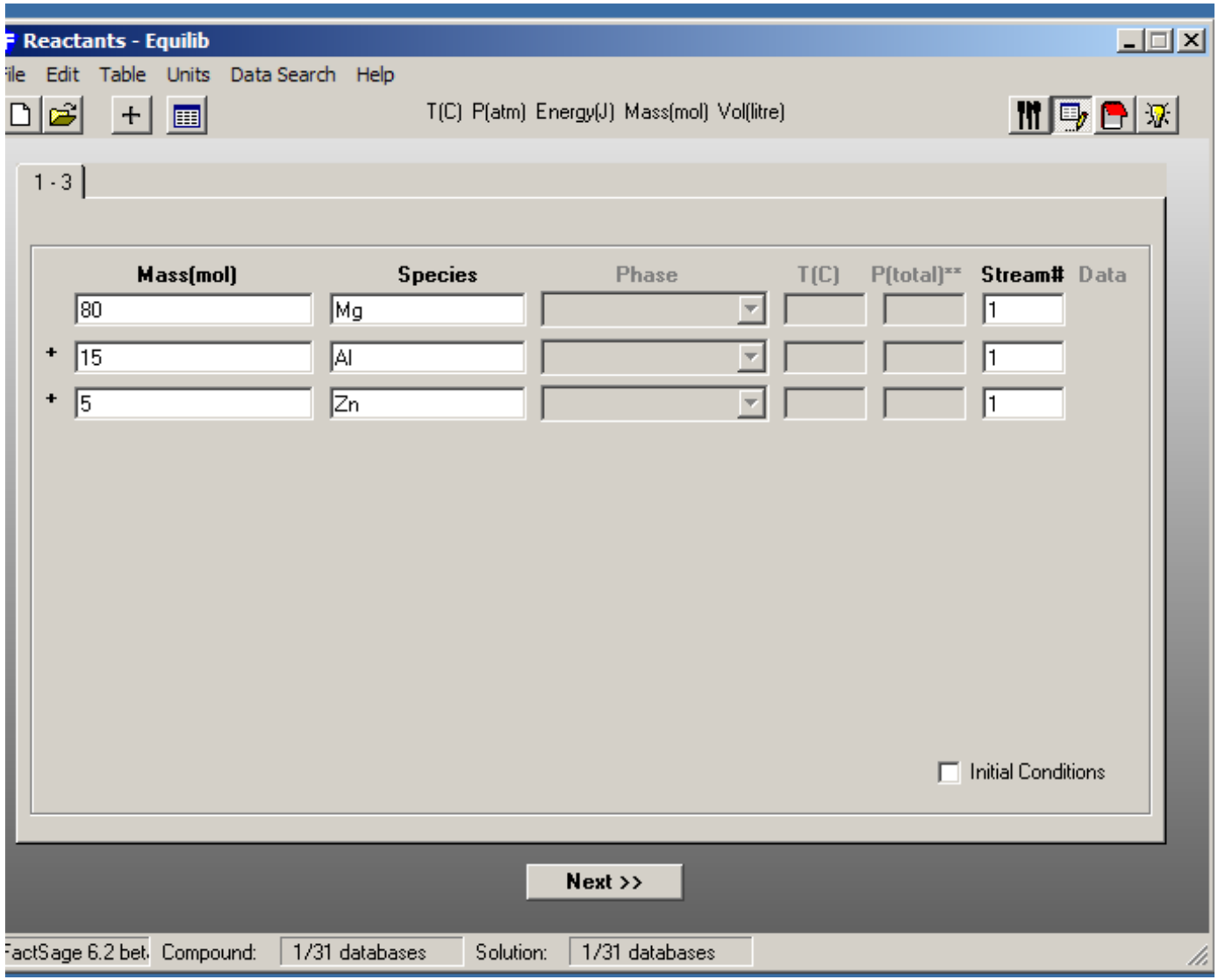
Alloy Design
- Solidification and Thermodynamics

