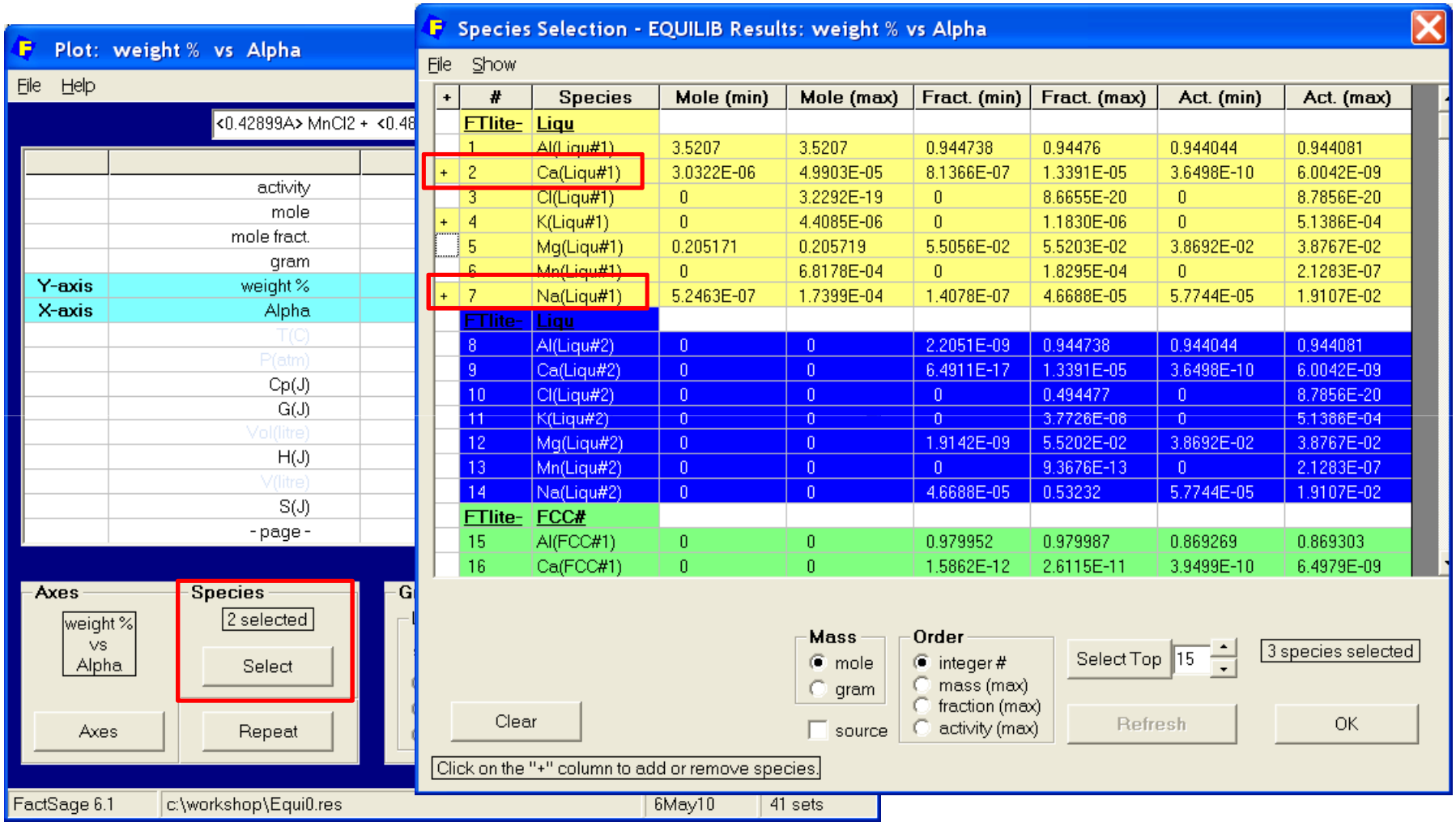

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