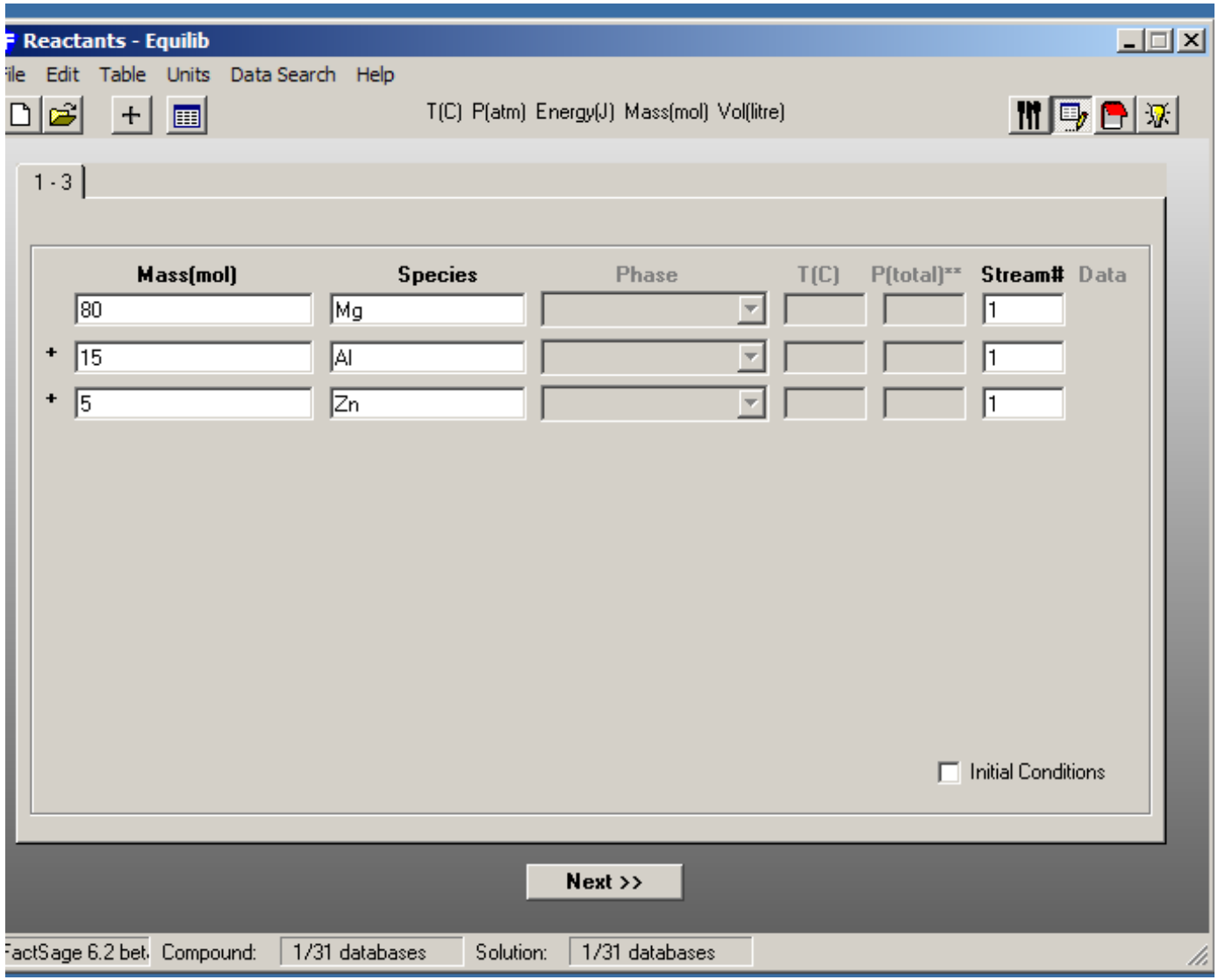
1 – 30 **Solidification**

42 – 57 **Thermodynamic Properties**

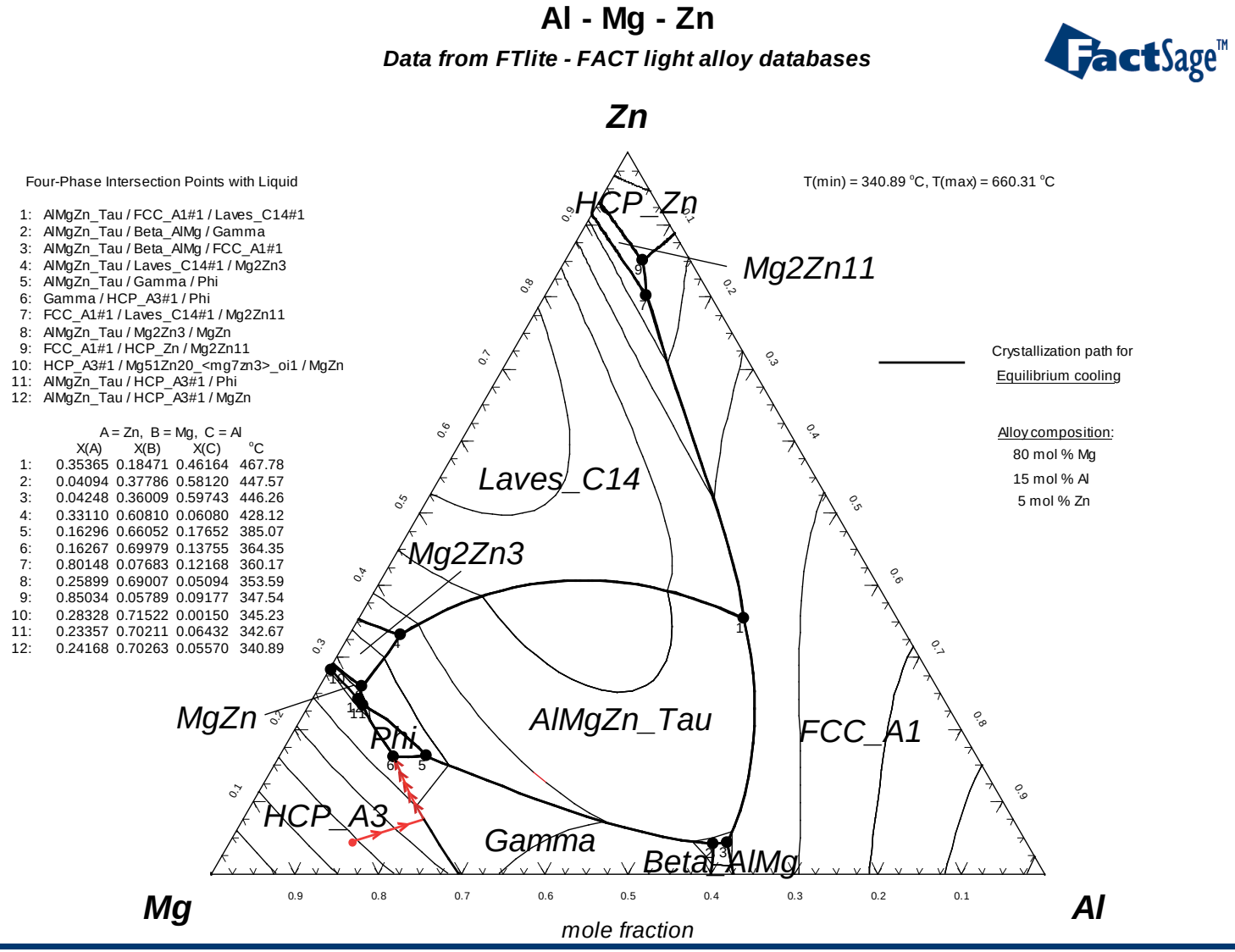
Solidification



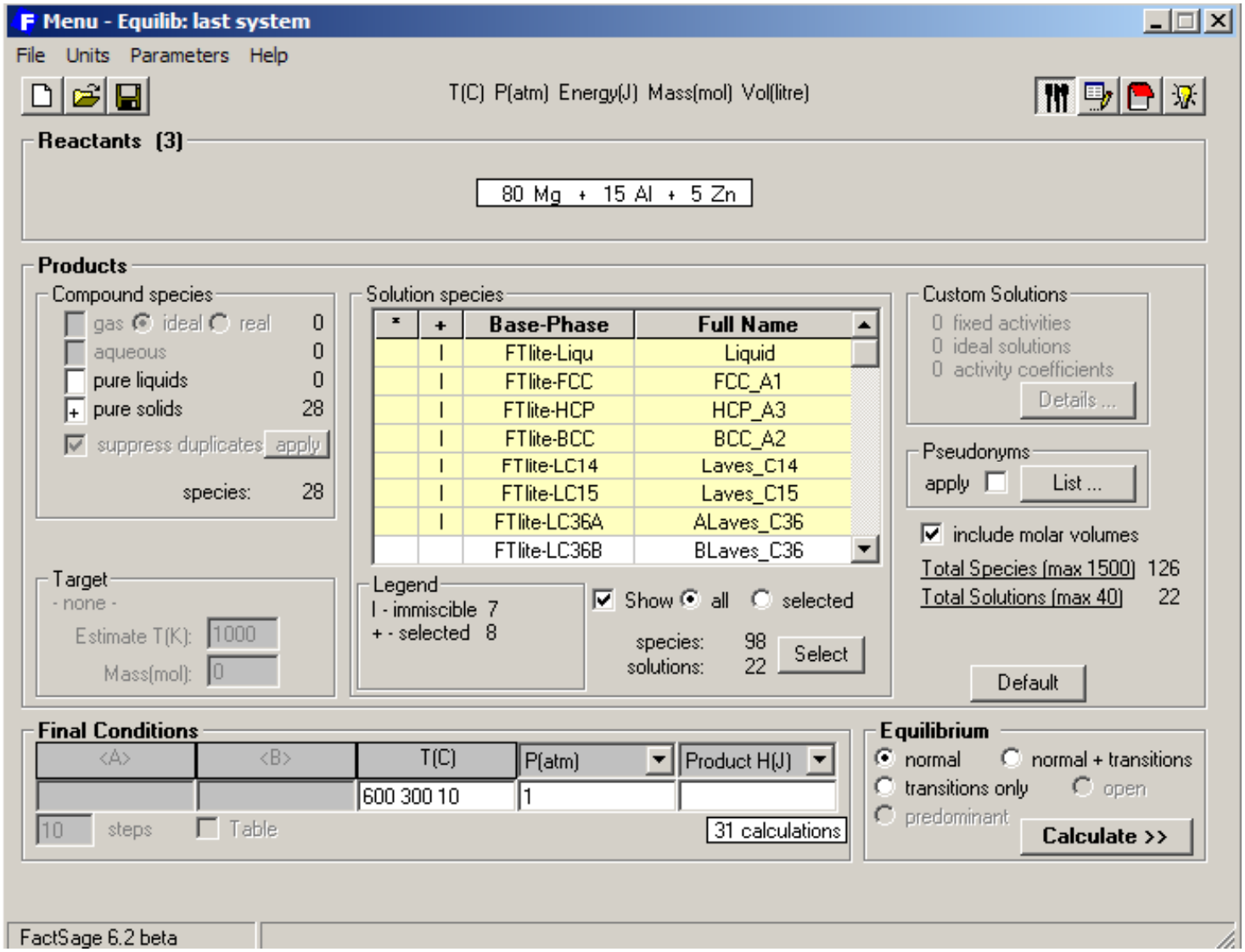
Solidification

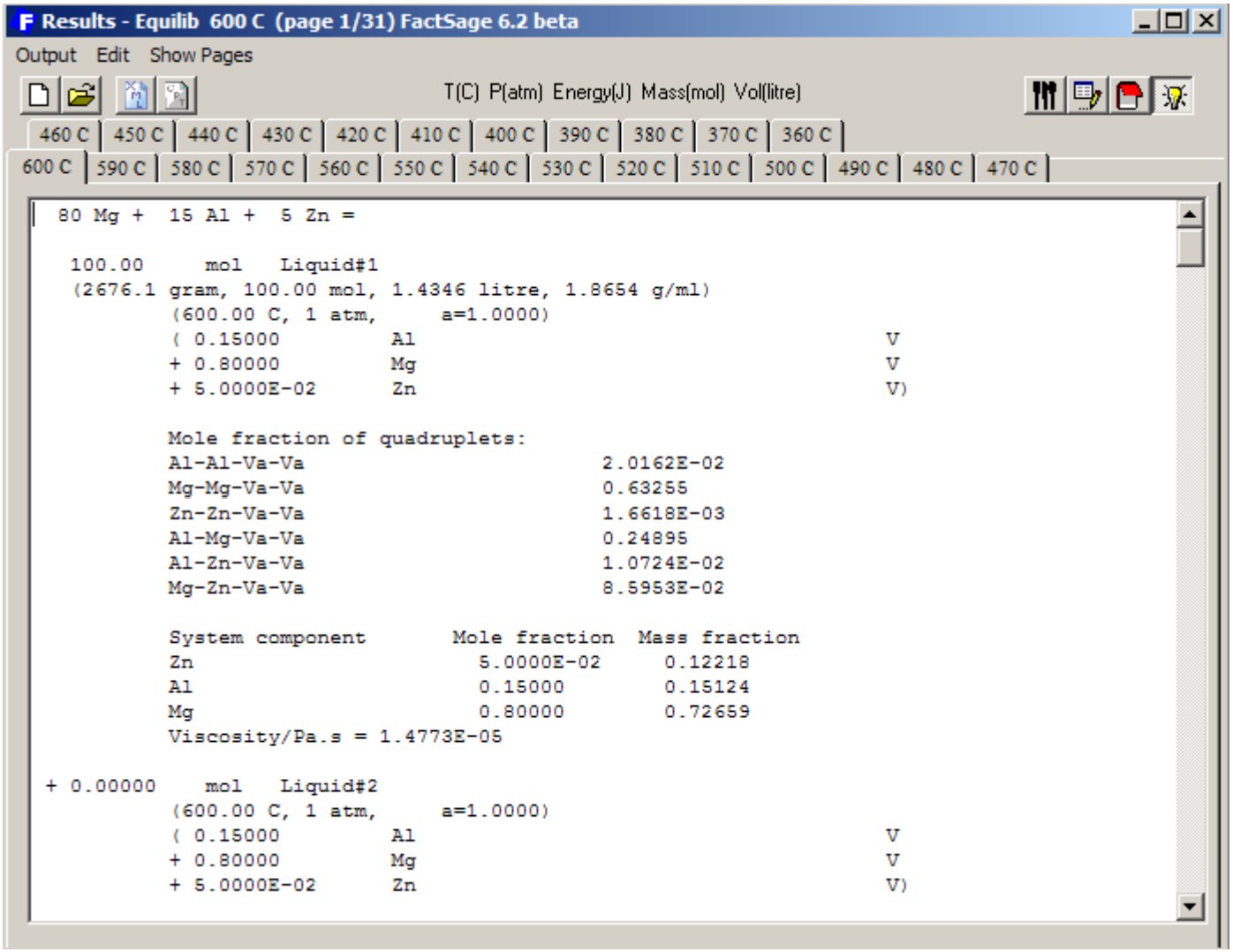


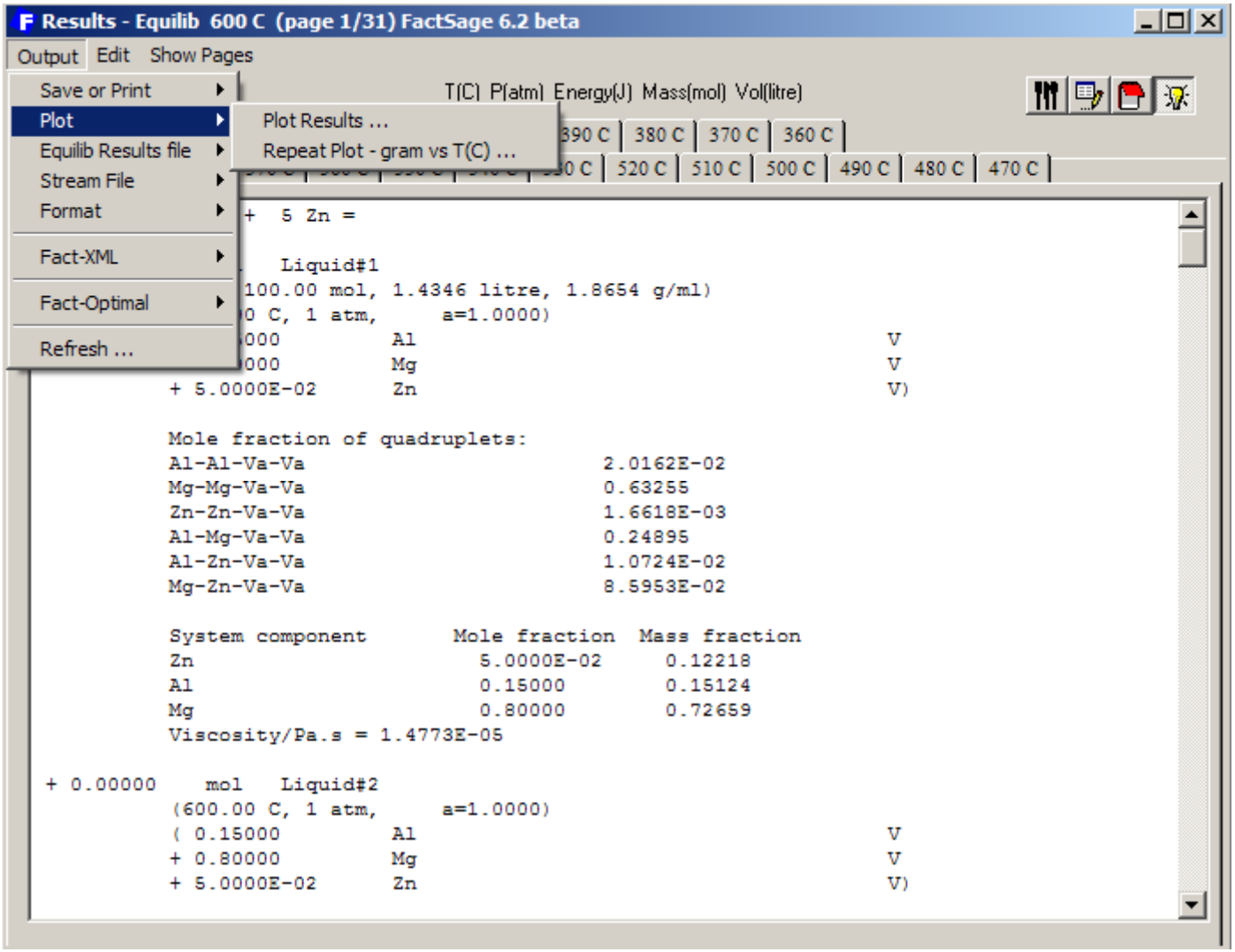
Equilibrium cooling path

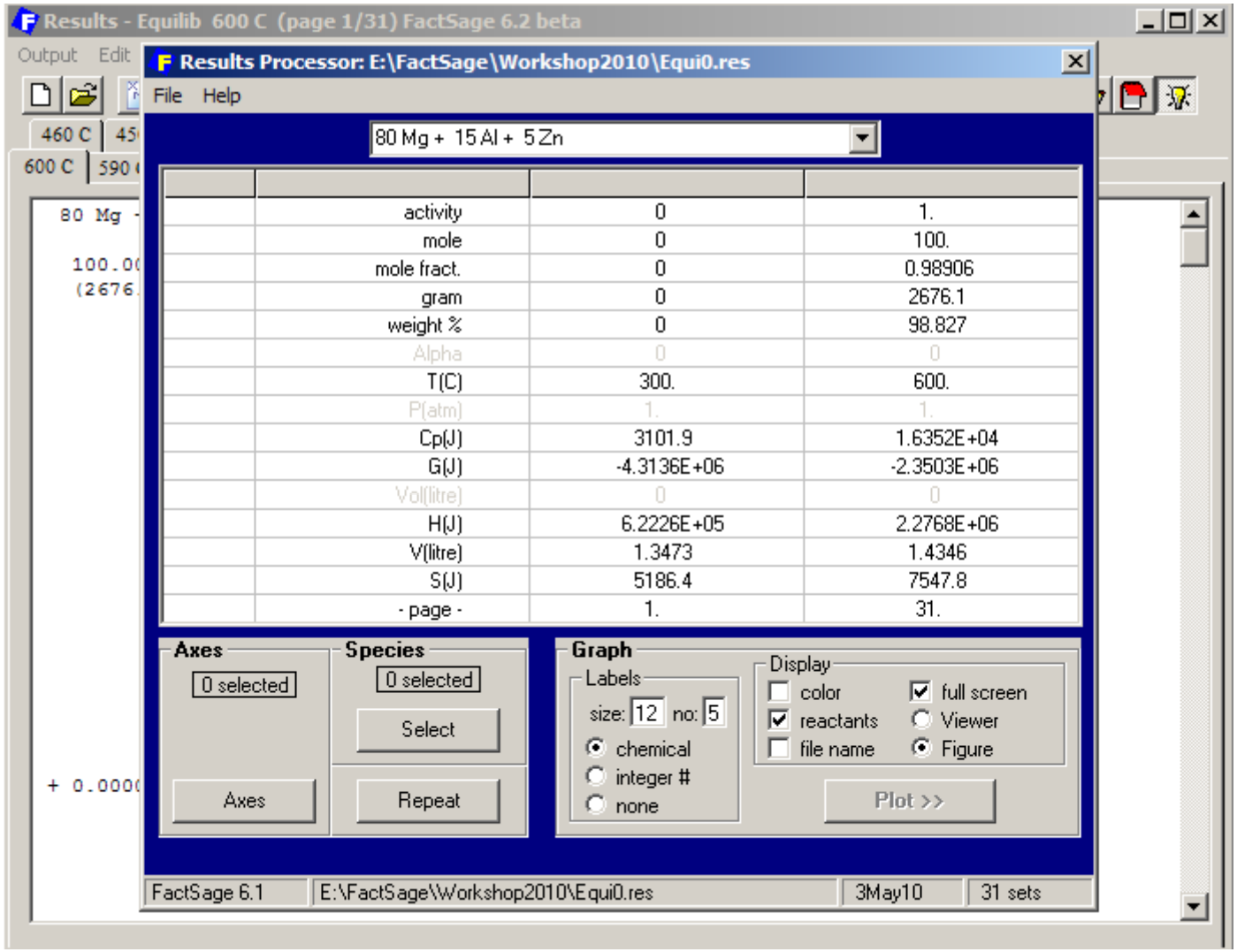


Select all solids and solutions

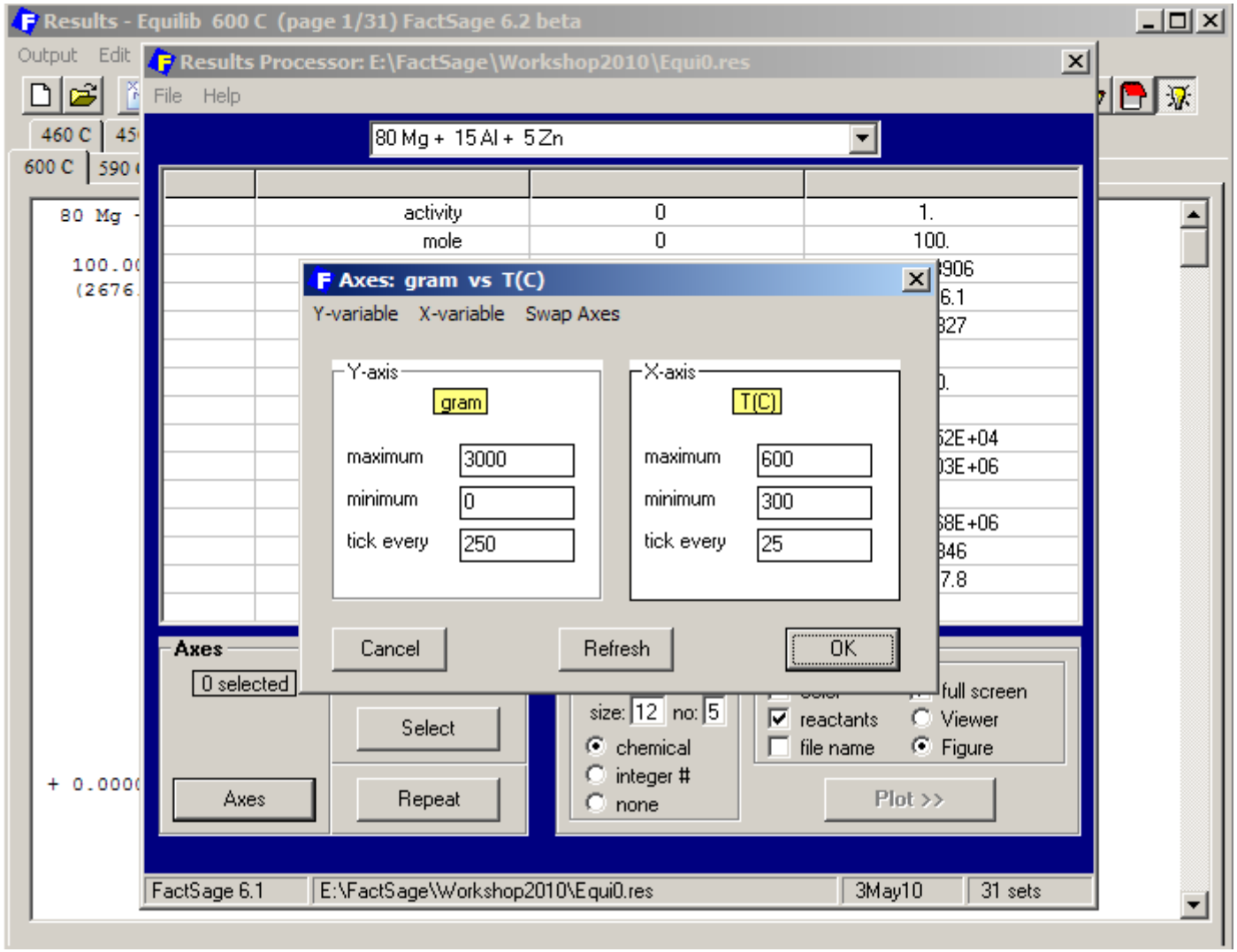



Results - Equilib 600 C (page 1/31) FactSage 6.2 beta
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)
460 C 450 C 440 C 430 C 420 C 410 C 400 C 390 C 380 C 370 C 360 C
600 C 590 C 580 C 570 C 560 C 550 C 540 C 530 C 520 C 510 C 500 C 490 C 480 C 470 C
80 Mg + 15 Al + 5 Zn =
100.00 mol Liquid#1
(2676.1 gram, 100.00 mol, 1.4346 litre, 1.8654 g/ml)
(600.00 C, 1 atm, a=1.0000)
(0.15000 Al V
+ 0.80000 Mg V
+ 5.0000E-02 Zn V)
Mole fraction of quadruplets:
Al-Al-Va-Va 2.0162E-02
Mg-Mg-Va-Va 0.63255
Zn-Zn-Va-Va 1.6618E-03
Al-Mg-Va-Va 0.24895
Al-Zn-Va-Va 1.0724E-02
Mg-Zn-Va-Va 8.5953E-02
System component Mole fraction Mass fraction
Zn 5.0000E-02 0.12218
Al 0.15000 0.15124
Mg 0.80000 0.72659
Viscosity/Pa.s = 1.4773E-05
+ 0.00000 mol Liquid#2
(600.00 C, 1 atm, a=1.0000)
(0.15000 Al V
+ 0.80000 Mg V
+ 5.0000E-02 Zn V)

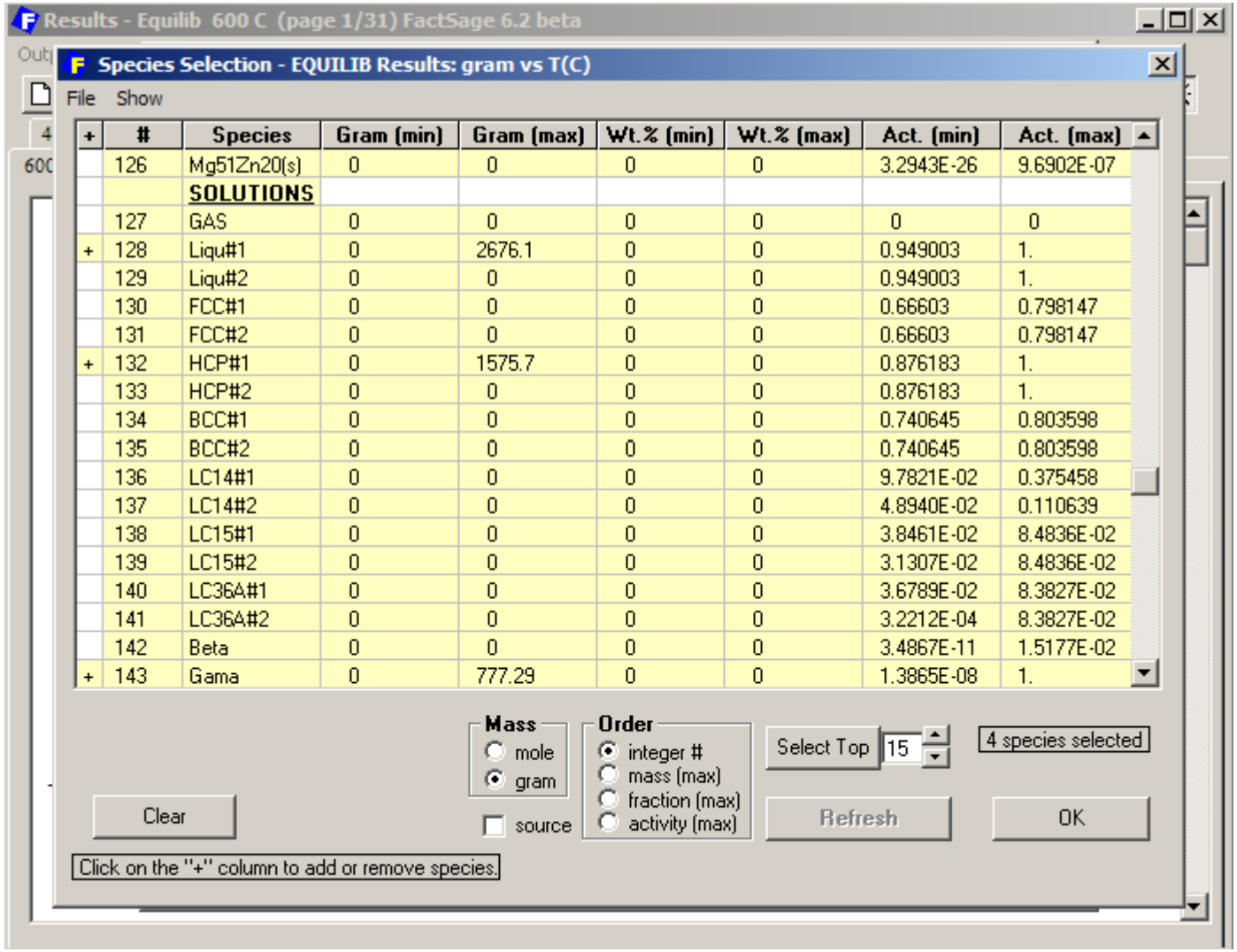

Results - Equilib 600 C (page 1/31) FactSage 6.2 beta
Output
Edit
Show Pages
Save or Print
Plot
Equilib Results file
Stream File
Format
Fact-XML
Fact-Optimal
Refresh ...
Plot Results ...
Repeat Plot - gram vs T(C) ...
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)
390 C
380 C
370 C
360 C
520 C
510 C
500 C
490 C
480 C
470 C
+ 5 Zn =
Liquid#1
100.00 mol, 1.4346 litre, 1.8654 g/ml)
0 C, 1 atm, a=1.0000)
000 Al V
000 Mg V
+ 5.0000E-02 Zn V)
Mole fraction of quadruplets:
Al-Al-Va-Va 2.0162E-02
Mg-Mg-Va-Va 0.63255
Zn-Zn-Va-Va 1.6618E-03
Al-Mg-Va-Va 0.24895
Al-Zn-Va-Va 1.0724E-02
Mg-Zn-Va-Va 8.5953E-02
System component Mole fraction Mass fraction
Zn 5.0000E-02 0.12218
Al 0.15000 0.15124
Mg 0.80000 0.72659
Viscosity/Pa.s = 1.4773E-05
+ 0.00000 mol Liquid#2
(600.00 C, 1 atm, a=1.0000)
(0.15000 Al V
+ 0.80000 Mg V
+ 5.0000E-02 Zn V)


Results - Equilib 600 C (page 1/31) FactSage 6.2 beta
Output Edit
460 C
600 C
80 Mg -
100.0(
(2676.
+ 0.000(
Results Processor: E:\FactSage\Workshop2010\Equi0.res
File Help
80 Mg + 15 Al + 5 Zn
activity 0 1.
mole 0 100.
mole fract. 0 0.98906
gram 0 2676.1
weight % 0 98.827
Alpha 0 0
T(C) 300. 600.
P(atm) 1. 1.
Cp(J) 3101.9 1.6352E+04
G(J) -4.3136E+06 -2.3503E+06
Vol(litre) 0 0
H(J) 6.2226E+05 2.2768E+06
V(litre) 1.3473 1.4346
S(J) 5186.4 7547.8
- page - 1. 31.
Axes
0 selected
Axes
Species
0 selected
Select
Repeat
Graph
Labels
size: 12 no: 5
chemical
integer #
none
Display
color
reactants
file name
full screen
Viewer
Figure
Plot >>
FactSage 6.1
E:\FactSage\Workshop2010\Equi0.res
3May10
31 sets

Selection of axes



Selection of species to be plotted
(choose all solids and elements for which Gram(Max)>0)



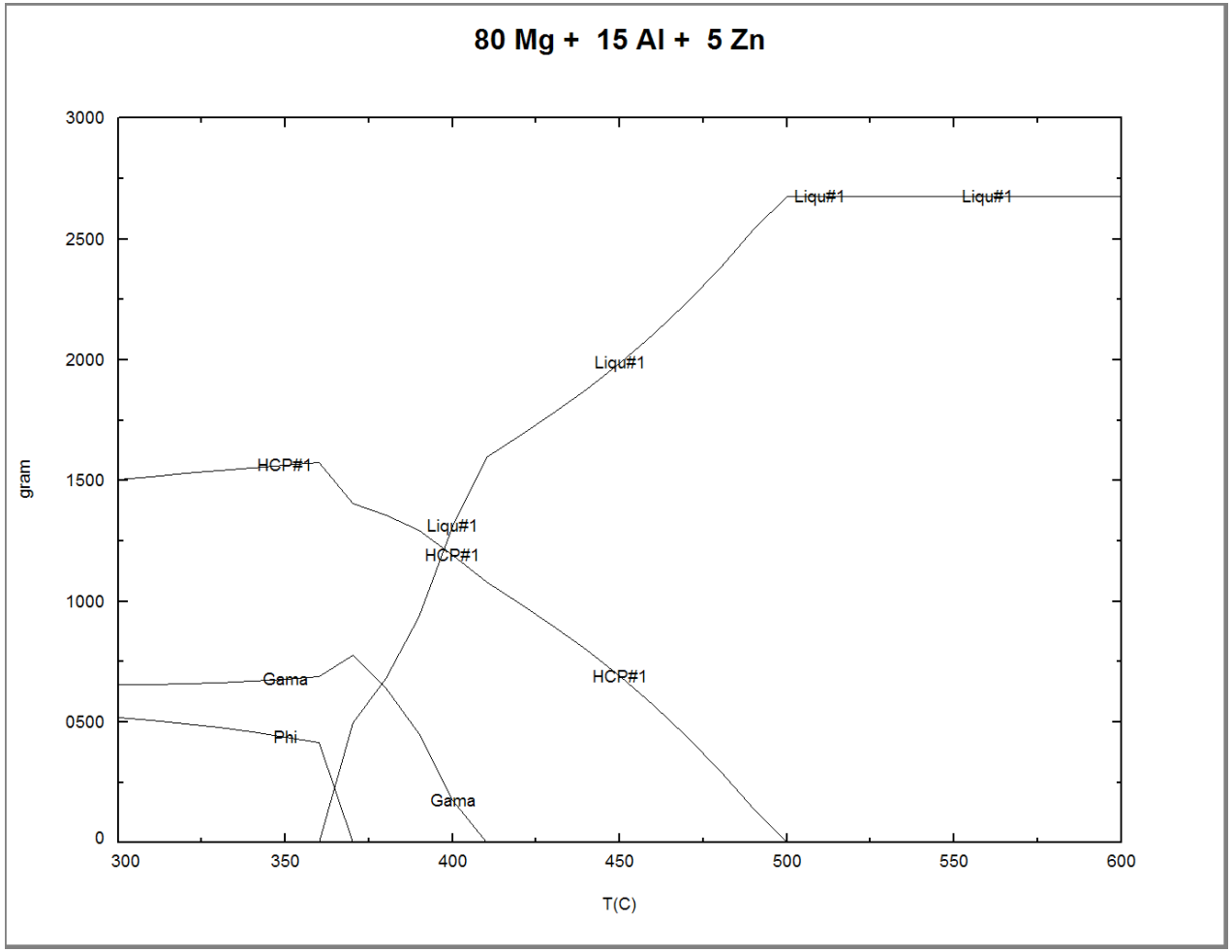
+	#	Species	Gram (min)	Gram (max)	Wt.% (min)	Wt.% (max)	Act. (min)	Act. (max)
	126	Mg51Zn20(s)	0	0	0	0	3.2943E-26	9.6902E-07
		SOLUTIONS						
	127	GAS	0	0	0	0	0	0
+	128	Liqu#1	0	2676.1	0	0	0.949003	1.
	129	Liqu#2	0	0	0	0	0.949003	1.
	130	FCC#1	0	0	0	0	0.66603	0.798147
	131	FCC#2	0	0	0	0	0.66603	0.798147
+	132	HCP#1	0	1575.7	0	0	0.876183	1.
	133	HCP#2	0	0	0	0	0.876183	1.
	134	BCC#1	0	0	0	0	0.740645	0.803598
	135	BCC#2	0	0	0	0	0.740645	0.803598
	136	LC14#1	0	0	0	0	9.7821E-02	0.375458
	137	LC14#2	0	0	0	0	4.8940E-02	0.110639
	138	LC15#1	0	0	0	0	3.8461E-02	8.4836E-02
	139	LC15#2	0	0	0	0	3.1307E-02	8.4836E-02
	140	LC36A#1	0	0	0	0	3.6789E-02	8.3827E-02
	141	LC36A#2	0	0	0	0	3.2212E-04	8.3827E-02
	142	Beta	0	0	0	0	3.4867E-11	1.5177E-02
+	143	Gama	0	777.29	0	0	1.3865E-08	1.

Amounts of Phases during Equilibrium Cooling

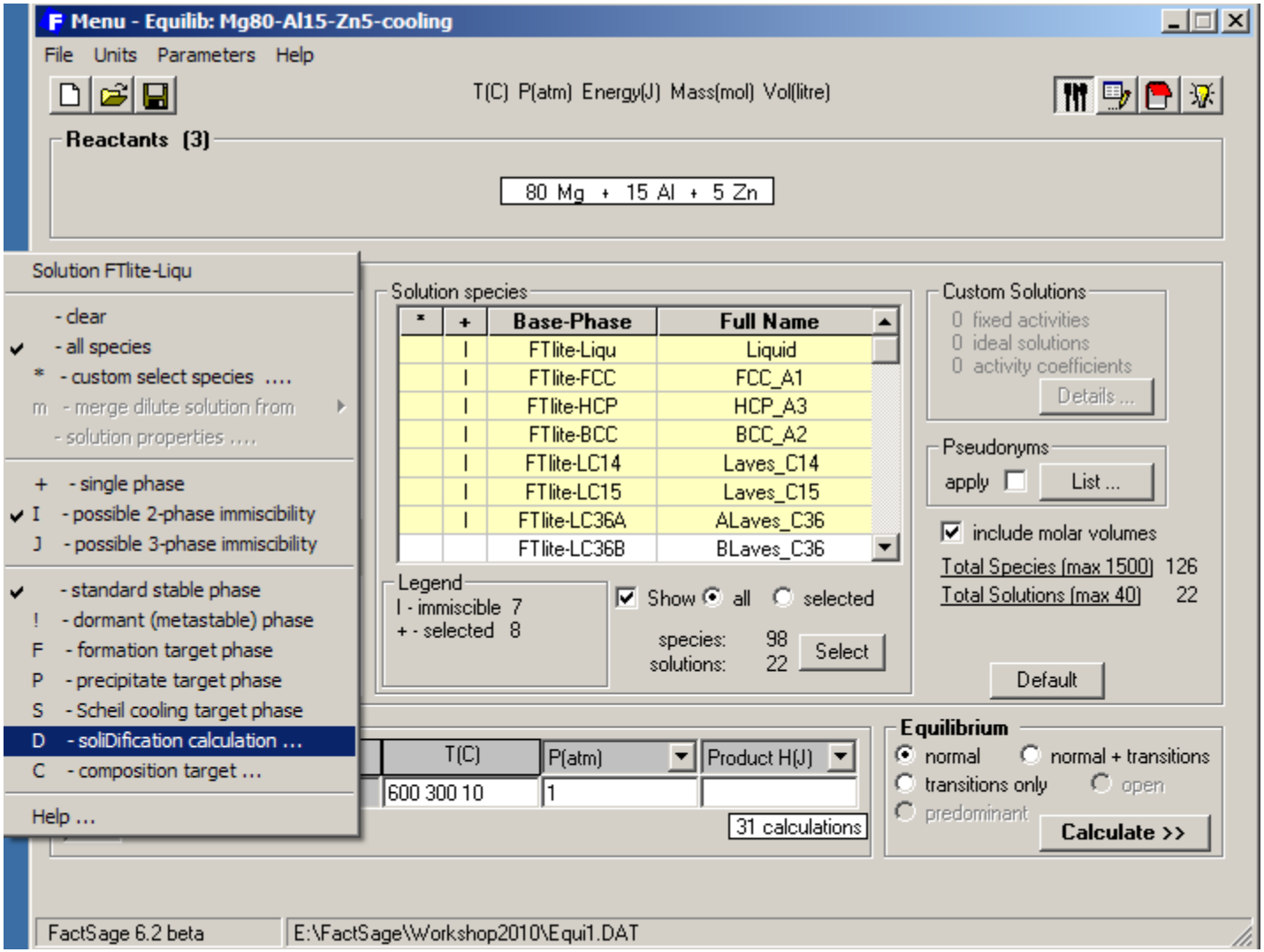
Liquidus at about 500 °C

Univariant at about 400 °C

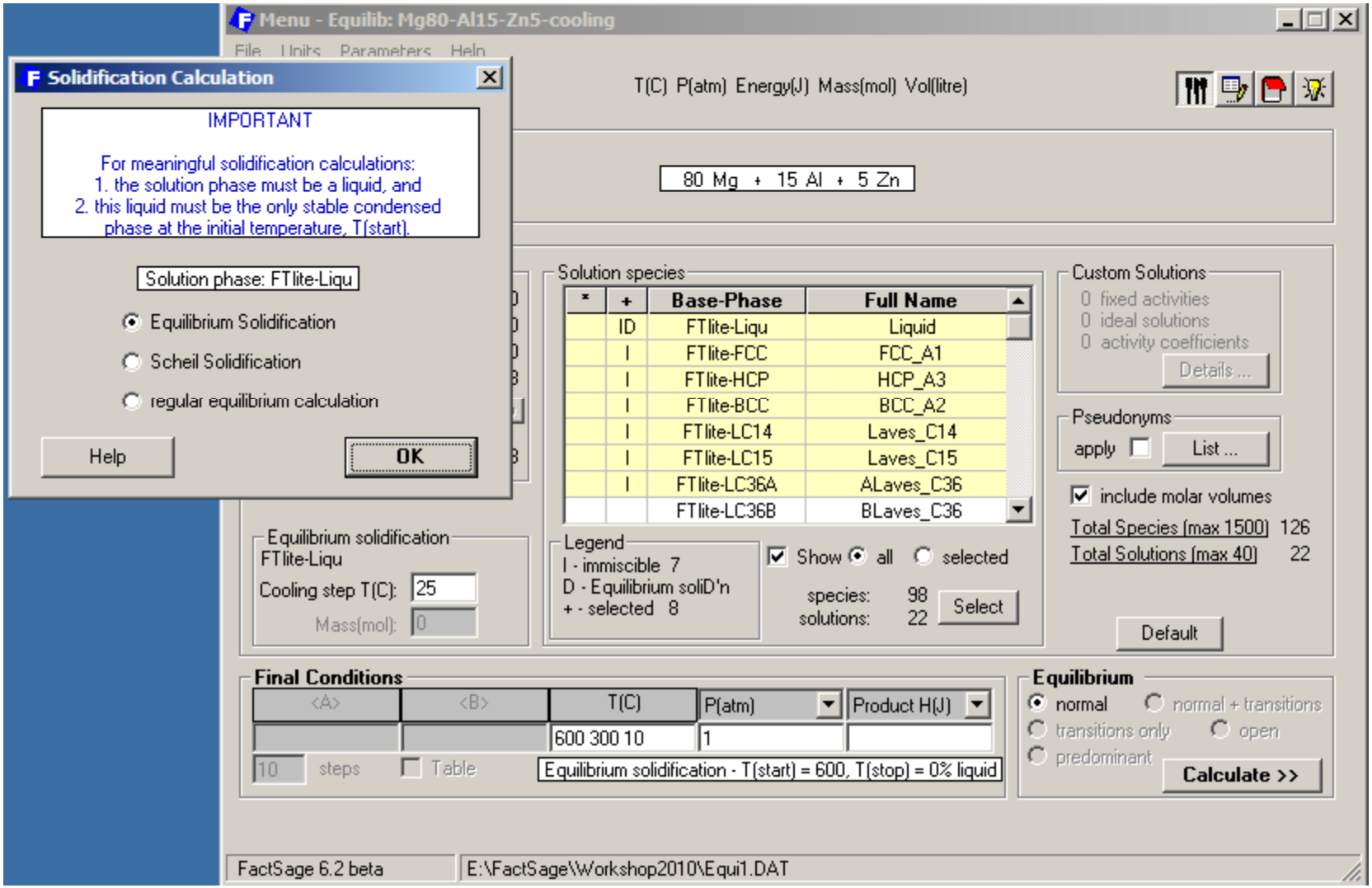
??? reaction at about 300 °C



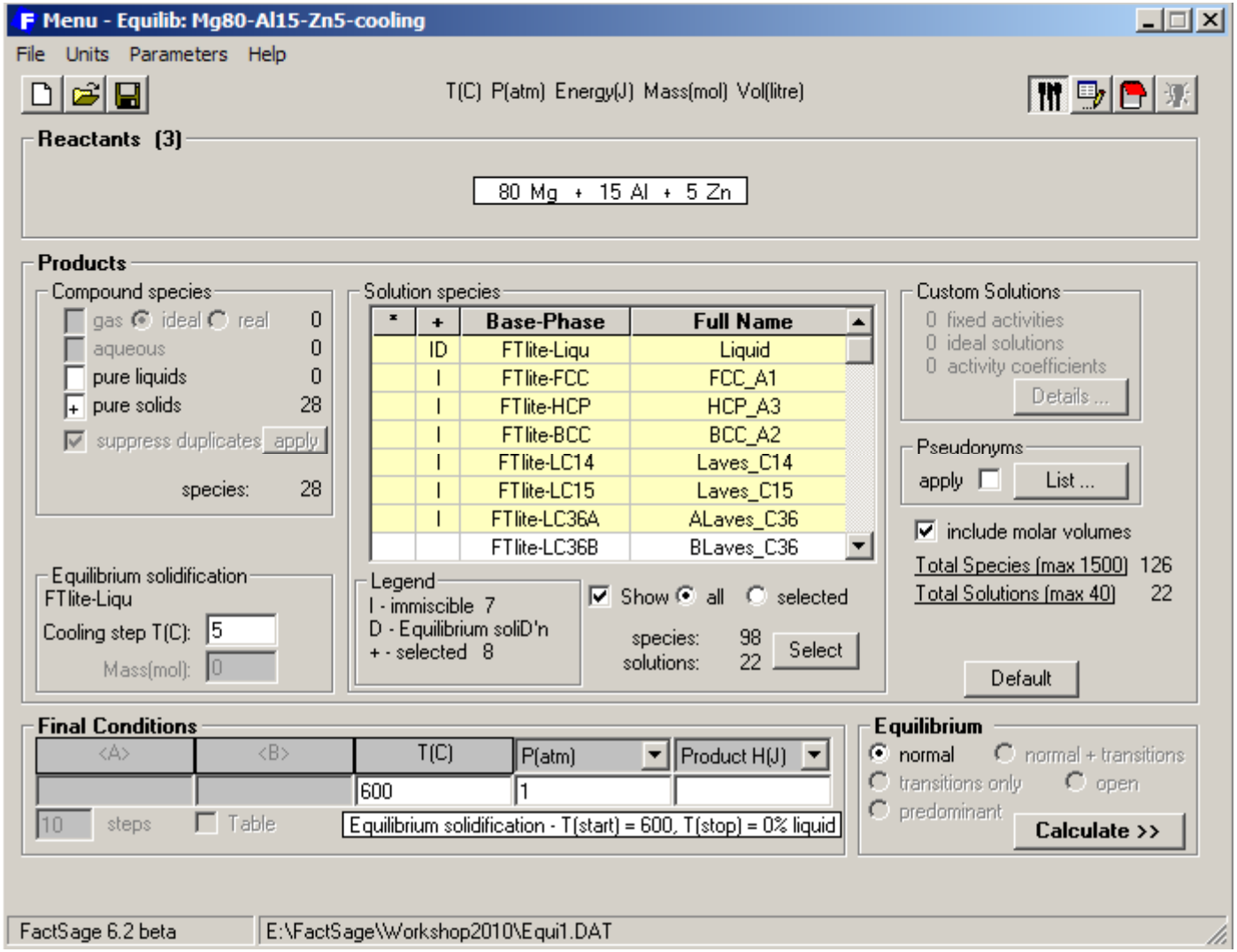
Using the “solidification software”



Select equilibrium solidification from liquid
(click on “include molar volumes” – See Manual Advanced Equilib 8)

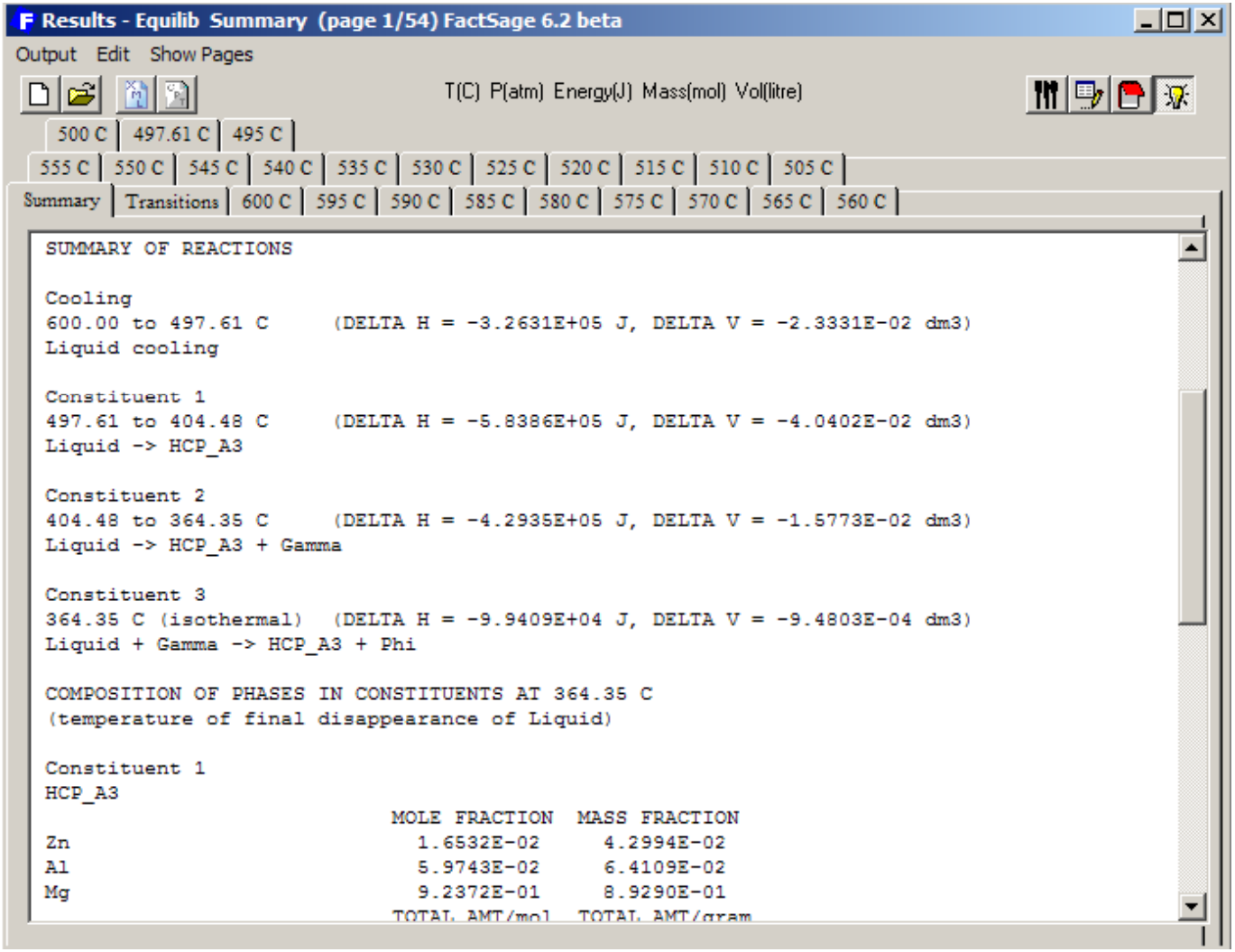


Select starting temperature

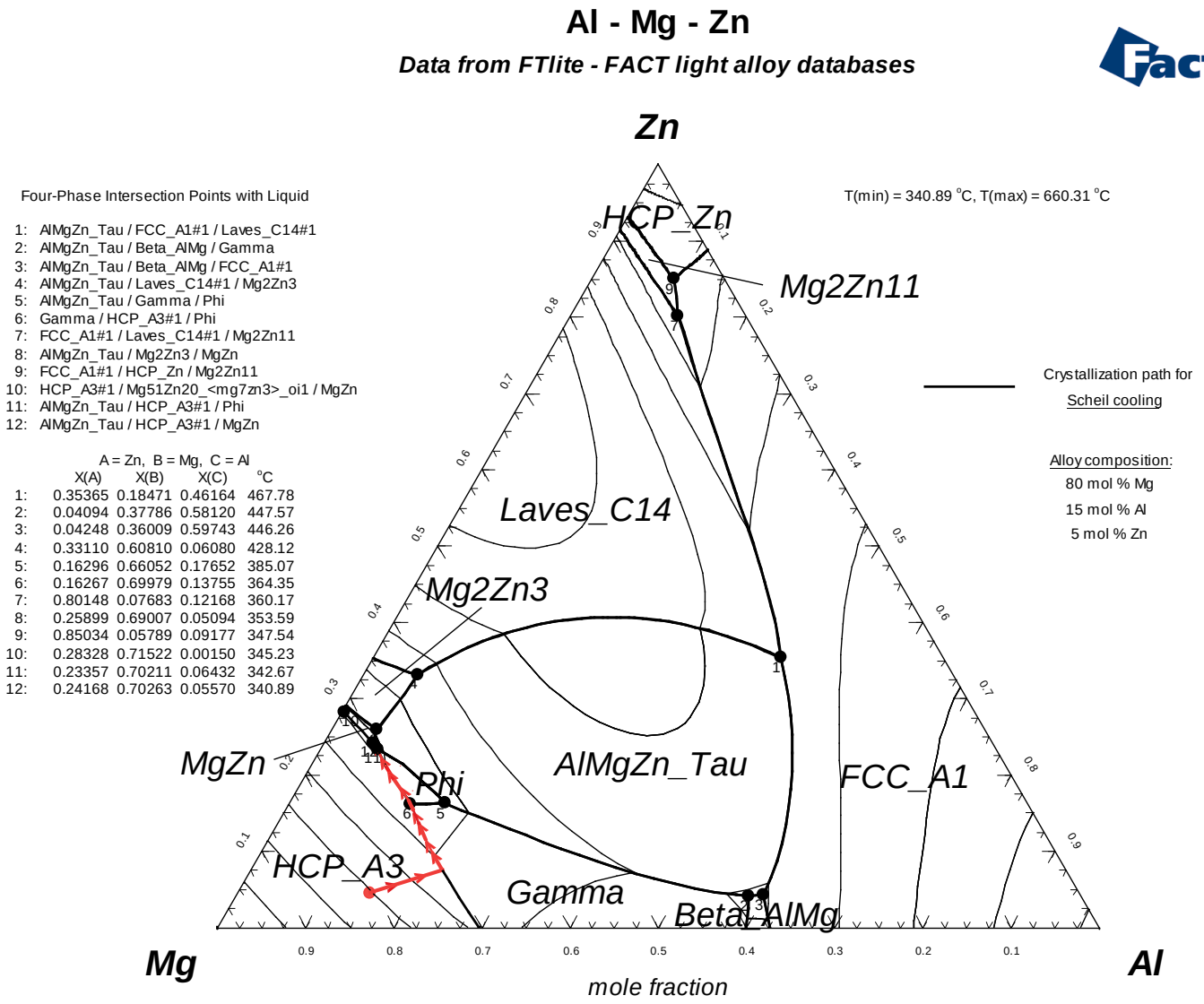


Output for Equilibrium Solidification

Note calculation of ΔH, ΔV (for ΔV be sure to click on "include molar volumes")
Calculation ends at temperature of final disappearance of liquid



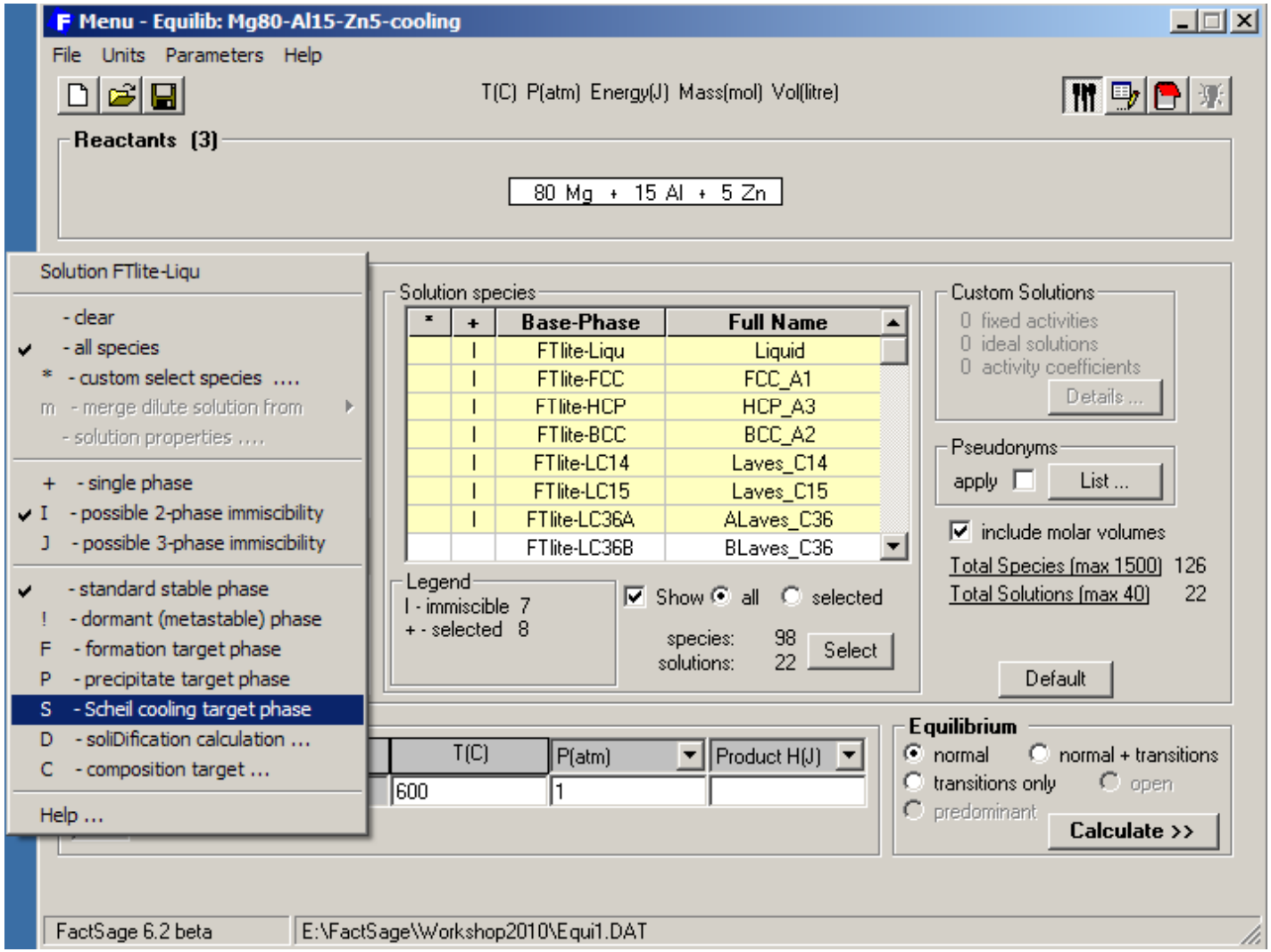
Scheil-Gulliver cooling path



Scheil-Gulliver Target for liquid

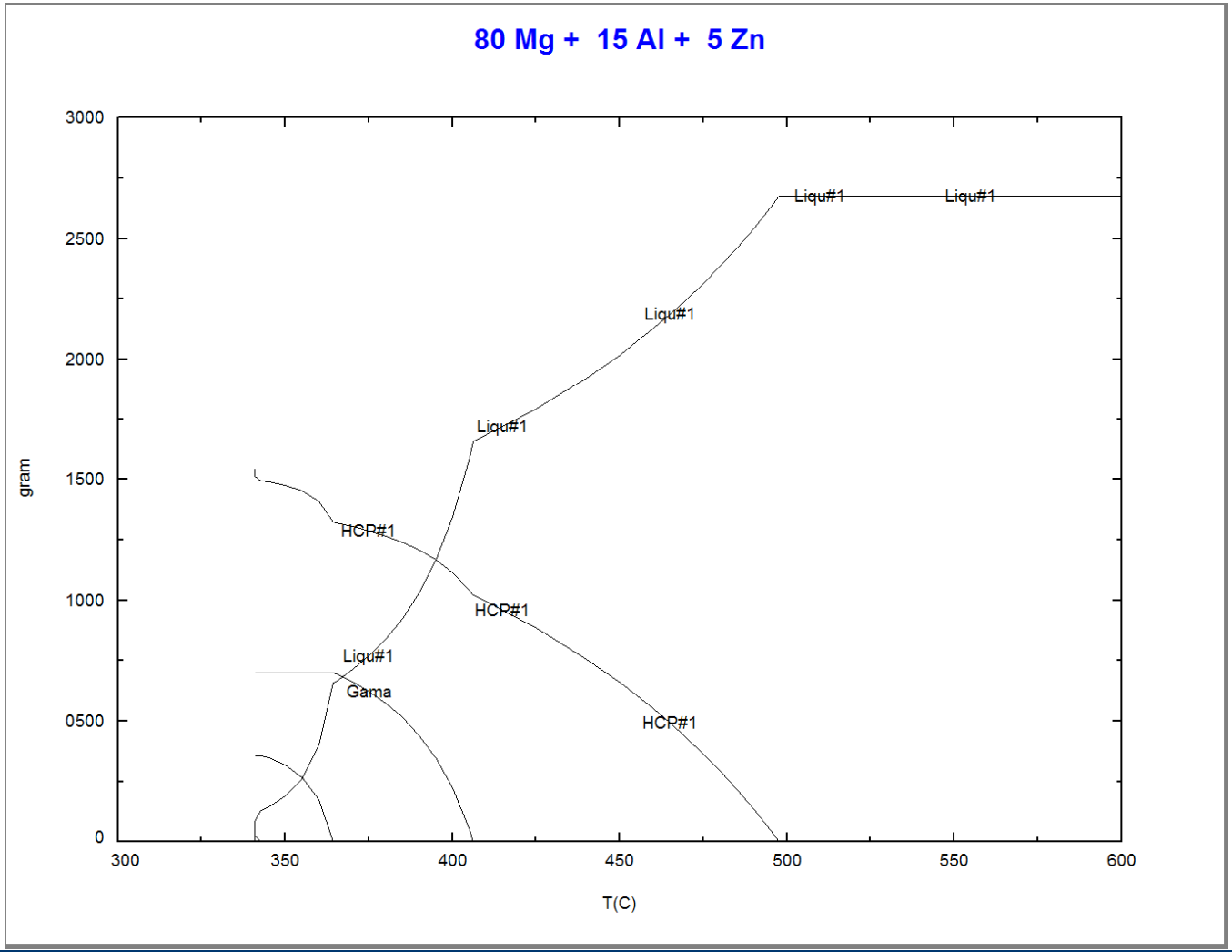
(Set starting temperature at 600 °C)

(See Manual Equilib Advanced 2.3)

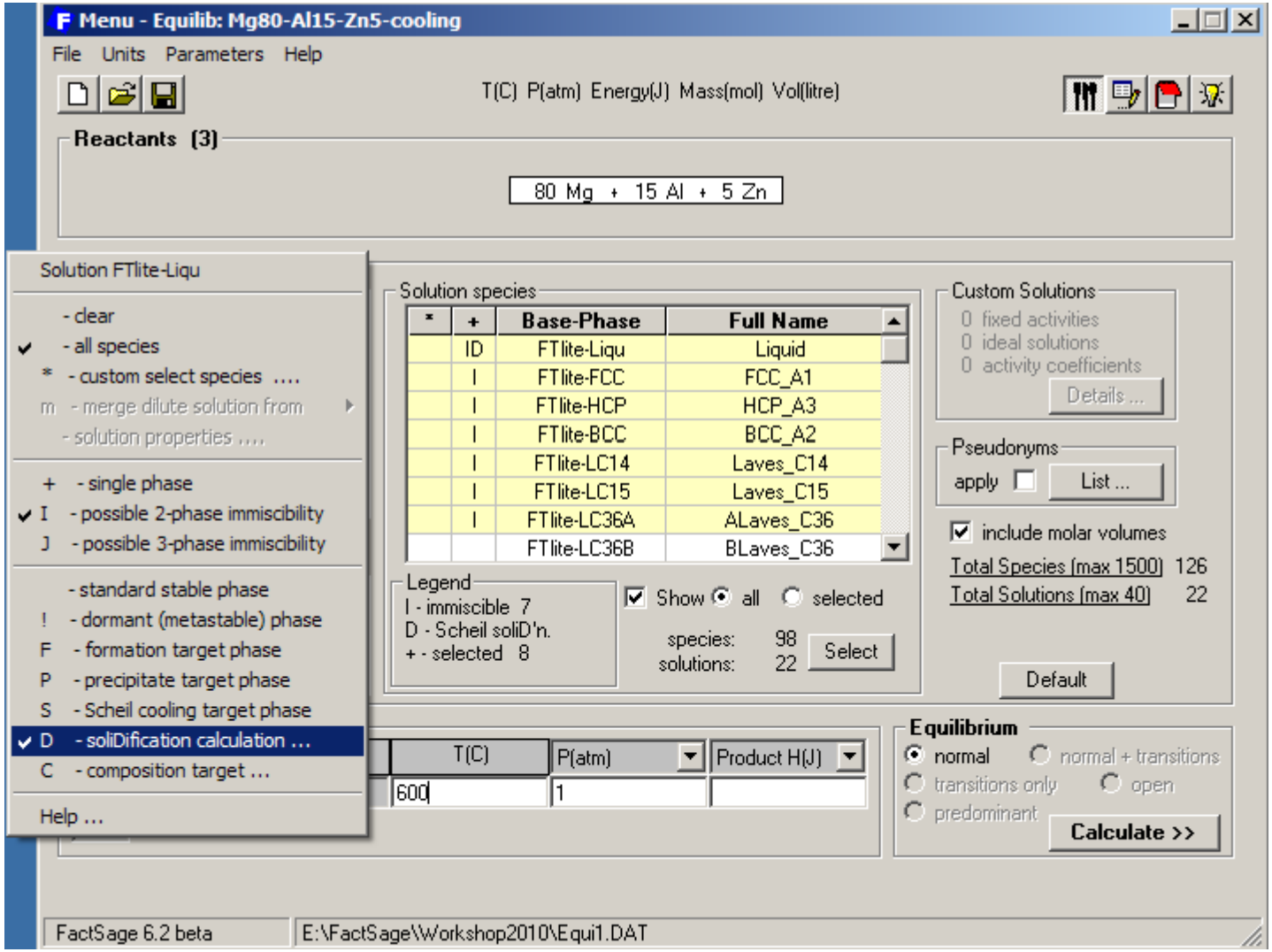


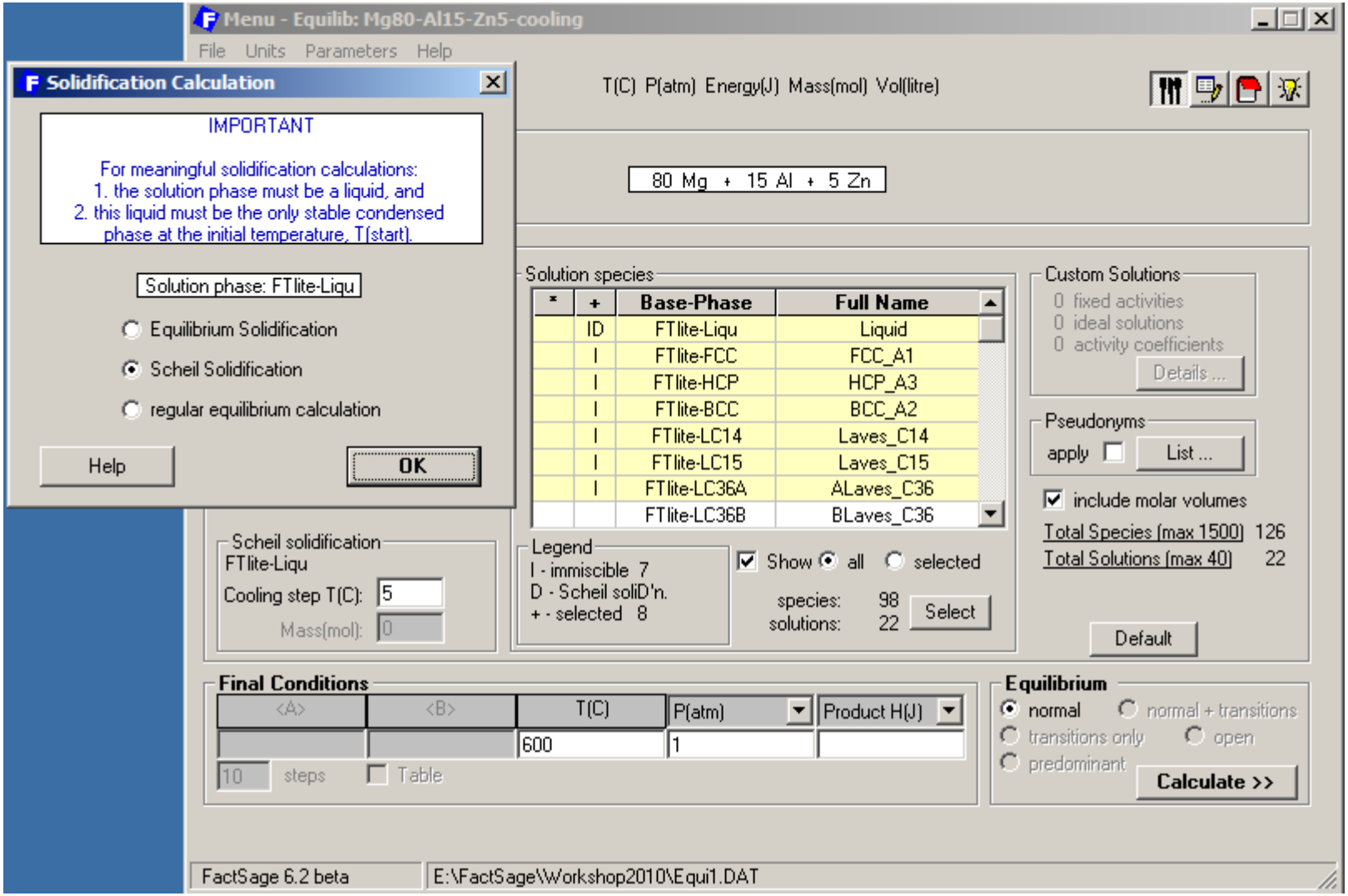
Graphical output of Scheil target calculation

- Calculation ends at temperature of final disappearance of liquid
- Graph shows phase distribution