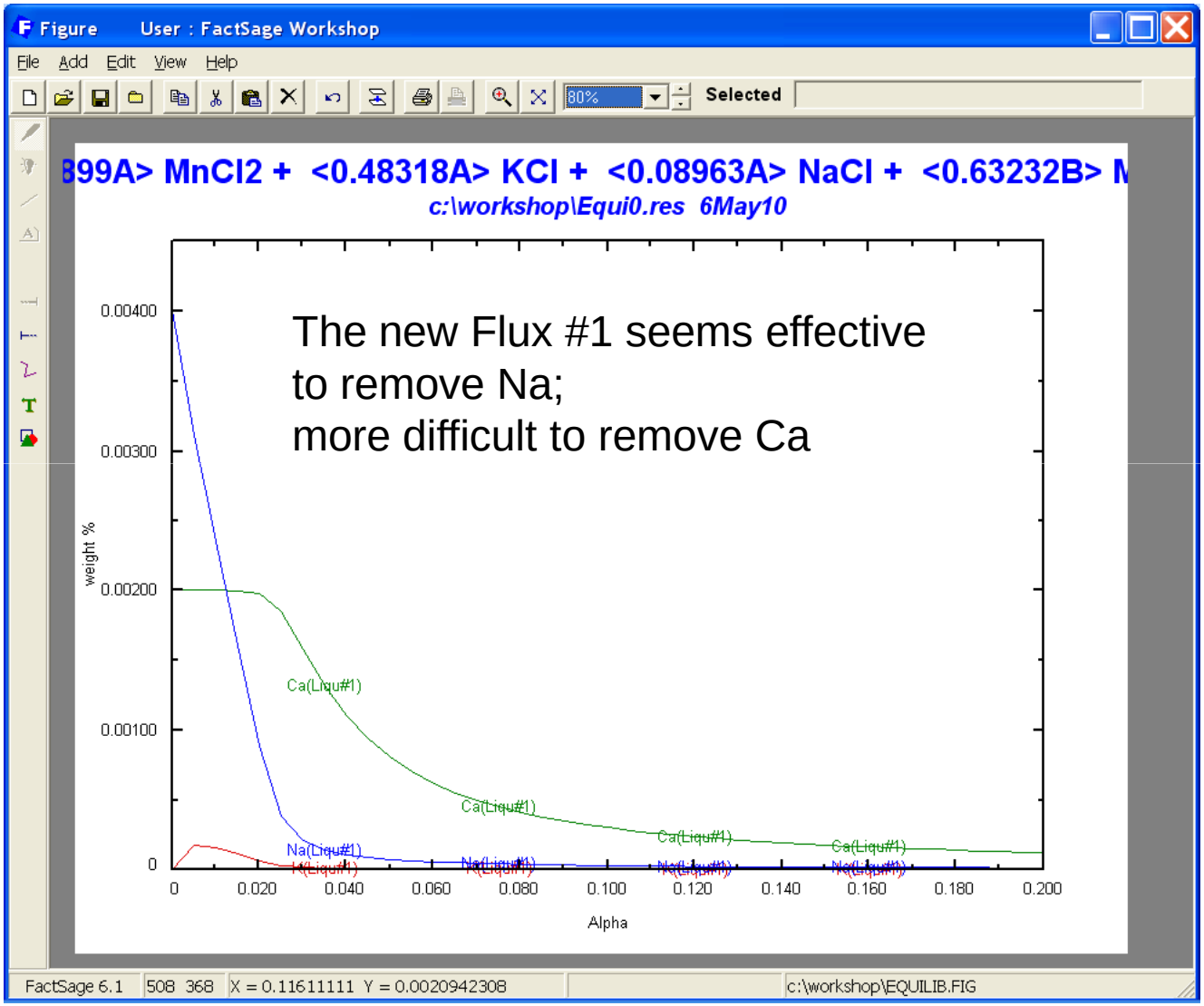

- **Example #2: Comparison of 2 salt fluxes for alkali removal**