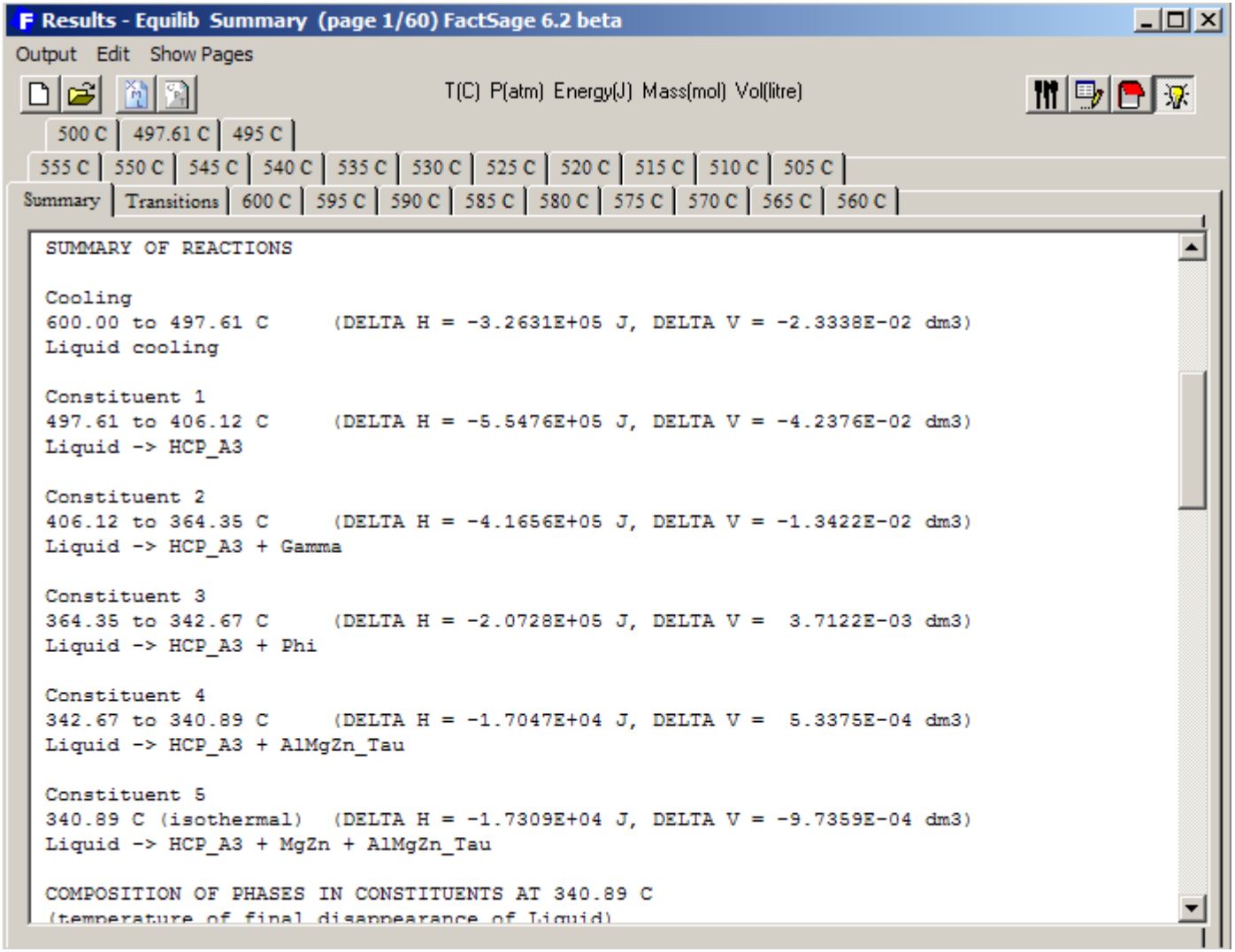


“Solidification” calculation for Scheil-Gulliver cooling




Menu - Equilib: Mg80-Al15-Zn5-cooling
File Units Parameters Help
Solidification Calculation
IMPORTANT
For meaningful solidification calculations:
1. the solution phase must be a liquid, and
2. this liquid must be the only stable condensed phase at the initial temperature, T[start].
Solution phase: FTlite-Liqu
Equilibrium Solidification
Scheil Solidification
regular equilibrium calculation
Help
OK
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)
80 Mg + 15 Al + 5 Zn
Solution species
* + Base-Phase Full Name
ID FTlite-Liqu Liquid
I FTlite-FCC FCC_A1
I FTlite-HCP HCP_A3
I FTlite-BCC BCC_A2
I FTlite-LC14 Laves_C14
I FTlite-LC15 Laves_C15
I FTlite-LC36A ALaves_C36
FTlite-LC36B BLaves_C36
Custom Solutions
0 fixed activities
0 ideal solutions
0 activity coefficients
Details ...
Pseudonyms
apply
List ...
include molar volumes
Total Species (max 1500) 126
Total Solutions (max 40) 22
Scheil solidification
FTlite-Liqu
Cooling step T(C): 5
Mass(mol): 0
Legend
I - immiscible 7
D - Scheil soliD'n.
+ - selected 8
Show all selected
species: 98
solutions: 22
Select
Default
Final Conditions
<A> <B> T(C) P(atm) Product H(J)
600 1
10 steps Table
Equilibrium
normal normal + transitions
transitions only open
predominant
Calculate >>
FactSage 6.2 beta
E:\FactSage\Workshop2010\Equi1.DAT

Output for Scheil-Gulliver Solidification



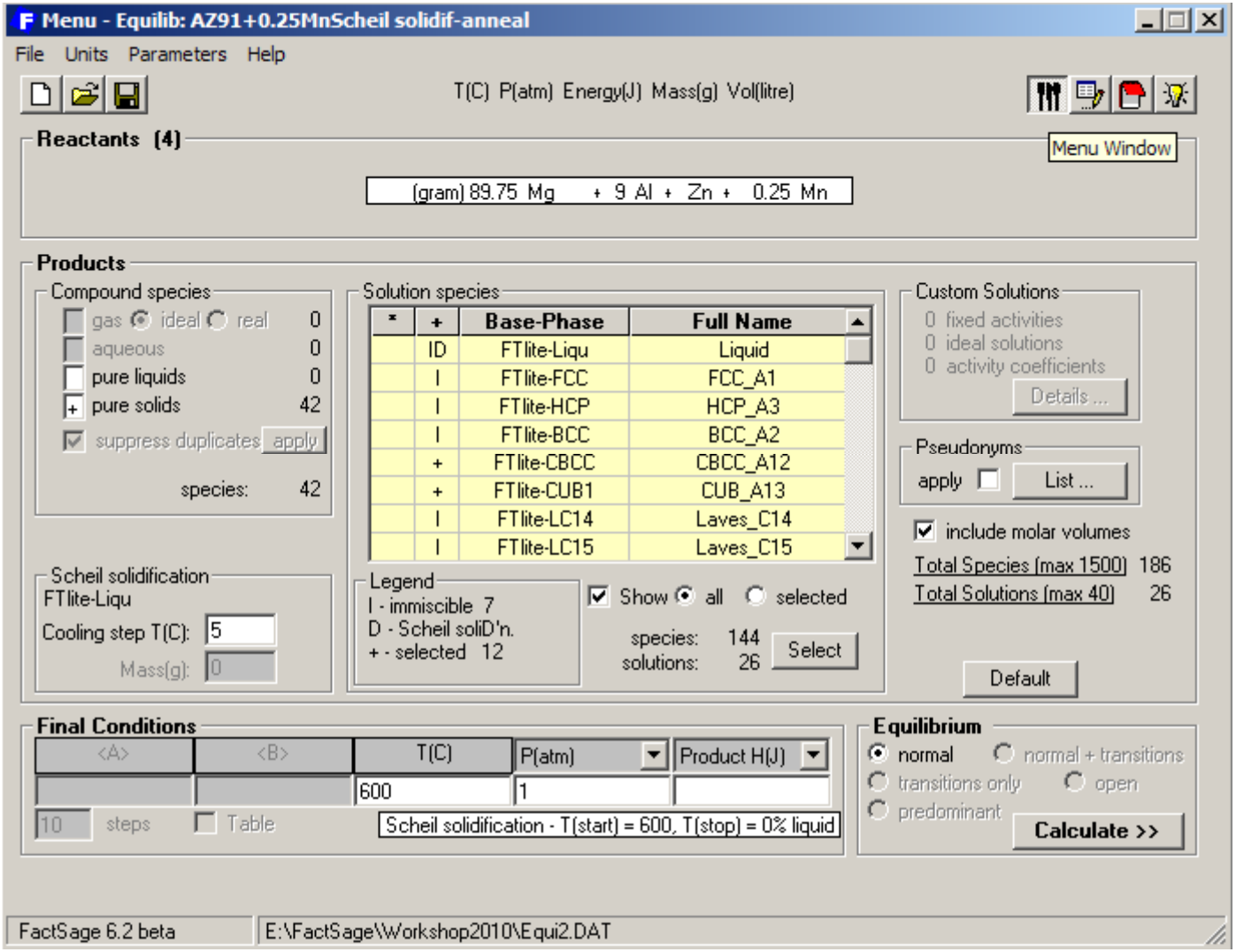
- Solidification software (extended Scheil cooling)
  - Scheil cooling + post equilibration of Scheil microstructure
- AZ91 alloy + 0.25 wt.% Mn

Tracking microstructure constituents

Output : Solidification temperature of 340.89°C

CONS.	PHASE	TOTAL AMT/gram	
1	1 'Al8Mn5'	5.2241E-04	Constituent 1 594.16 to 594.06 C Liq. -> 'Al8Mn5'
2	1 HCP	6.4599E+01	Constituent 2 594.06 to 524.15 C Liq. -> HCP + 'Al8Mn5'
2	2 'Al8Mn5'	2.8231E-01	
3	1 HCP	1.5644E+01	Constituent 3 524.15 to 447.46 C Liq. -> HCP + Al11Mn4
3	2 Al11Mn4	1.4638E-01	
4	1 HCP	1.7084E+00	Constituent 4 447.46 to 431.74 C Liq. -> HCP + 'Al4Mn'
4	2 'Al4Mn'	1.7892E-02	
5	1 HCP	4.9213E+00	Constituent 5 431.74 to 364.34 C Liq. -> HCP + 'Al12Mg17' + 'Al4Mn'
5	2 'Al12Mg17'	1.1878E+01	
5	3 'Al4Mn'	2.6558E-02	
6	1 HCP	1.9669E-01	Constituent 6 364.34 to 342.66 C Liq. -> HCP + Phi + 'Al4Mn' + Al11Mn4
6	2 Phi	4.0423E-01	
6	3 'Al4Mn'	1.7904E-05	
6	4 Al11Mn4	3.8196E-05	
7	1 HCP	2.4177E-02	Constituent 7 342.66 to 340.89 C Liq. -> HCP + Tau + Al11Mn4
7	2 Tau	3.5706E-02	
7	3 Al11Mn4	1.4894E-06	
8	1 HCP	4.2084E-02	Constituent 8 340.89 C (isothermal) Liq. -> HCP + MgZn + Tau + Al11Mn4
8	2 MgZn	5.1501E-02	
8	3 Tau	2.1364E-02	
8	4 Al11Mn4	2.3786E-06	

Input for Scheil Solidification AZ91 + 0.25% Mn



- Solidification software (extended Scheil cooling)
  - Scheil cooling + post equilibration (annealing) of Scheil microstructure
- AZ91 alloy + 0.25 wt.% Mn

Tracking microstructure constituents

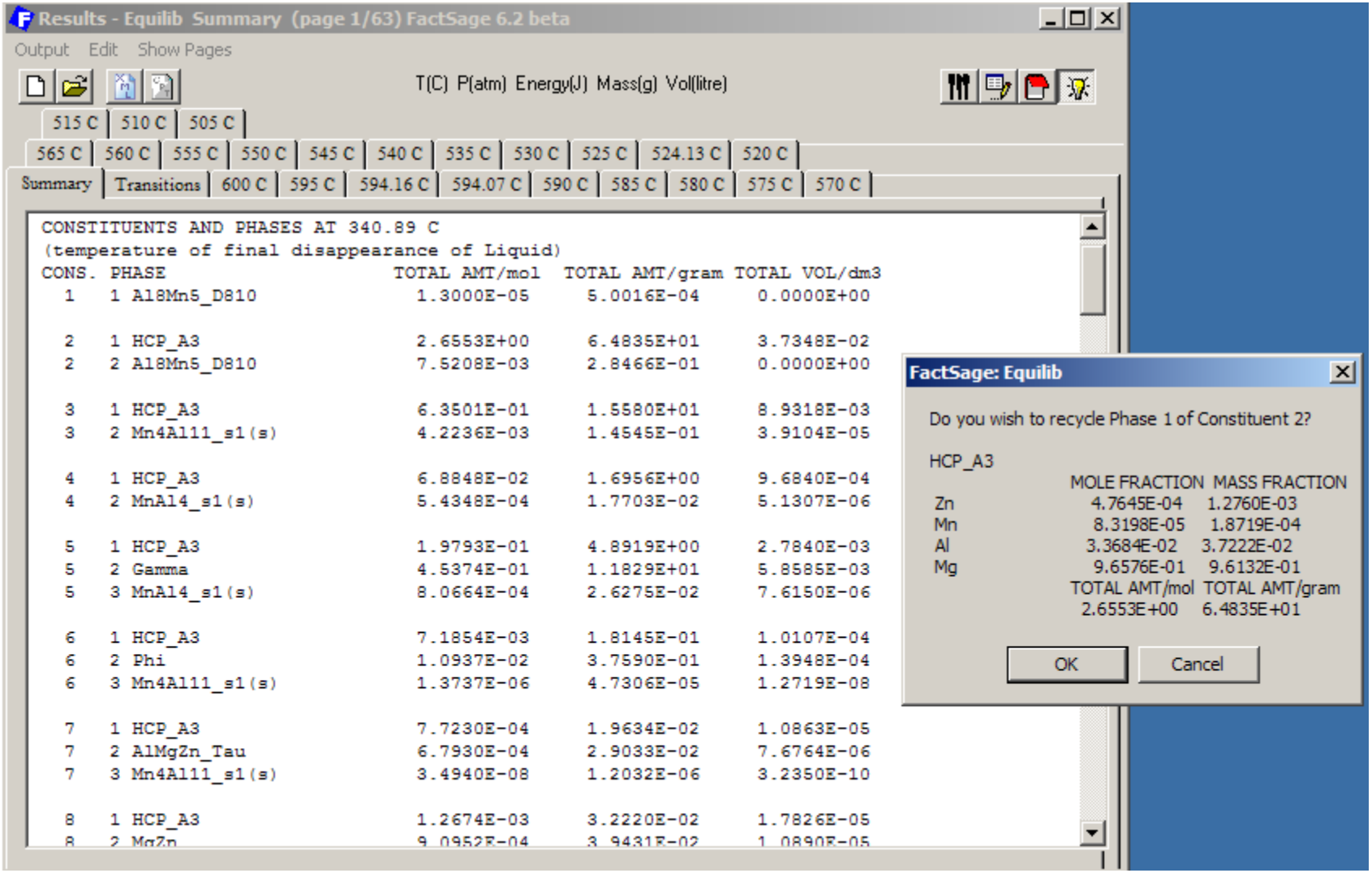
Output : Solidification temperature of 340.89°C

CONS.	PHASE	TOTAL AMT/gram
1	1 'Al8Mn5'	5.2241E-04
2	1 HCP	6.4599E+01
2	2 'Al8Mn5'	2.8231E-01
3	1 HCP	1.5644E+01
3	2 Al11Mn4	1.4638E-01
4	1 HCP	1.7084E+00
4	2 'Al4Mn'	1.7892E-02
5	1 HCP	4.9213E+00
5	2 'Al12Mg17'	1.1878E+01
5	3 'Al4Mn'	2.6558E-02
6	1 HCP	1.9669E-01
6	2 Phi	4.0423E-01
6	3 'Al4Mn'	1.7904E-05
6	4 Al11Mn4	3.8196E-05
7	1 HCP	2.4177E-02
7	2 Tau	3.5706E-02
7	3 Al11Mn4	1.4894E-06
8	1 HCP	4.2084E-02
8	2 MgZn	5.1501E-02
8	3 Tau	2.1364E-02
8	4 Al11Mn4	2.3786E-06

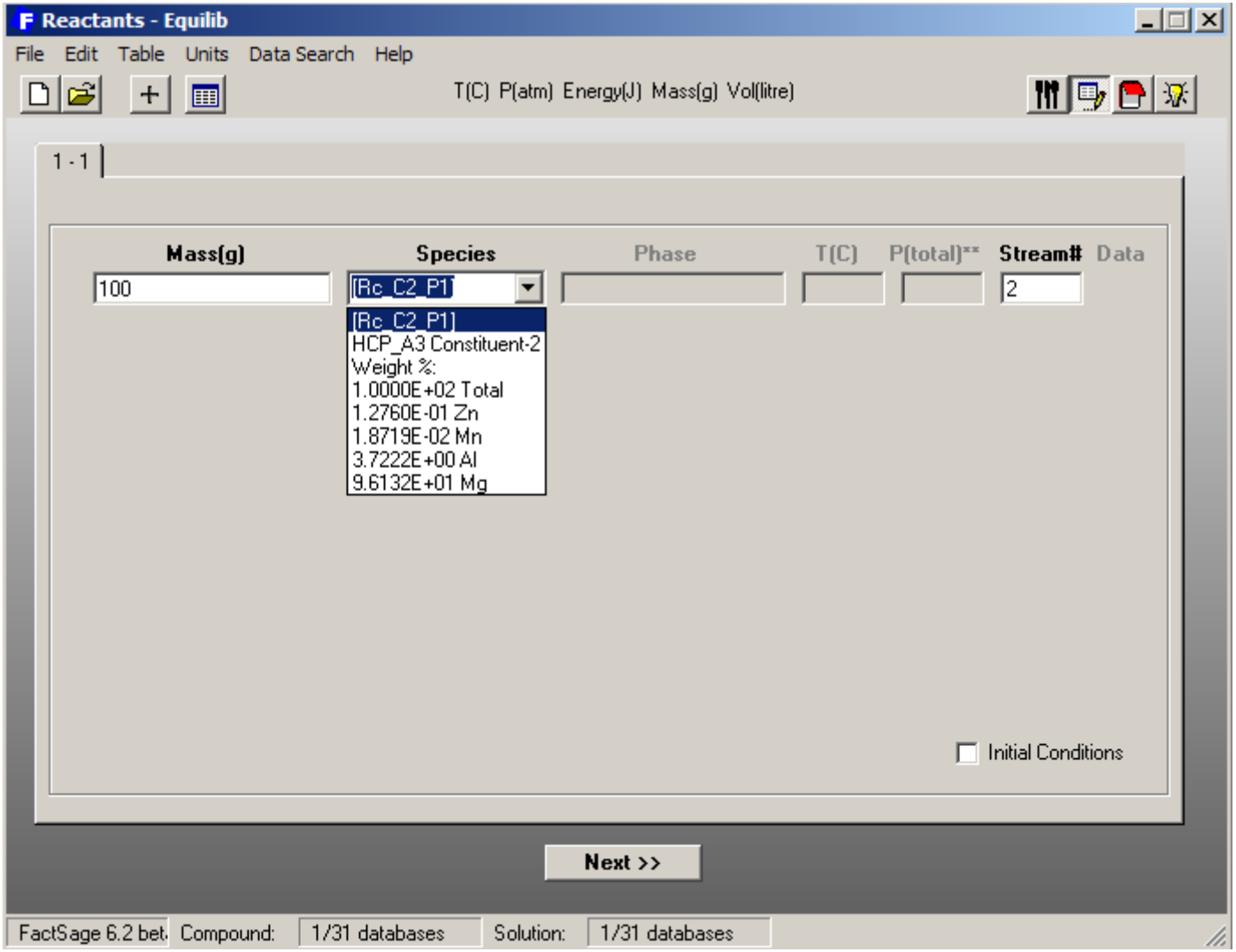
Amount & Average Composition of the **HCP phase**

	wt. %	Mg	Al	Zn	Mn
2	64.599	96.19	3.67	0.125	195 ppm
3	15.644	92.25	7.45	0.298	14.7 ppm
4	1.708	89.22	10.34	0.440	1.2 ppm
5	4.921	88.95	10.03	1.021	0.7 ppm
6	0.197	89.77	5.14	5.086	0.1 ppm
7	0.024	90.55	2.93	6.519	0.2 ppm
8	0.042	90.57	2.90	6.538	0.2 ppm

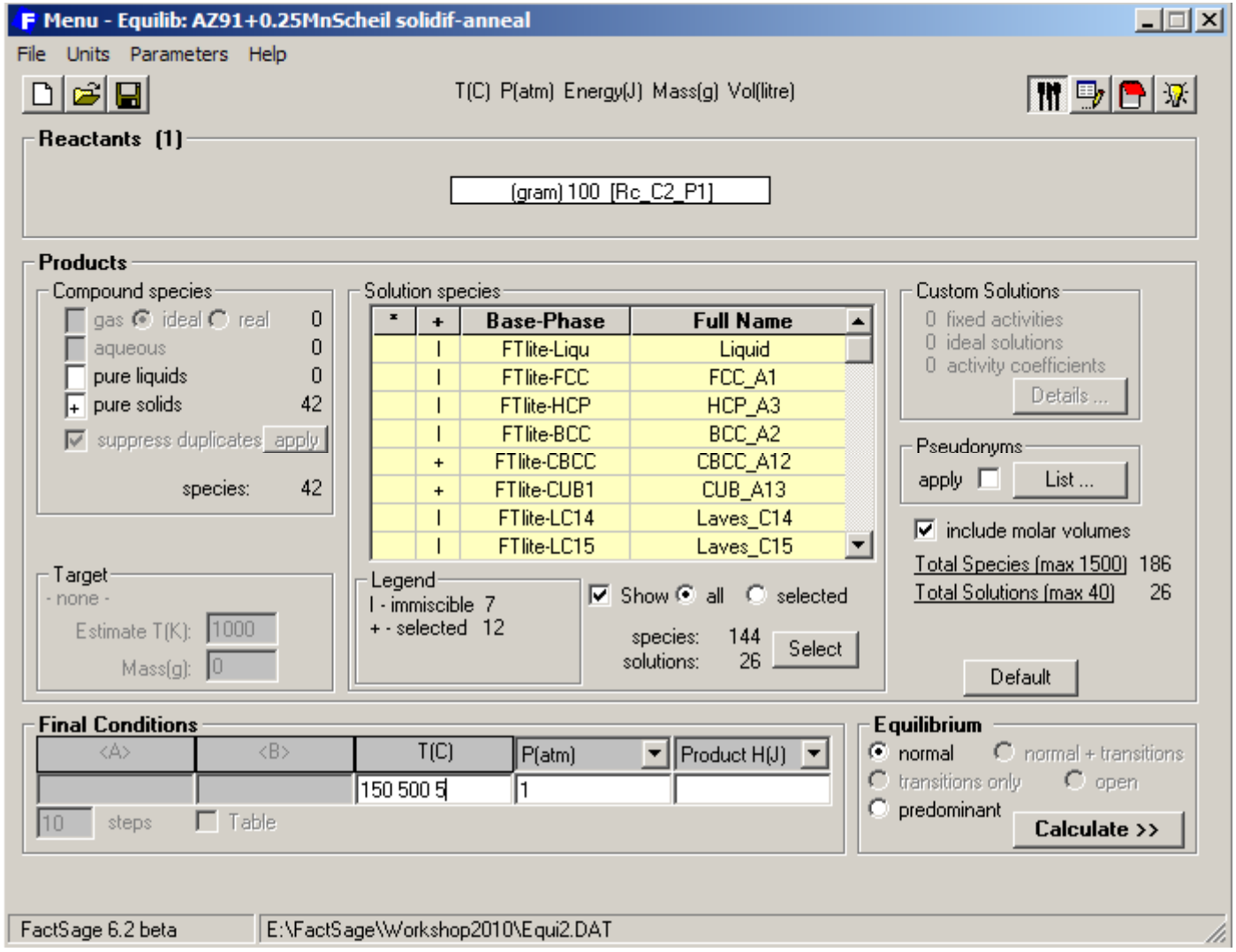
Selecting HCP phase of constituent 2 for subsequent annealing



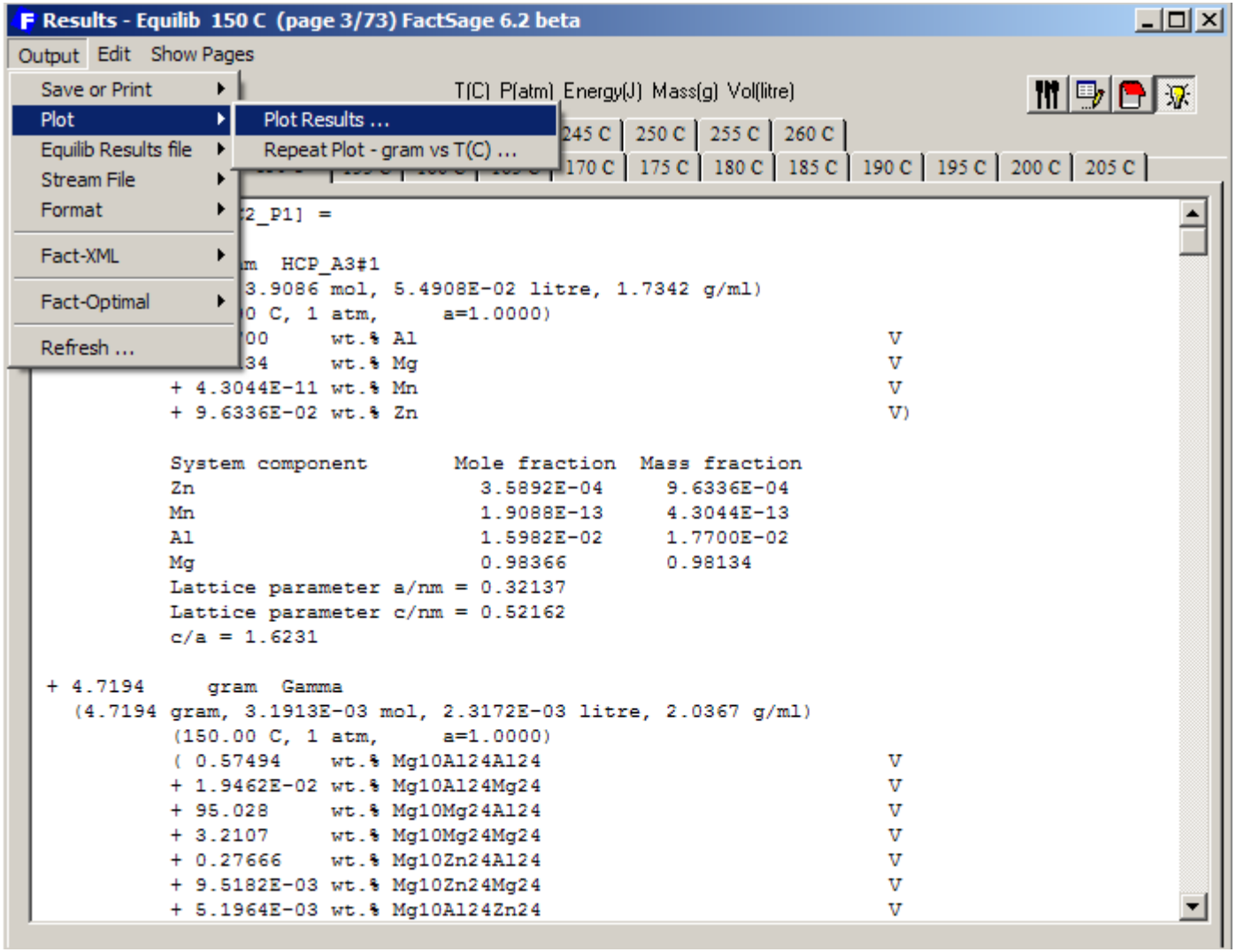
Imported automatically into Equilib (change mass to 100 g)



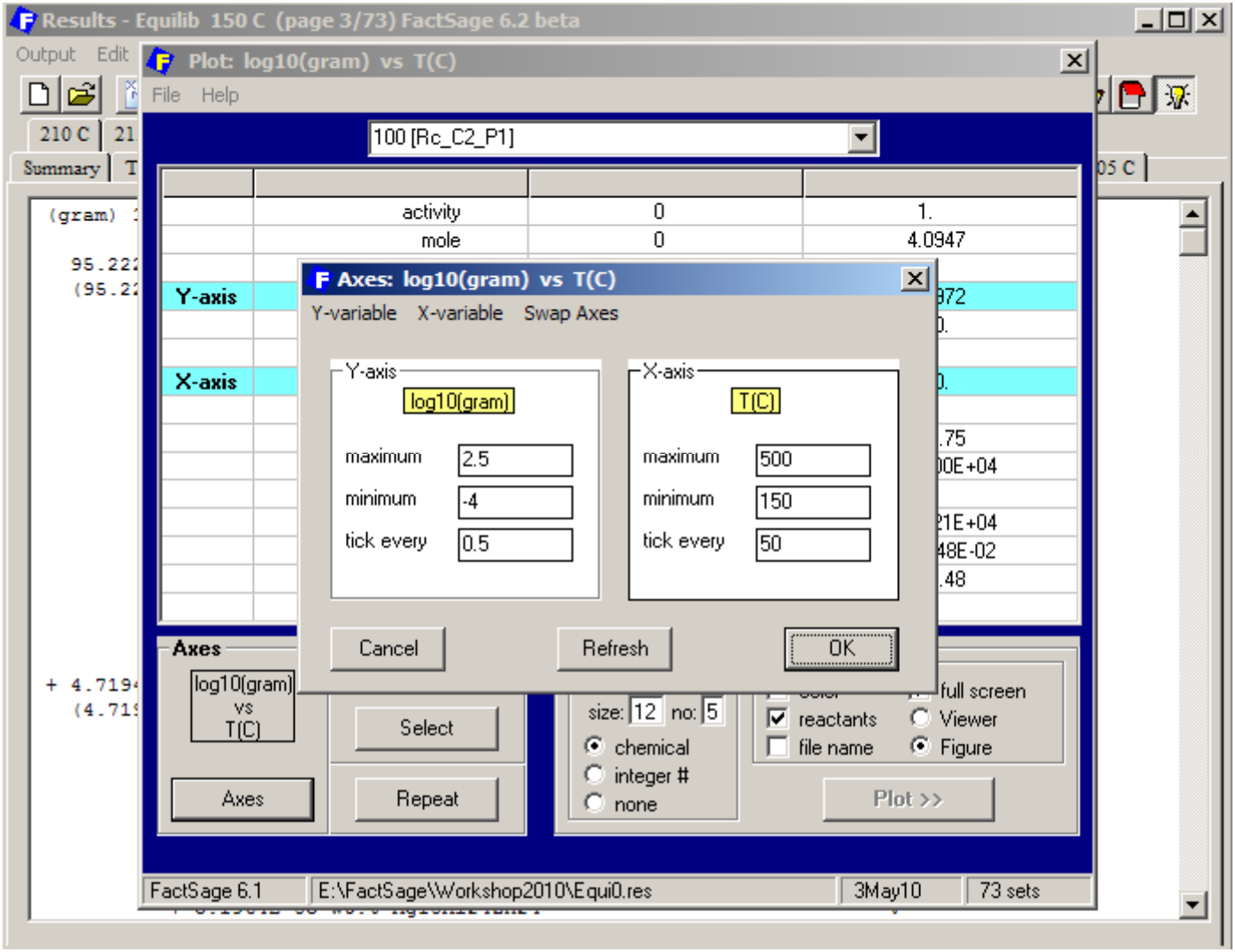
Anneal at 150 to 500 °C



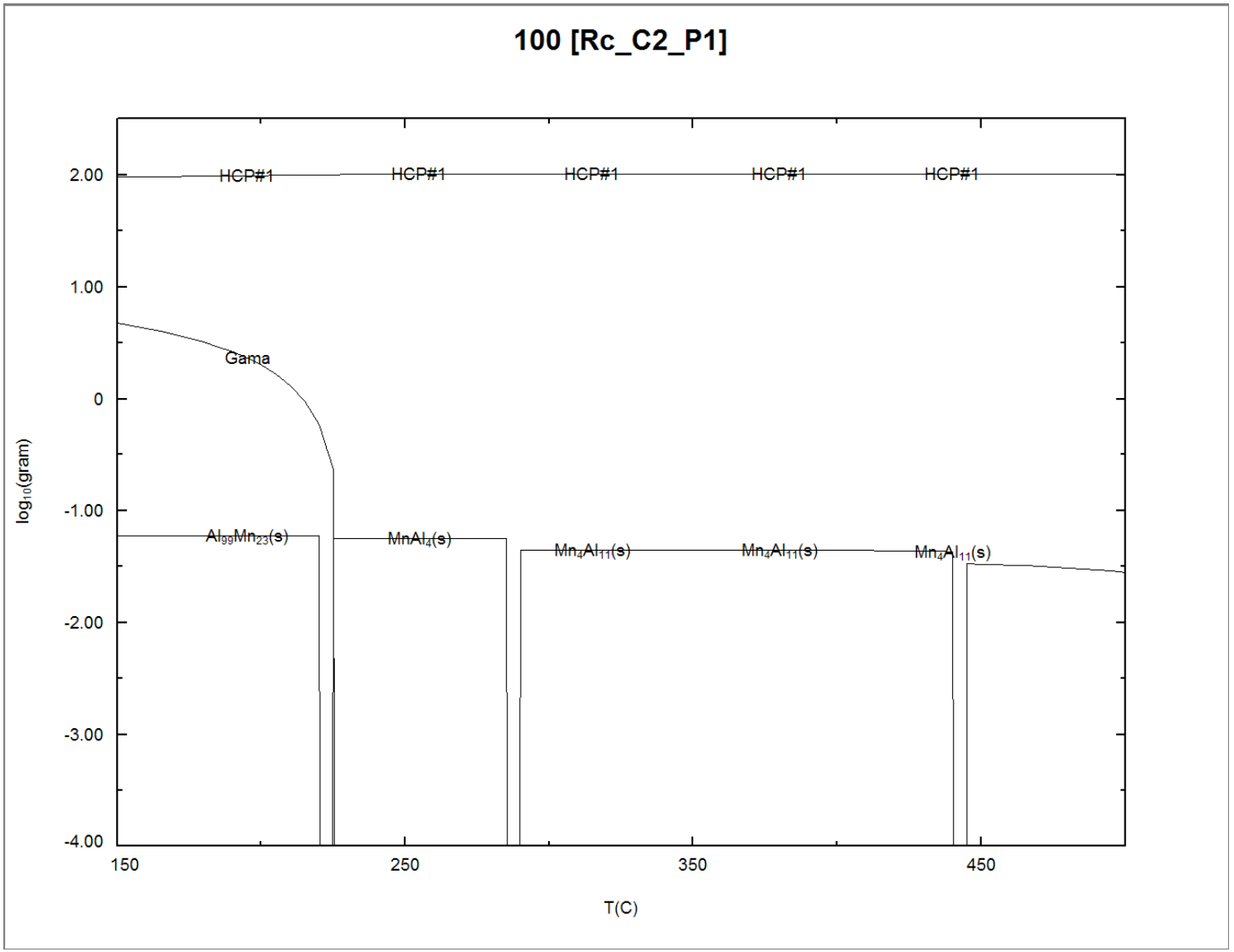
Plot equilibrium products in HCP phase of constituent 2 after annealing



- Select axes


Results - Equilib 150 C (page 3/73) FactSage 6.2 beta
Output Edit
Plot: log10(gram) vs T(C)
File Help
100 [Rc_C2_P1]
activity 0 1.
mole 0 4.0947
Y-axis
X-axis
Axes: log10(gram) vs T(C)
Y-variable X-variable Swap Axes
Y-axis
log10(gram)
maximum 2.5
minimum -4
tick every 0.5
X-axis
T(C)
maximum 500
minimum 150
tick every 50
Cancel
Refresh
OK
Axes
log10(gram) vs T(C)
Axes
Select
Repeat
size: 12 no: 5
chemical
integer #
none
reactants
file name
full screen
Viewer
Figure
Plot >>
FactSage 6.1
E:\FactSage\Workshop2010\Equi0.res
3May10
73 sets

Equilibrium phase distribution in HCP phase of constituent 2 after annealing (HCP + precipitates)



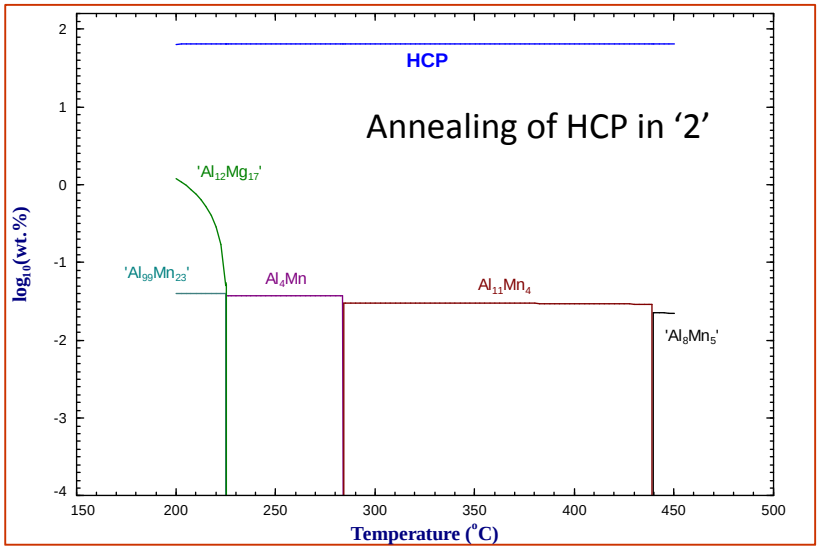
- Solidification software (extended Scheil cooling)
  - Scheil cooling + post equilibration of Scheil microstructure
- AZ91 alloy + 0.25 wt.% Mn

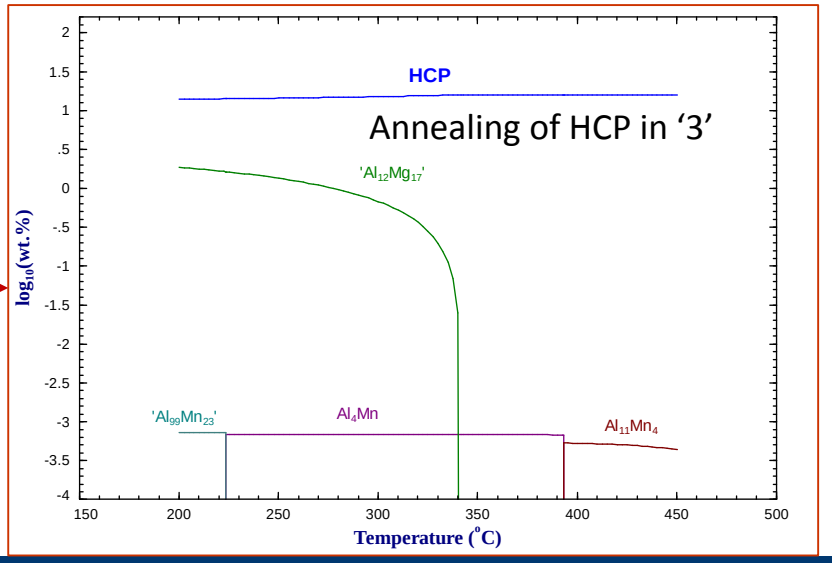
Tracking microstructure constituents

Annealing
Phases *vs* T for HCP in the different microstructural constituents

Amount & Average Composition of the **HCP phase** at 340.89°C

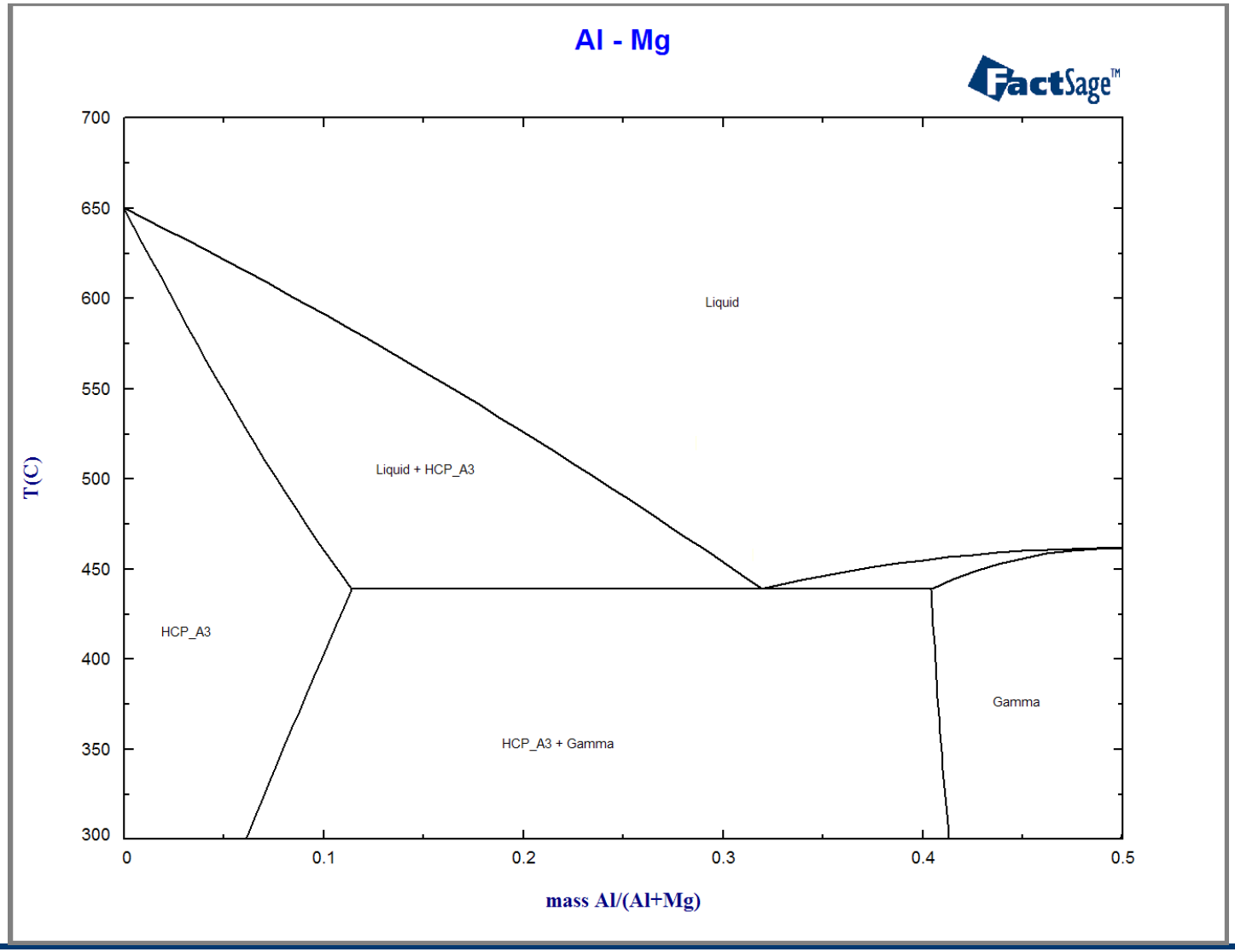
	wt. %	Mg	Al	Zn	Mn
2	64.599	96.19	3.67	0.125	195 ppm
3	15.644	92.25	7.45	0.298	14.7 ppm
4	1.708	89.22	10.34	0.440	1.2 ppm
5	4.921	88.95	10.03	1.021	0.7 ppm
6	0.197	89.77	5.14	5.086	0.1 ppm
7	0.024	90.55	2.93	6.519	0.2 ppm
8	0.042	90.57	2.90	6.538	0.2 ppm

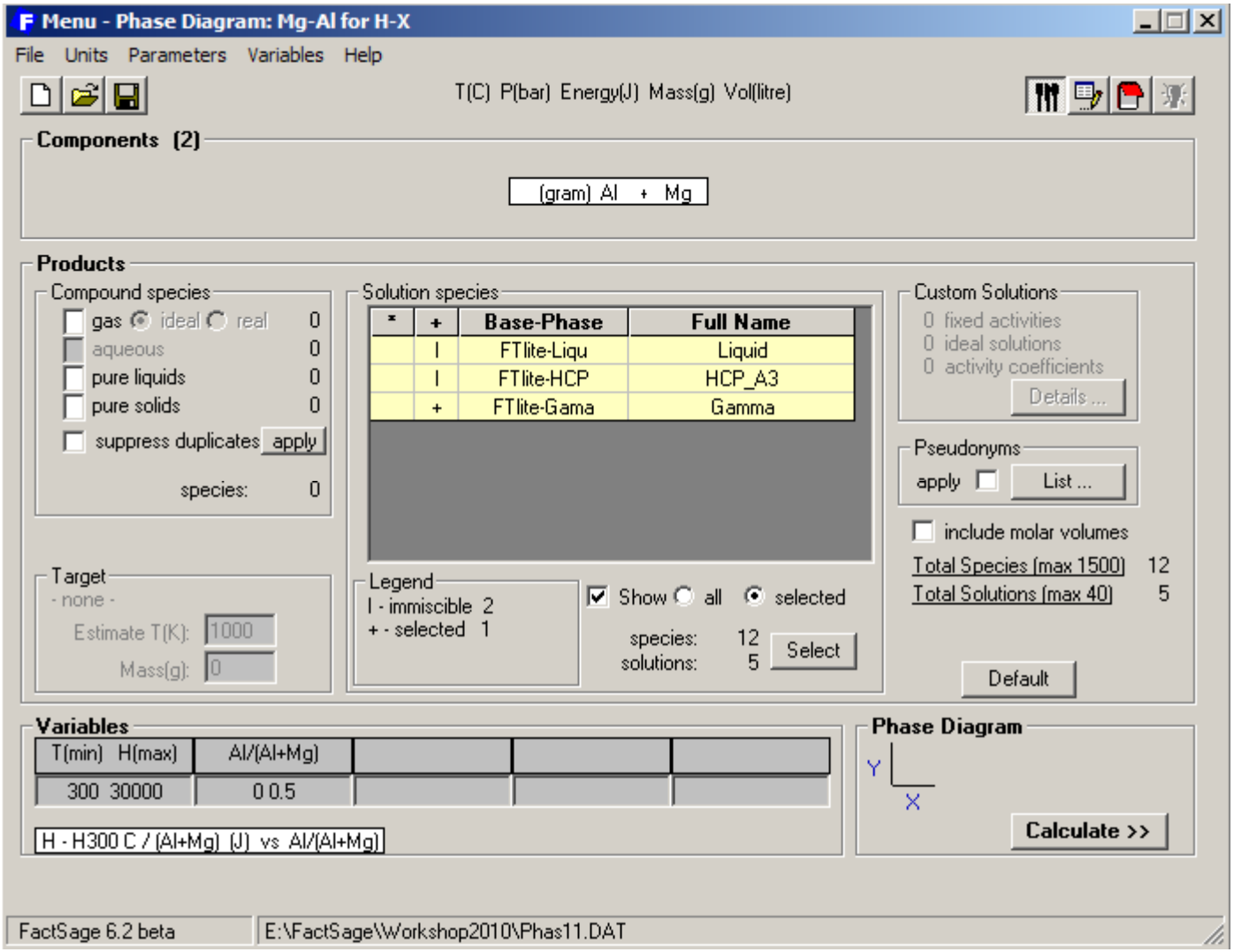




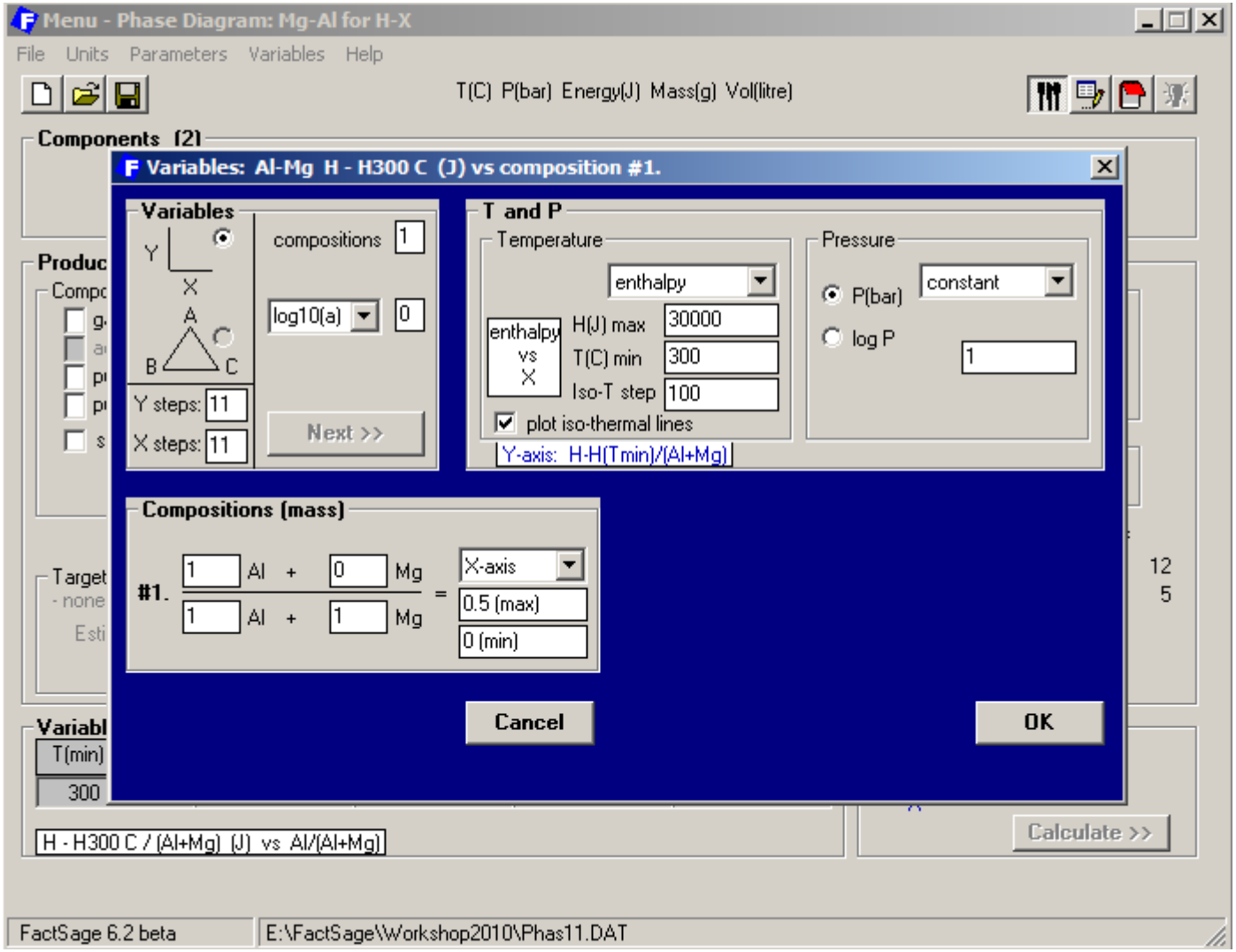
Enthalpy – Composition Phase Diagrams

- Mg-Al T-X diagram

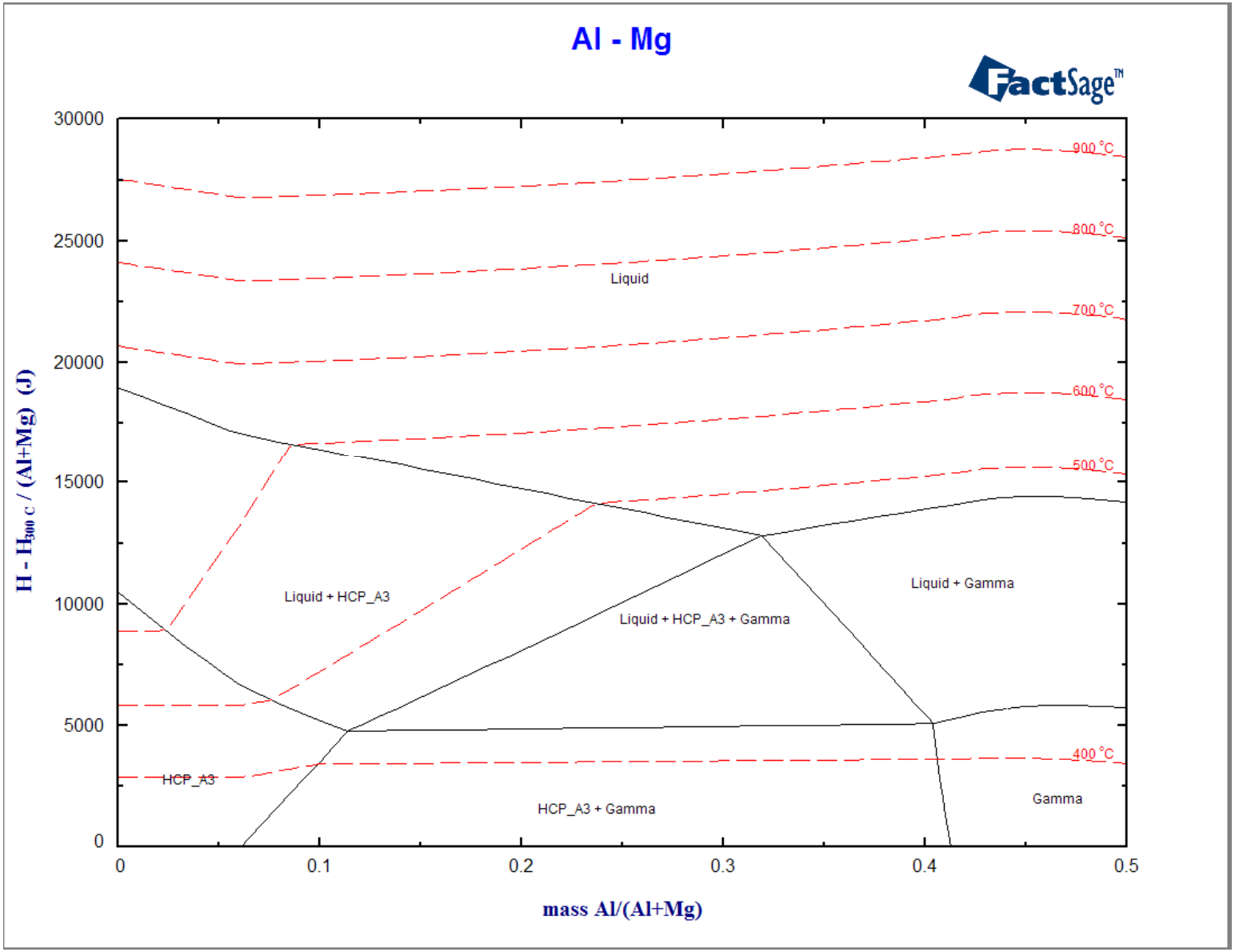



Menu - Phase Diagram: Mg-Al for H-X
File Units Parameters Variables Help
T(C) P(bar) Energy(J) Mass(g) Vol(litre)
Components (2)
(gram) Al + Mg
Products
Compound species
gas ideal real 0
aqueous 0
pure liquids 0
pure solids 0
suppress duplicates apply
species: 0
Solution species
* + Base-Phase Full Name
I FTlite-Liqu Liquid
I FTlite-HCP HCP_A3
+ FTlite-Gama Gamma
Custom Solutions
0 fixed activities
0 ideal solutions
0 activity coefficients
Details ...
Pseudonyms
apply List ...
include molar volumes
Total Species (max 1500) 12
Total Solutions (max 40) 5
Default
Target
- none -
Estimate T(K): 1000
Mass(g): 0
Legend
I - immiscible 2
+ - selected 1
Show all selected
species: 12
solutions: 5
Select
Variables
T(min) H(max) Al/(Al+Mg)
300 30000 0 0.5
H - H300 C / (Al+Mg) (J) vs Al/(Al+Mg)
Phase Diagram
Y
X
Calculate >>
FactSage 6.2 beta
E:\FactSage\Workshop2010\Phas11.DAT

Selecting variables for H-X diagram



Calculated Mg-Al H-X diagram



Al - Mg - Zn

Data from FTlite - FACT light alloy databases

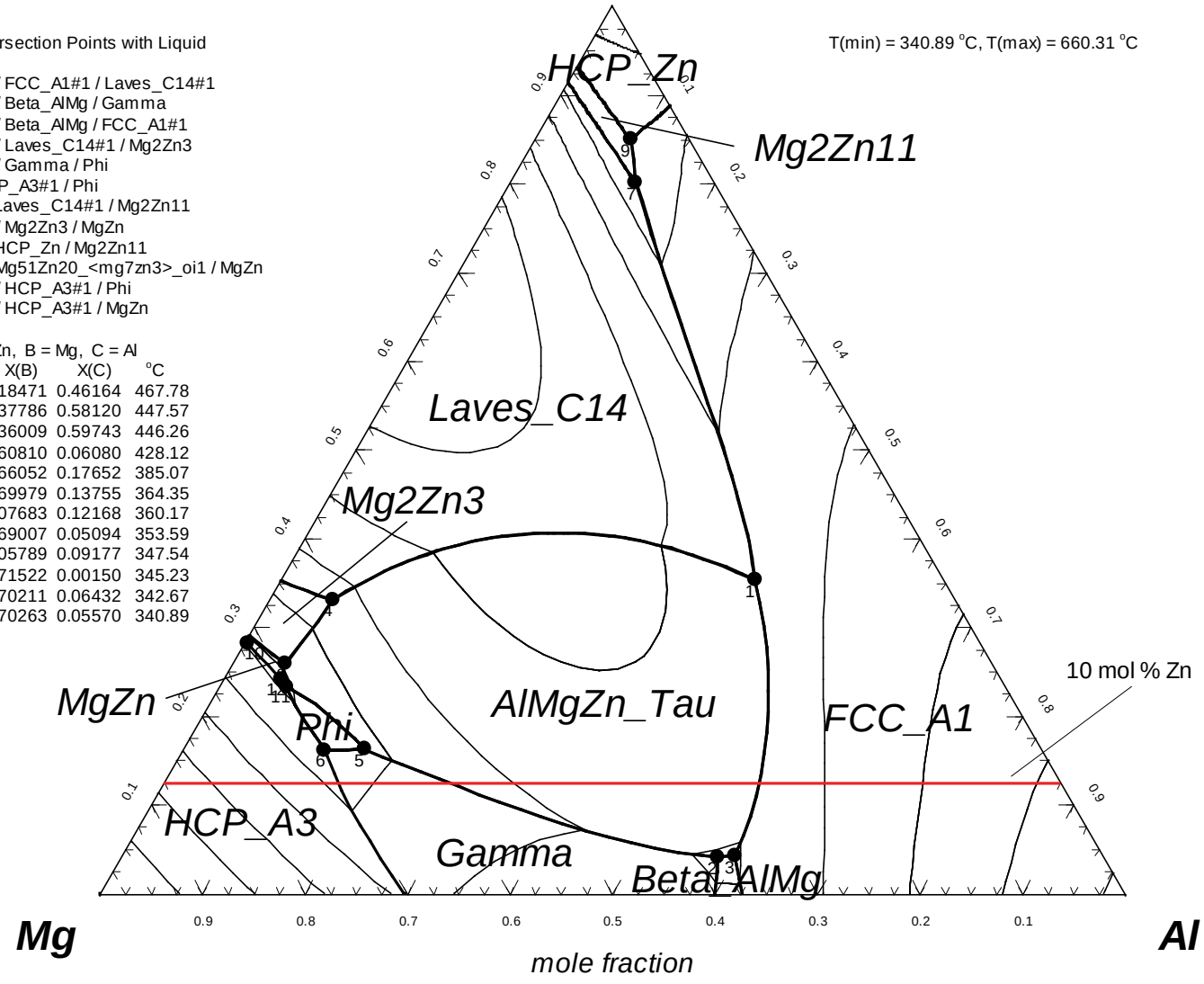
Four-Phase Intersection Points with Liquid

1: AlMgZn_Tau / FCC_A1#1 / Laves_C14#1
2: AlMgZn_Tau / Beta_AlMg / Gamma
3: AlMgZn_Tau / Beta_AlMg / FCC_A1#1
4: AlMgZn_Tau / Laves_C14#1 / Mg2Zn3
5: AlMgZn_Tau / Gamma / Phi
6: Gamma / HCP_A3#1 / Phi
7: FCC_A1#1 / Laves_C14#1 / Mg2Zn11
8: AlMgZn_Tau / Mg2Zn3 / MgZn
9: FCC_A1#1 / HCP_Zn / Mg2Zn11
10: HCP_A3#1 / Mg51Zn20_<mg7zn3>_oi1 / MgZn
11: AlMgZn_Tau / HCP_A3#1 / Phi
12: AlMgZn_Tau / HCP_A3#1 / MgZn

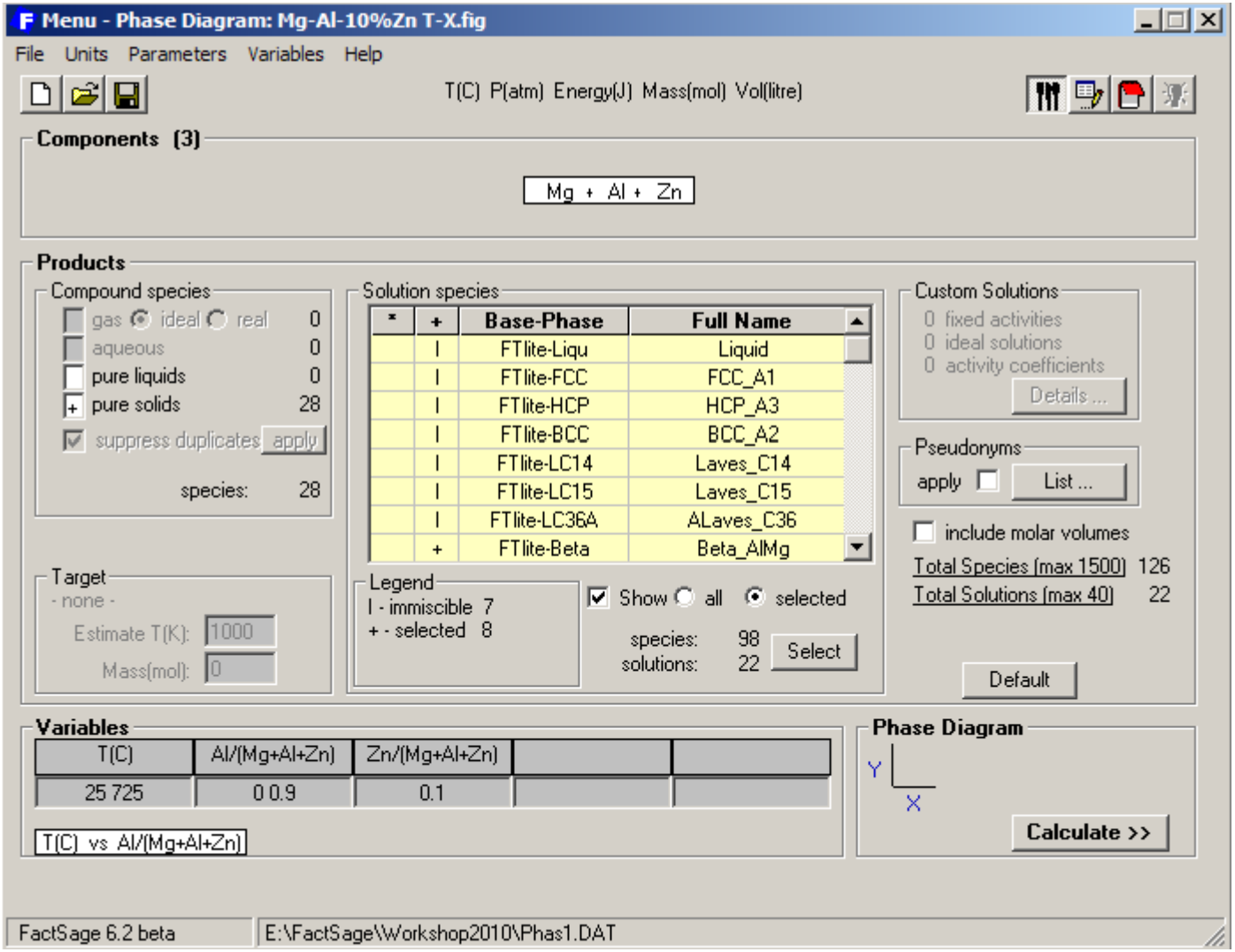
A = Zn, B = Mg, C = Al

	X(A)	X(B)	X(C)	°C
1:	0.35365	0.18471	0.46164	467.78
2:	0.04094	0.37786	0.58120	447.57
3:	0.04248	0.36009	0.59743	446.26
4:	0.33110	0.60810	0.06080	428.12
5:	0.16296	0.66052	0.17652	385.07
6:	0.16267	0.69979	0.13755	364.35
7:	0.80148	0.07683	0.12168	360.17
8:	0.25899	0.69007	0.05094	353.59
9:	0.85034	0.05789	0.09177	347.54
10:	0.28328	0.71522	0.00150	345.23
11:	0.23357	0.70211	0.06432	342.67
12:	0.24168	0.70263	0.05570	340.89

T(min) = 340.89 °C, T(max) = 660.31 °C

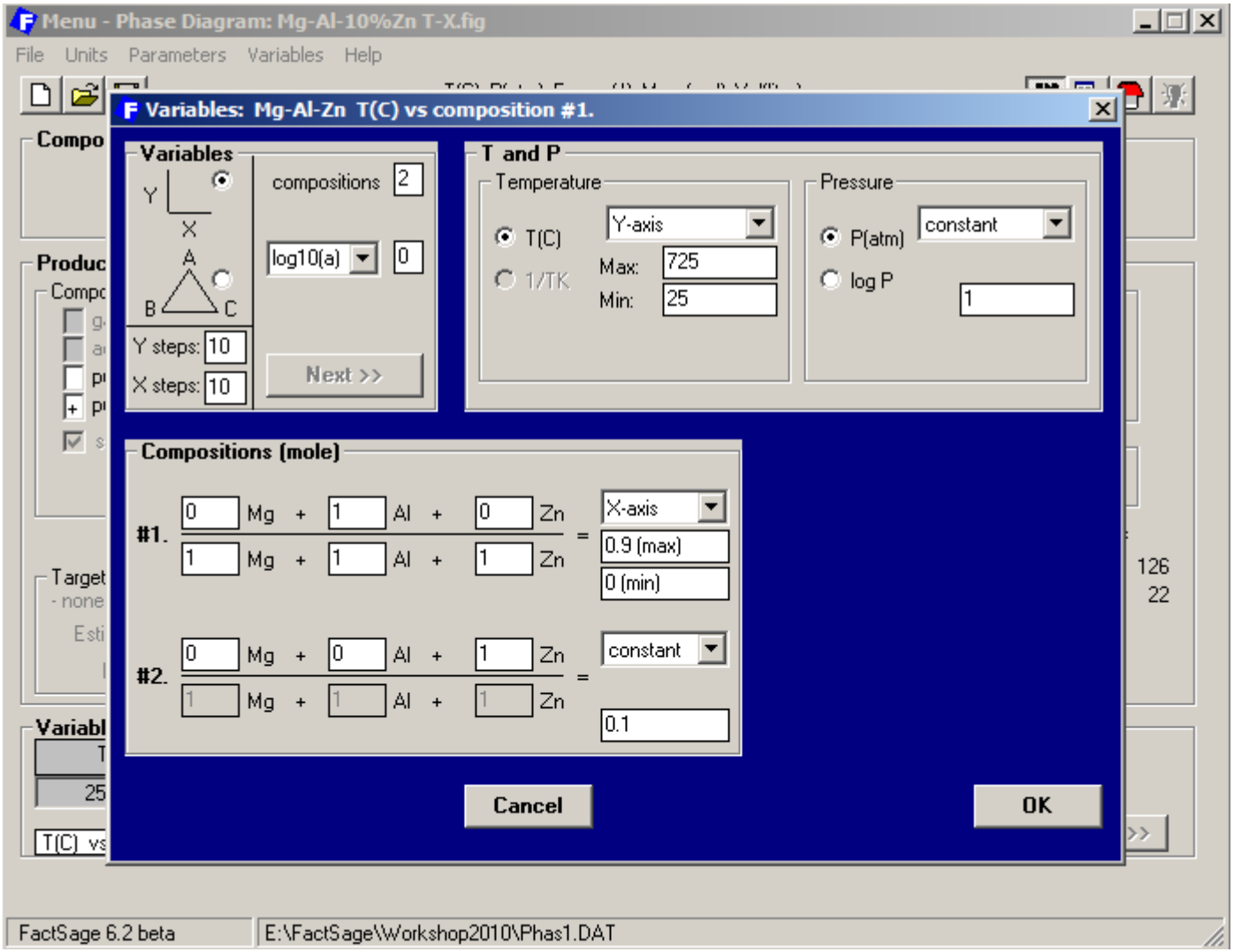


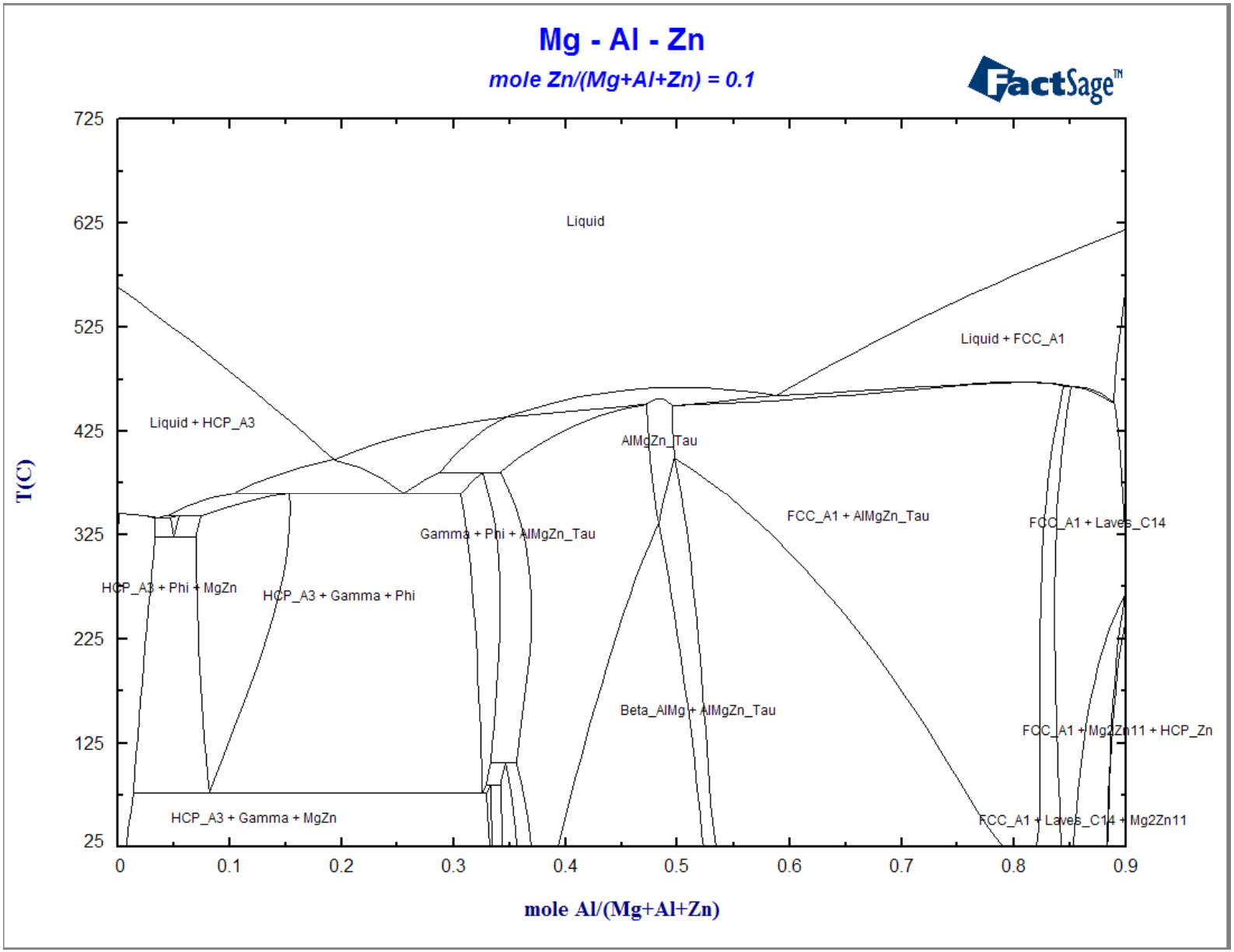
Mg-Al-Zn species selection for T-X diagram
(choose all solids and solutions)



Mg-Al-Zn T-X diagram at X_{Zn} = 0.1

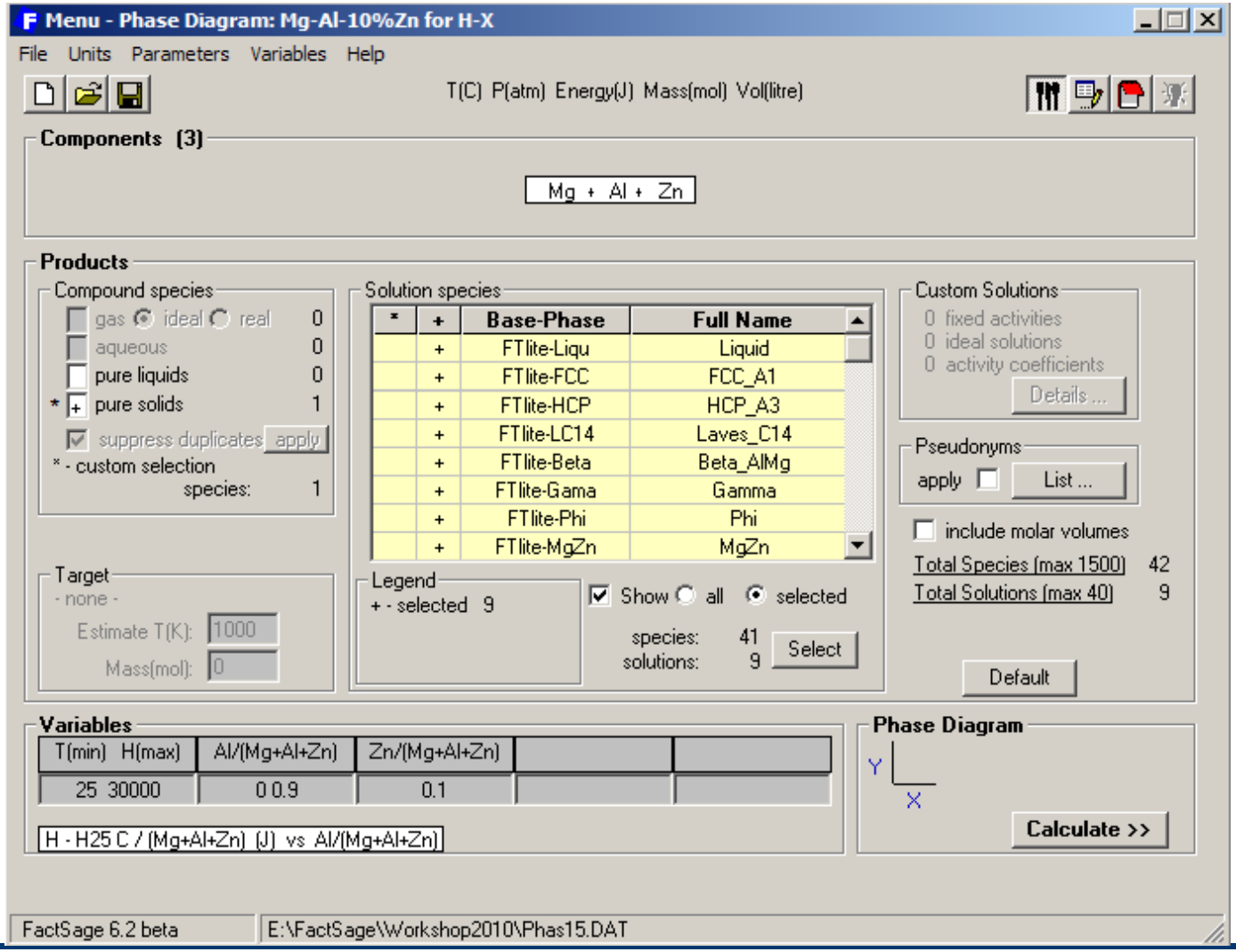
- Selection of variables



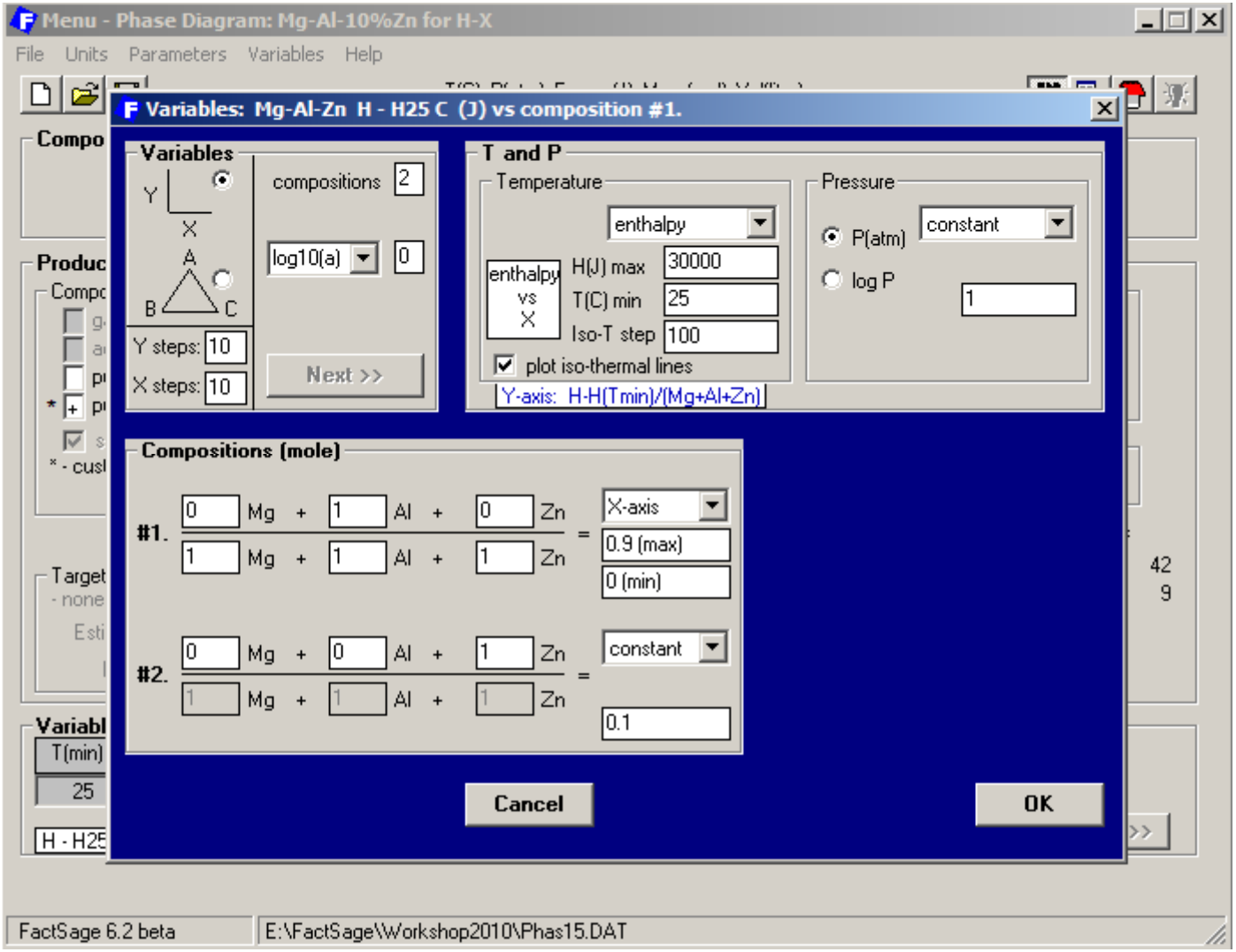

Mg - Al - Zn
mole Zn/(Mg+Al+Zn) = 0.1
FactSage™
725
625
525
425
325
225
125
25
T(C)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
mole Al/(Mg+Al+Zn)
Liquid
Liquid + FCC_A1
Liquid + HCP_A3
AlMgZn_Tau
FCC_A1 + AlMgZn_Tau
FCC_A1 + Laves_C14
Gamma + Phi + AlMgZn_Tau
HCP_A3 + Phi + MgZn
HCP_A3 + Gamma + Phi
Beta_AlMg + AlMgZn_Tau
FCC_A1 + Mg2Zn11 + HCP_Zn
HCP_A3 + Gamma + MgZn
FCC_A1 + Laves_C14 + Mg2Zn11

Selection of variable for H-X diagram

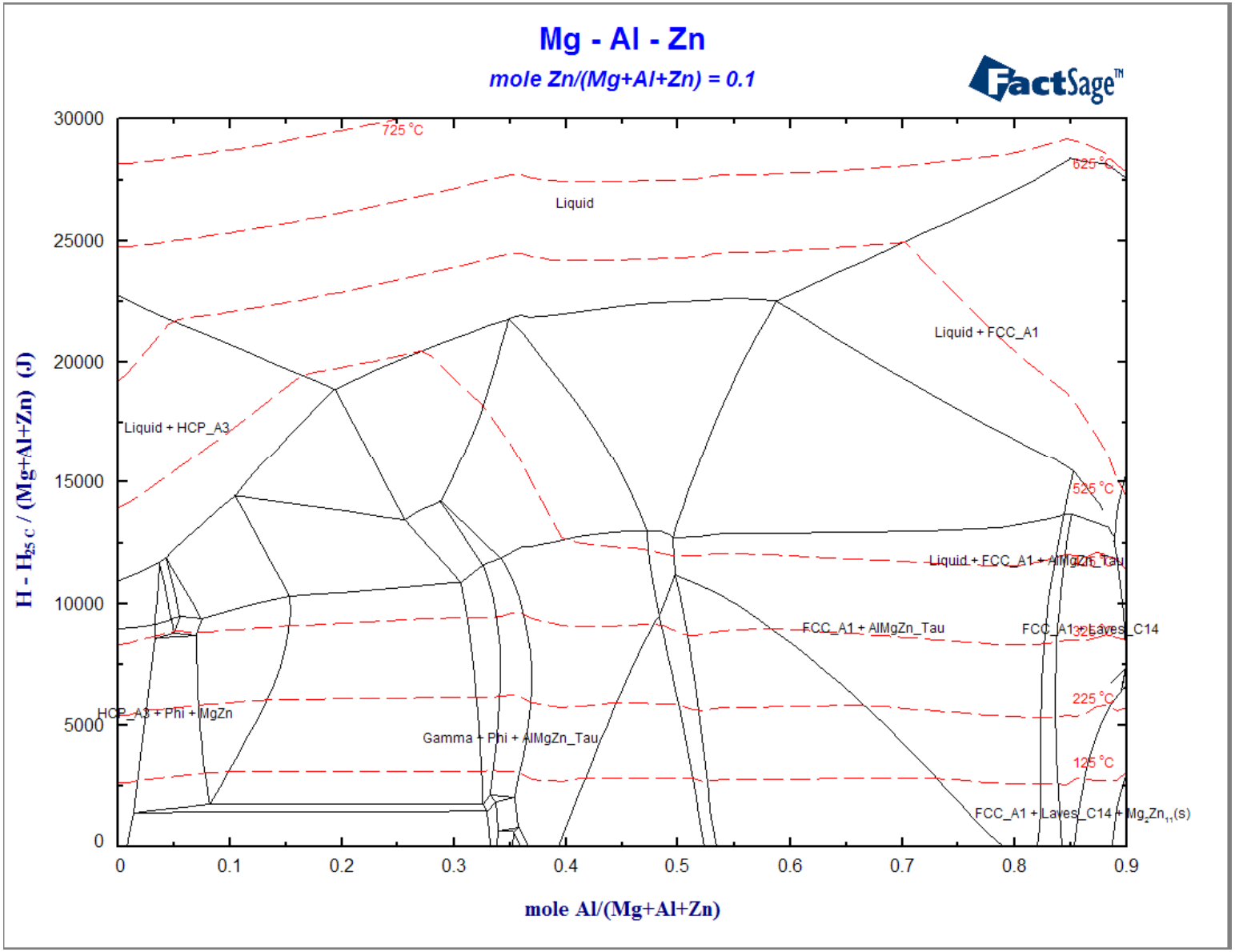
- In order to reduce calculation time, select only those species which appear on T-X diagram and remove I-option where possible



- Selection of variables for Mg-Al-Zn H-X diagram at X_{Zn} = 0.1

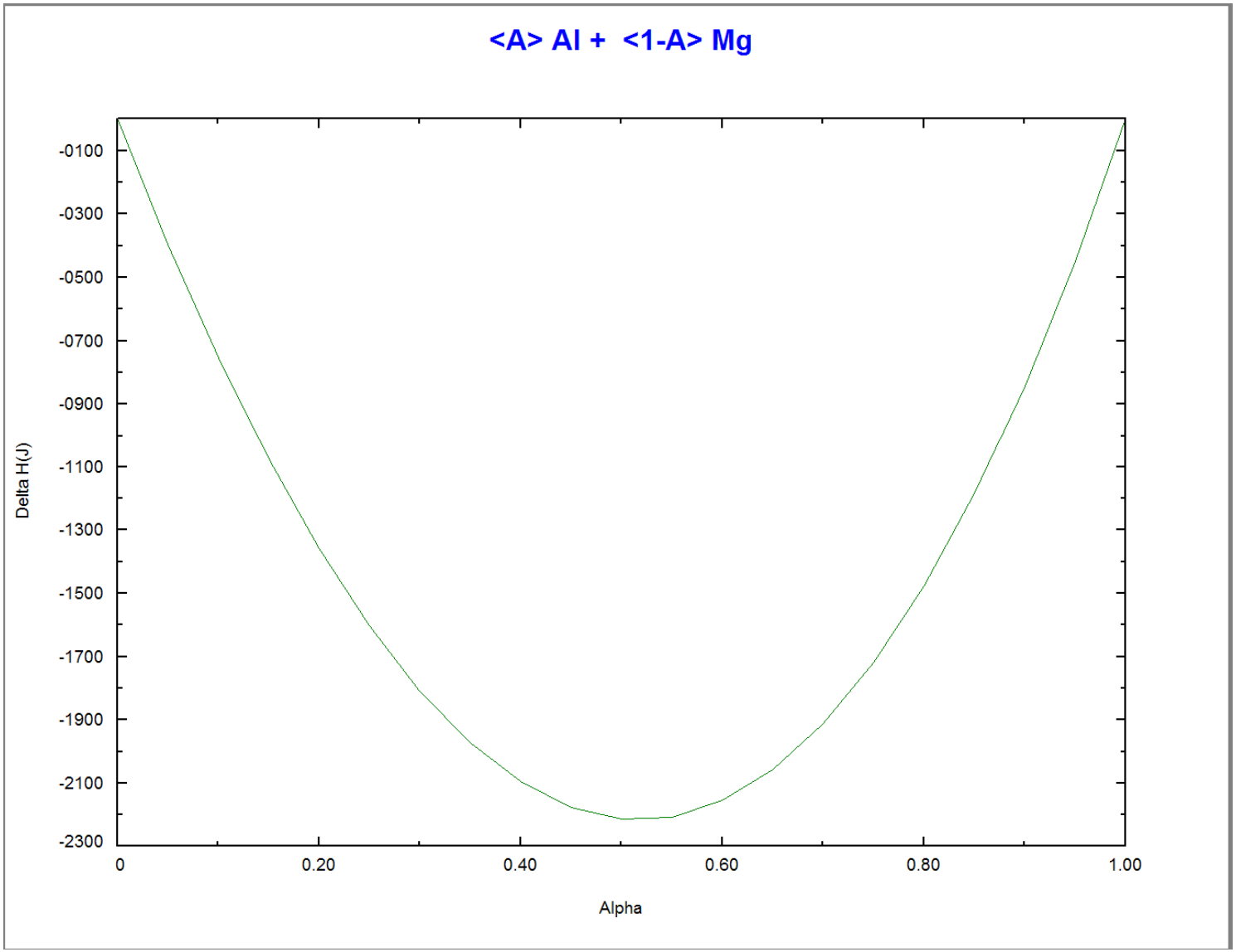


Calculated Mg-Al-Zn H-X diagram at X_{Zn} = 0.1

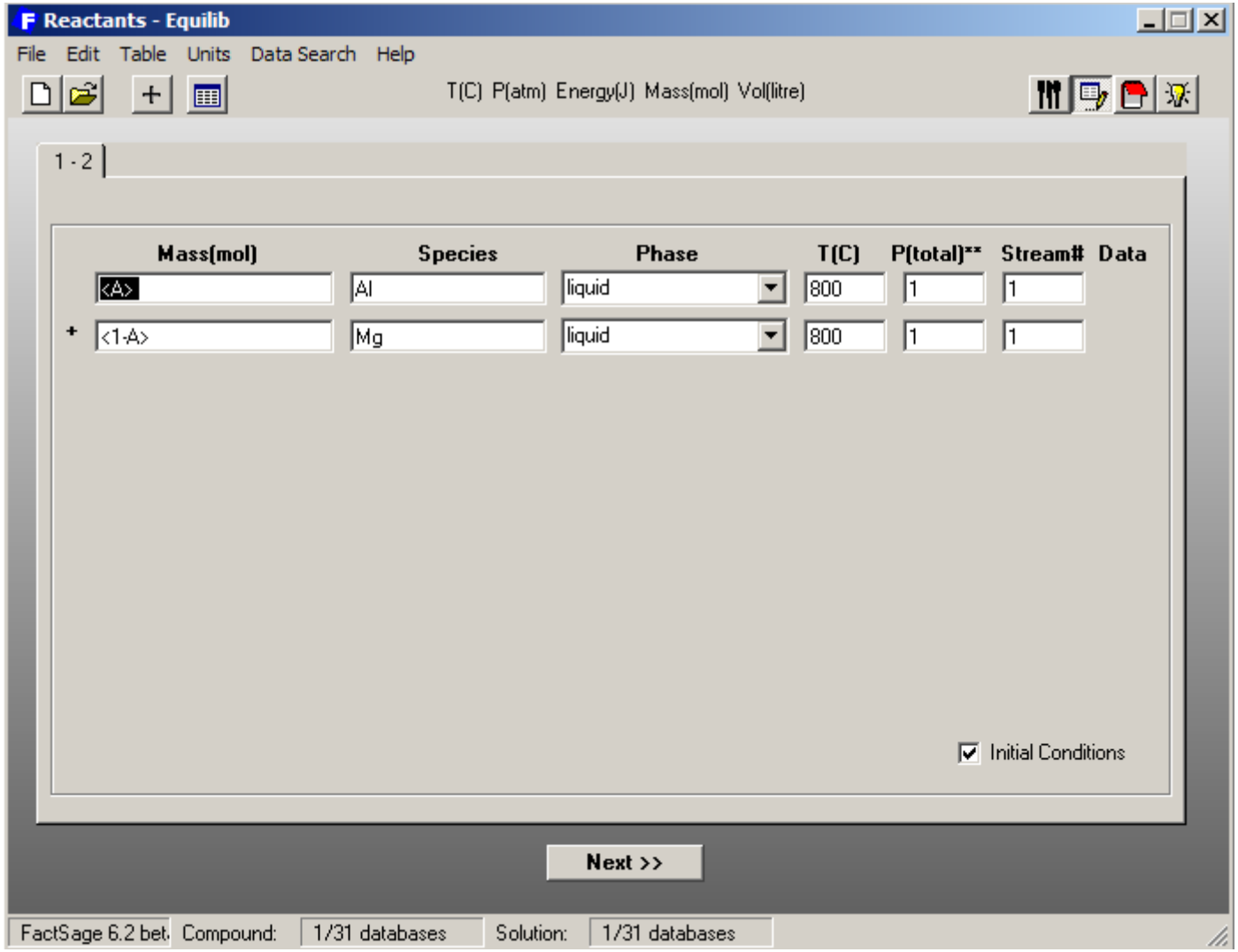


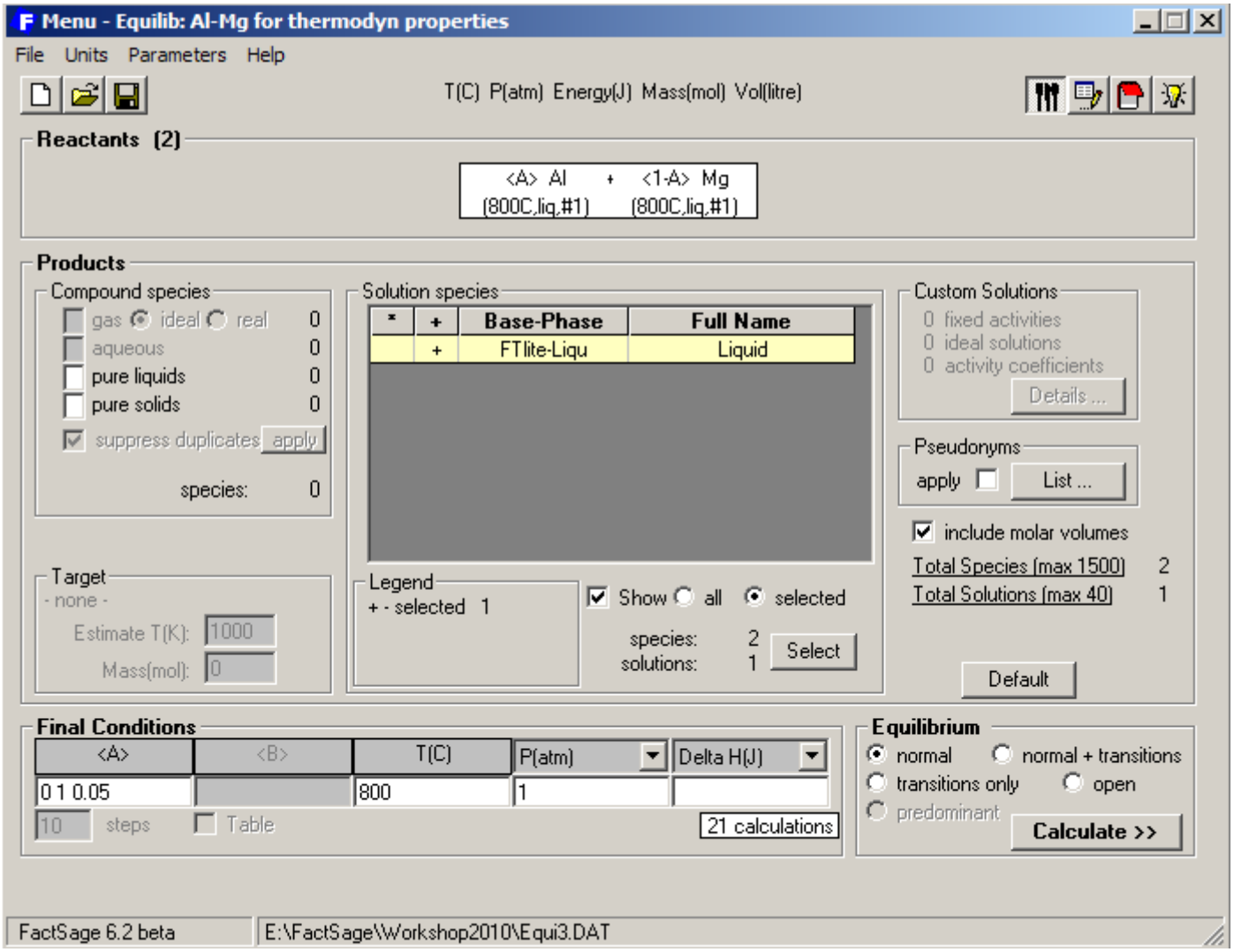
CALCULATING THERMODYNAMIC PROPERTIES

Calculated enthalpy of mixing of liquid Mg and liquid Al at 800 °C

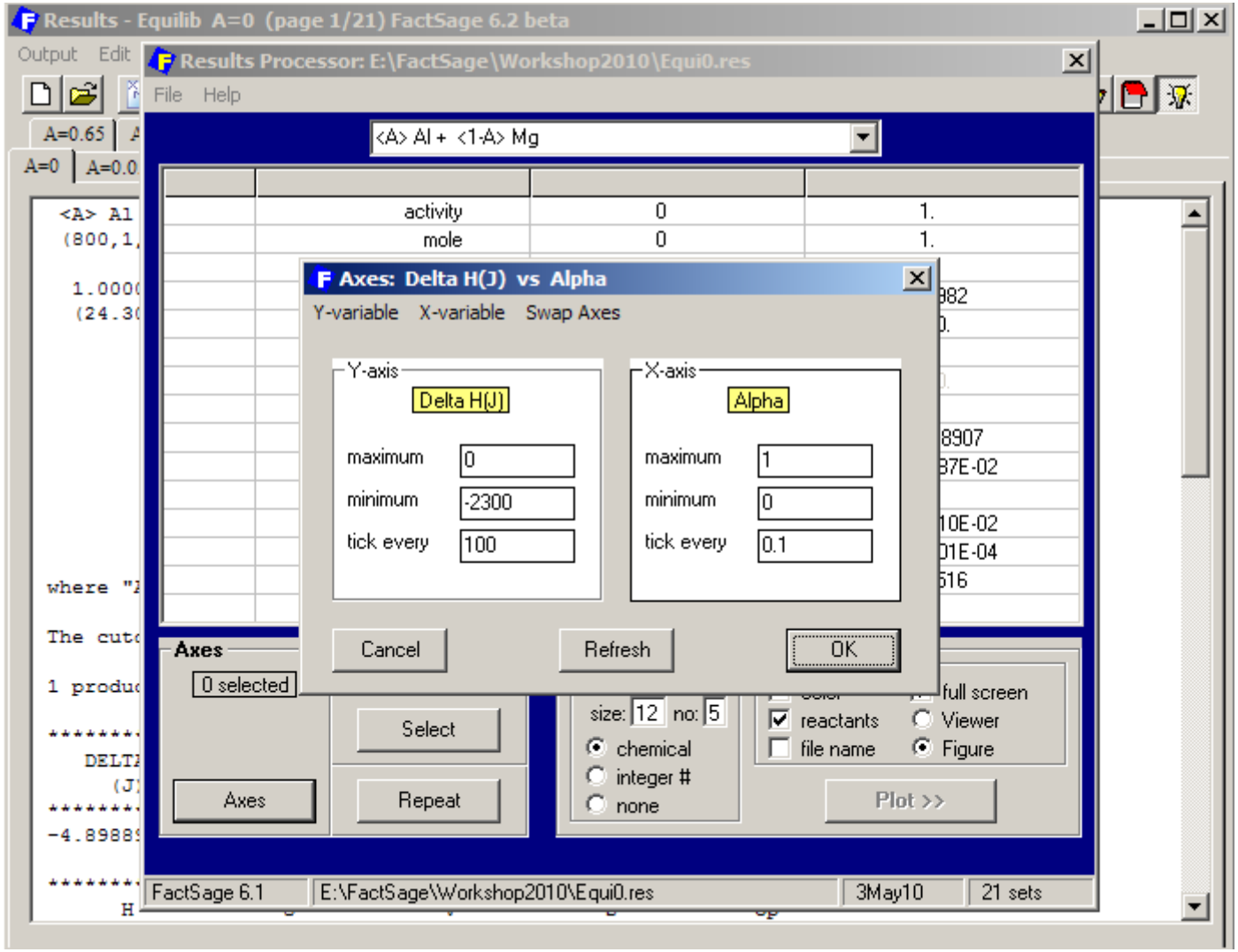


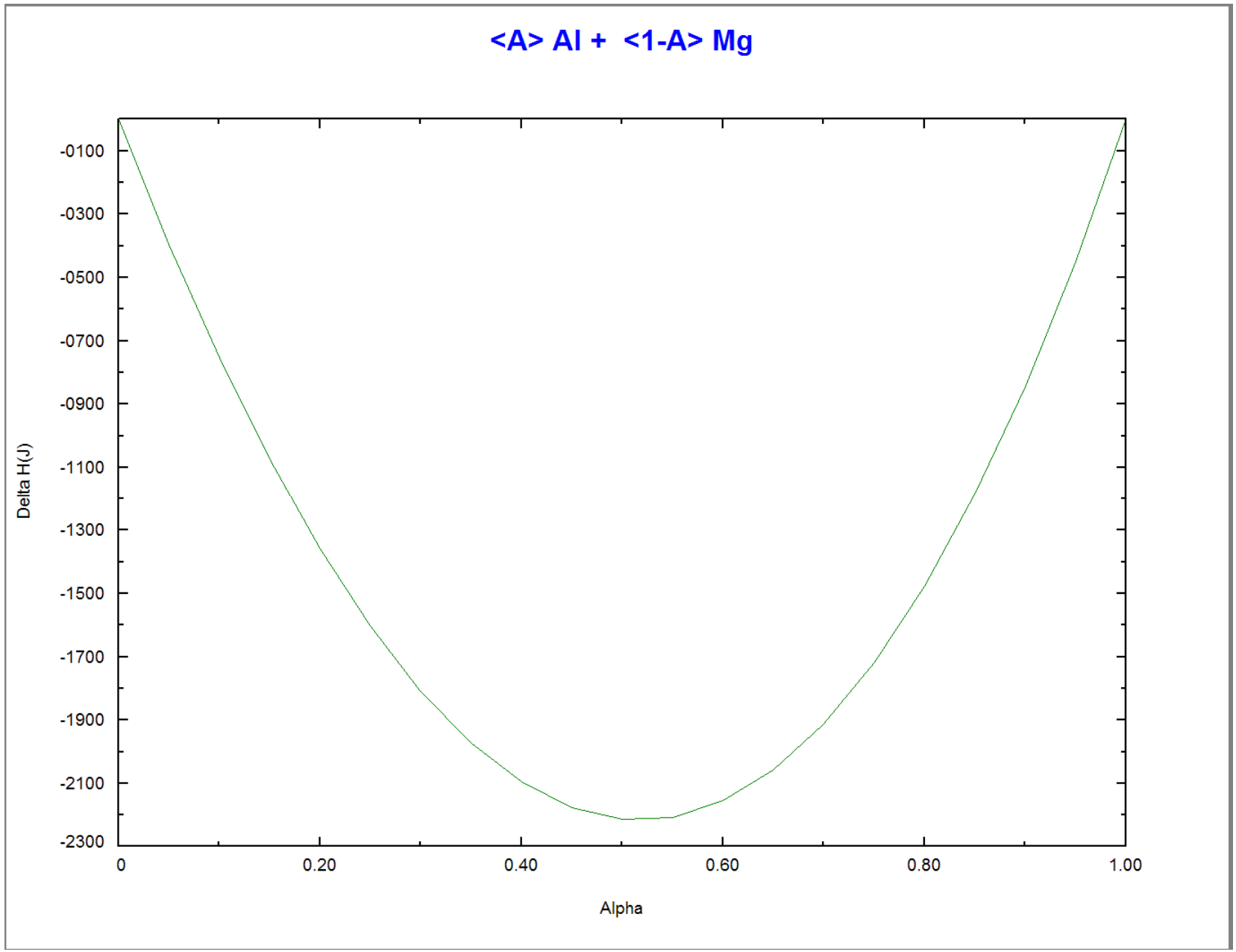
- Select “initial conditions” as pure Al and Mg liquids at 800 ^{o}C




Menu - Equilib: Al-Mg for thermodyn properties
File Units Parameters Help
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)
Reactants (2)
<A> Al (800C,liq,#1) + <1-A> Mg (800C,liq,#1)
Products
Compound species
gas ideal real 0
aqueous 0
pure liquids 0
pure solids 0
suppress duplicates apply
species: 0
Solution species
* + Base-Phase Full Name
+ FTlite-Liqu Liquid
Custom Solutions
0 fixed activities
0 ideal solutions
0 activity coefficients
Details ...
Pseudonyms
apply List ...
include molar volumes
Total Species (max 1500) 2
Total Solutions (max 40) 1
Target
- none -
Estimate T(K): 1000
Mass(mol): 0
Legend
+ - selected 1
Show all selected
species: 2
solutions: 1
Select
Default
Final Conditions
<A> <B> T(C) P(atm) Delta H(J)
0 1 0.05 800 1
10 steps Table
21 calculations
Equilibrium
normal normal + transitions
transitions only open
predominant
Calculate >>
FactSage 6.2 beta
E:\FactSage\Workshop2010\Equi3.DAT

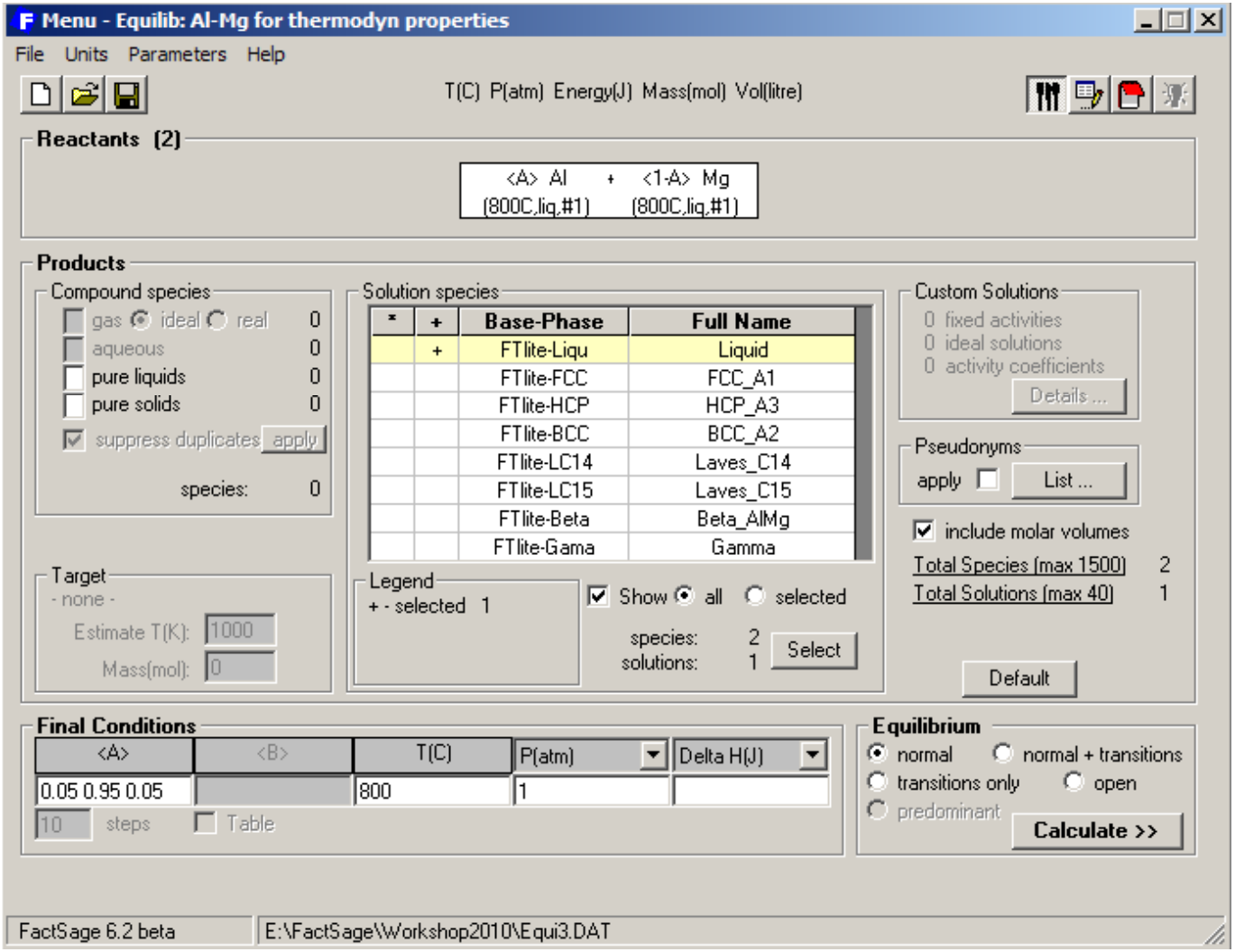
Plot results – selection of axes




<A> Al + <1-A> Mg
-0100
-0300
-0500
-0700
-0900
-1100
-1300
-1500
-1700
-1900
-2100
-2300
Delta H(J)
0
0.20
0.40
0.60
0.80
1.00
Alpha

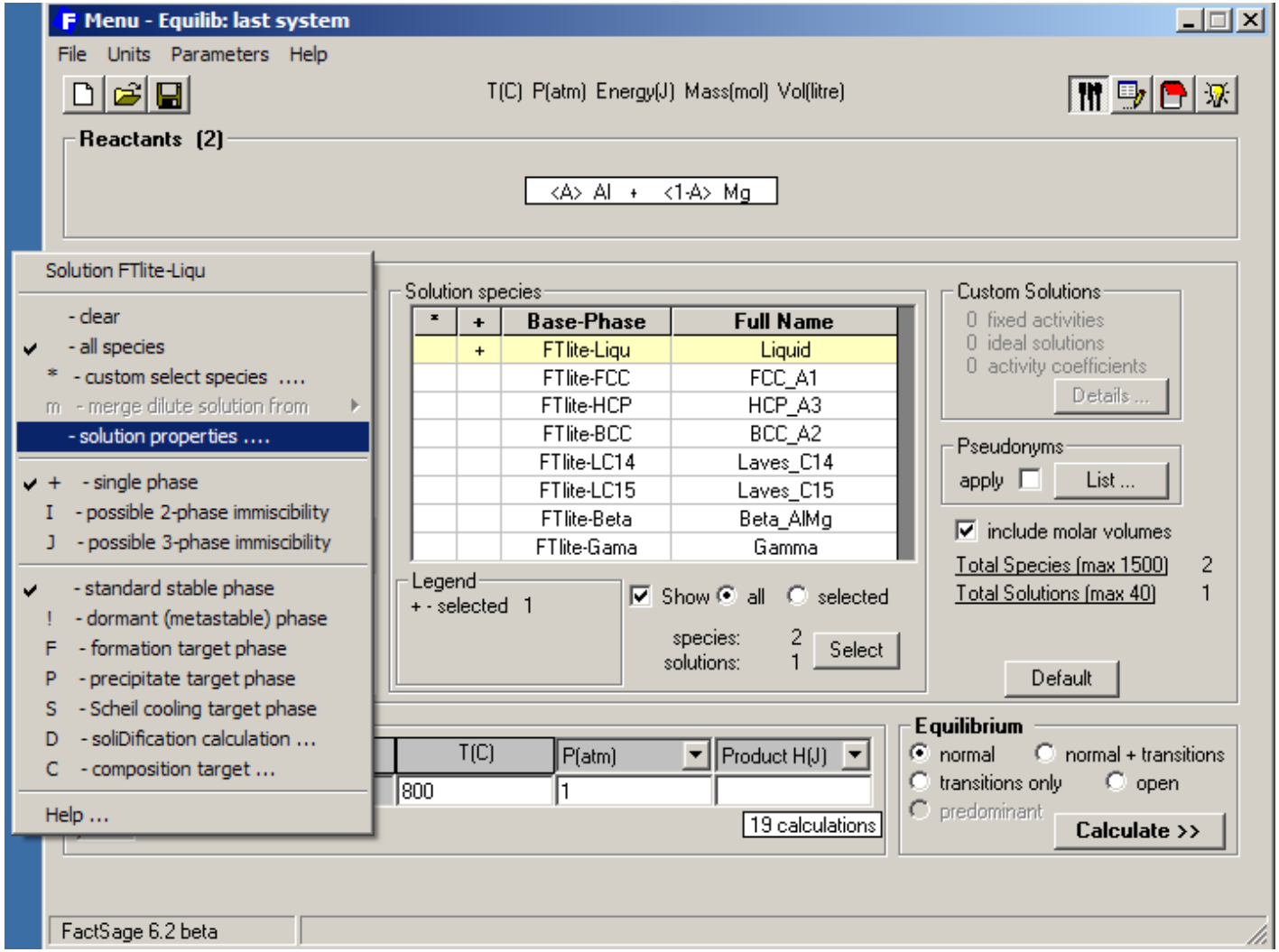
Solution Properties (see Manual Equilib Advanced 4)

- Select compositions for calculation of solution properties of liquid at 800 °C
(do not select <A> = 0 or <A> = 1)

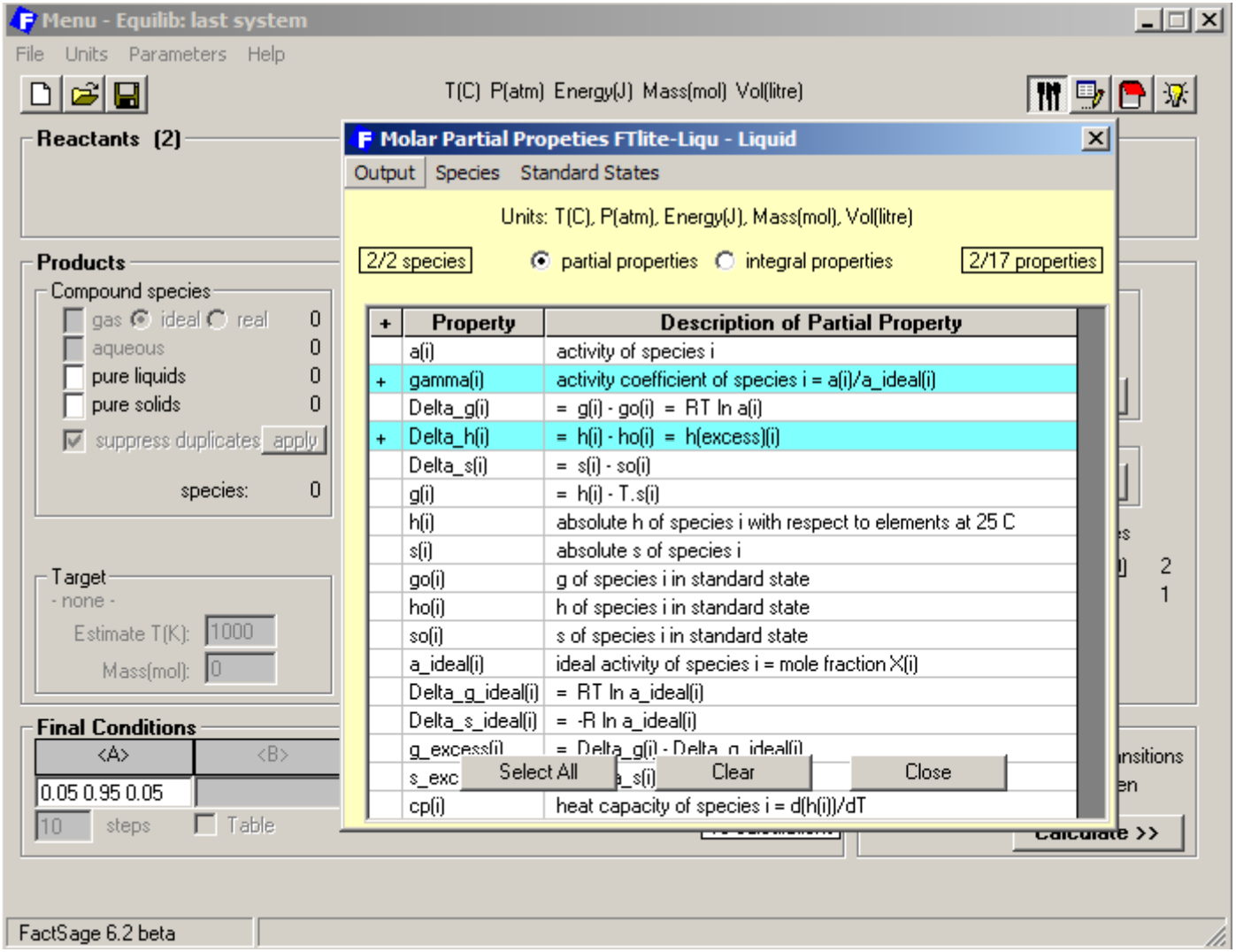


Solution Properties

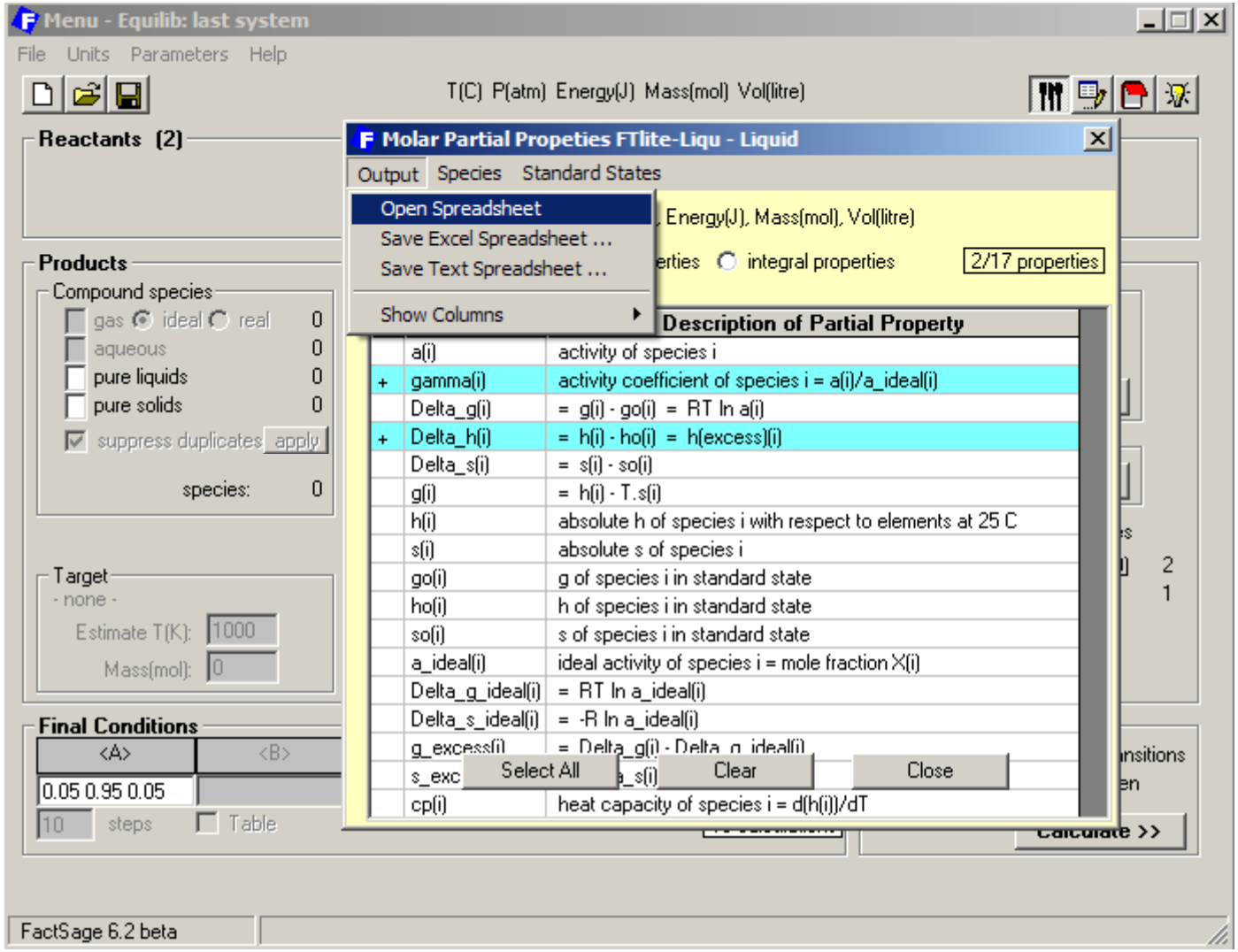
- After calculation, return to menu window and right click on phase for which properties are to be calculated



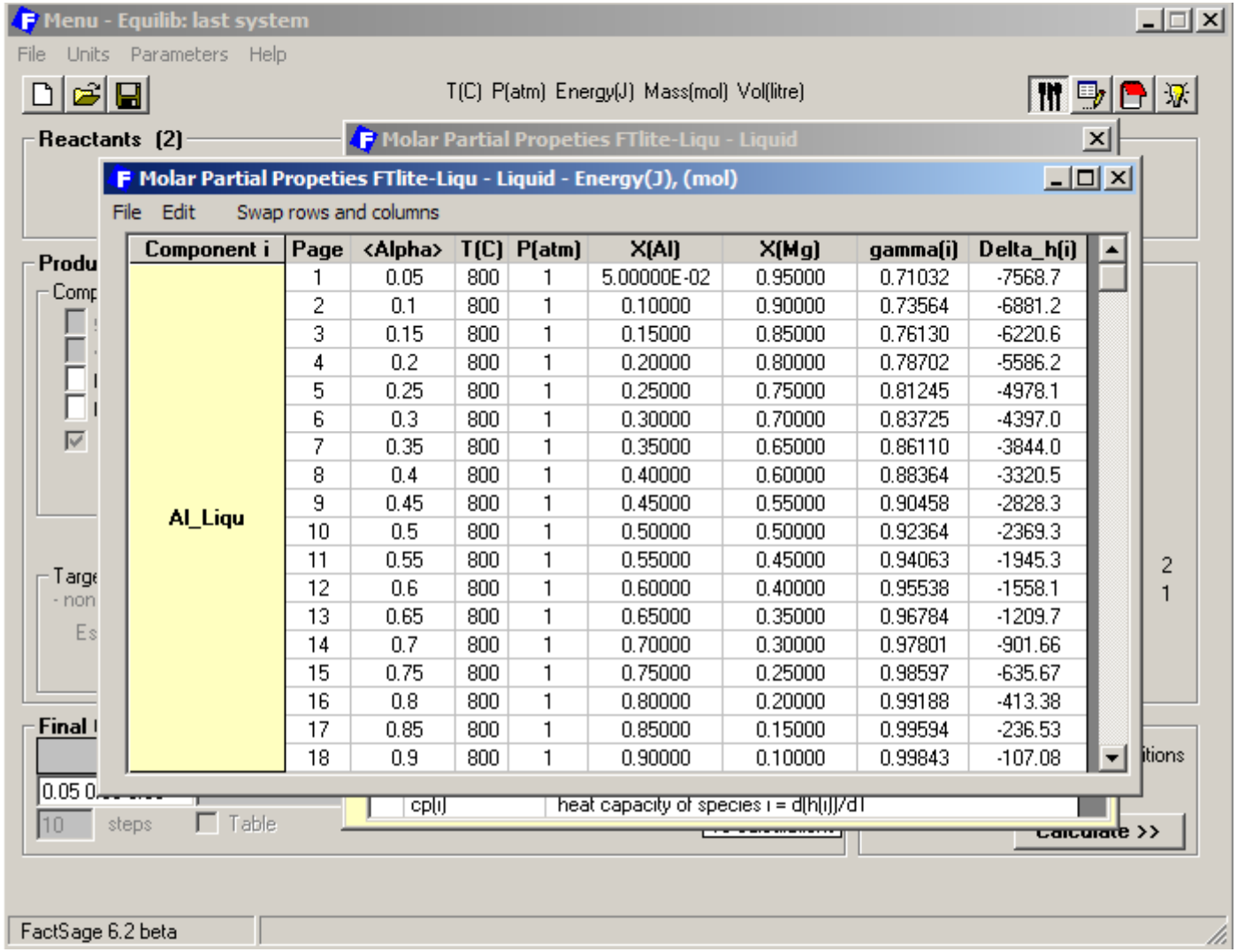
- Select properties to be calculated



- Open spreadsheet



- Spreadsheet showing calculated solution properties



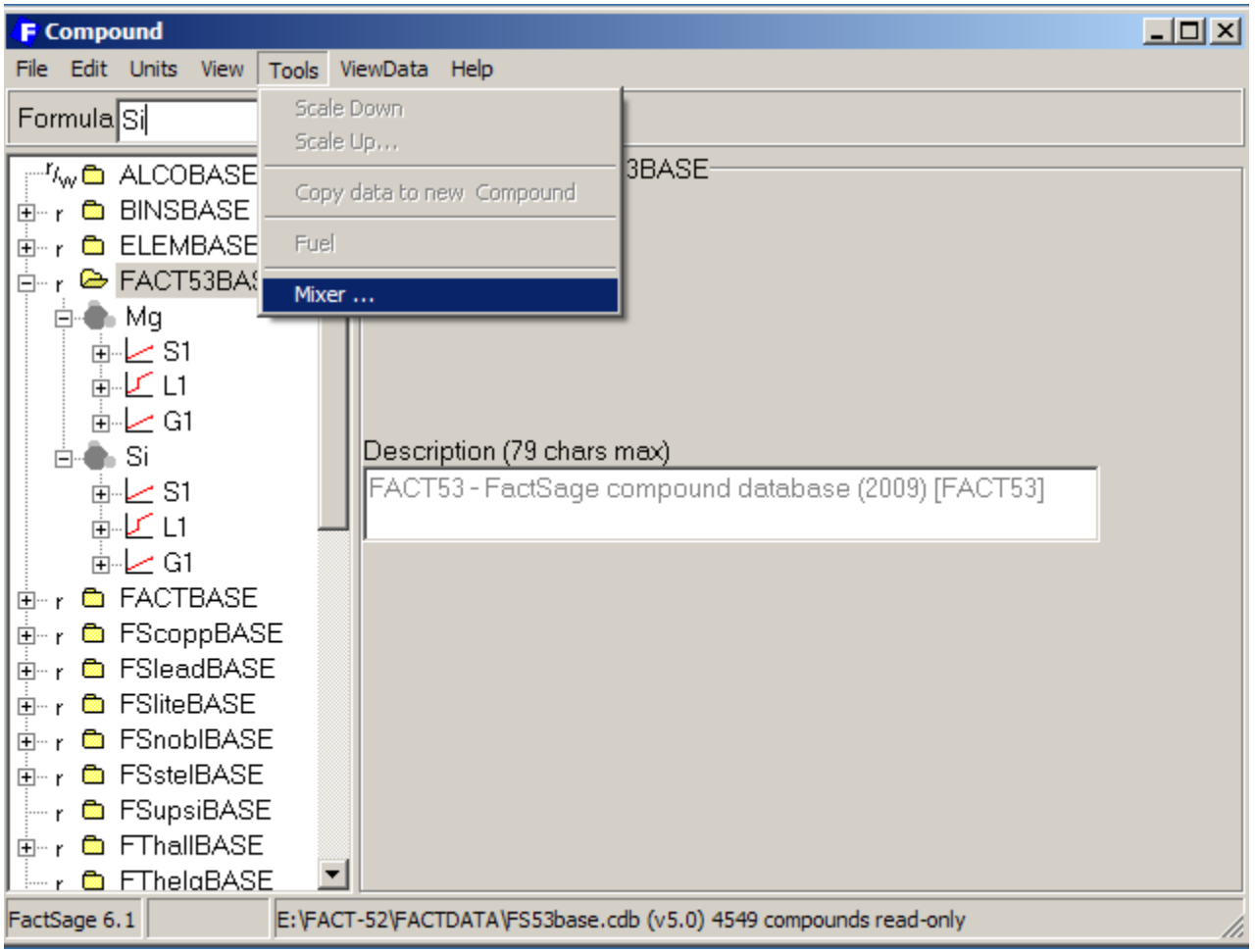
Component i	Page	<Alpha>	T(C)	P(atm)	X(Al)	X(Mg)	gamma(i)	Delta_h(i)
Al_Liqu	1	0.05	800	1	5.00000E-02	0.95000	0.71032	-7568.7
	2	0.1	800	1	0.10000	0.90000	0.73564	-6881.2
	3	0.15	800	1	0.15000	0.85000	0.76130	-6220.6
	4	0.2	800	1	0.20000	0.80000	0.78702	-5586.2
	5	0.25	800	1	0.25000	0.75000	0.81245	-4978.1
	6	0.3	800	1	0.30000	0.70000	0.83725	-4397.0
	7	0.35	800	1	0.35000	0.65000	0.86110	-3844.0
	8	0.4	800	1	0.40000	0.60000	0.88364	-3320.5
	9	0.45	800	1	0.45000	0.55000	0.90458	-2828.3
	10	0.5	800	1	0.50000	0.50000	0.92364	-2369.3
	11	0.55	800	1	0.55000	0.45000	0.94063	-1945.3
	12	0.6	800	1	0.60000	0.40000	0.95538	-1558.1
	13	0.65	800	1	0.65000	0.35000	0.96784	-1209.7
	14	0.7	800	1	0.70000	0.30000	0.97801	-901.66
	15	0.75	800	1	0.75000	0.25000	0.98597	-635.67
	16	0.8	800	1	0.80000	0.20000	0.99188	-413.38
	17	0.85	800	1	0.85000	0.15000	0.99594	-236.53
	18	0.9	800	1	0.90000	0.10000	0.99843	-107.08

- Using COMPOUND module to create compound Mg_2Si in a private database with

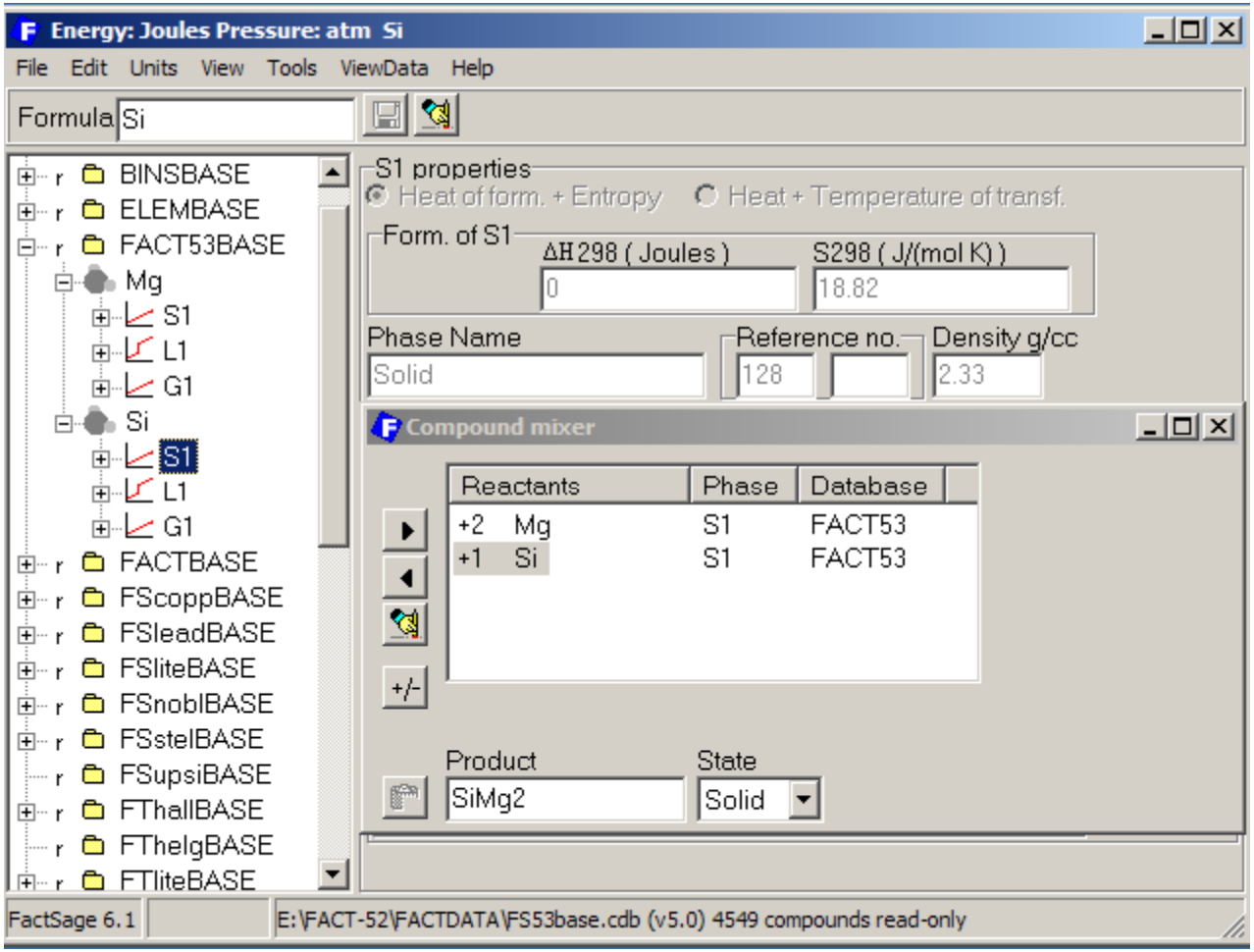
$2Mg + Si = Mg_2Si$ $\Delta H = -68000$ J/mol $\Delta S = -13.0$ J/mol^{-1}

relative to Mg(s1) and Si(s1) from FS53 database

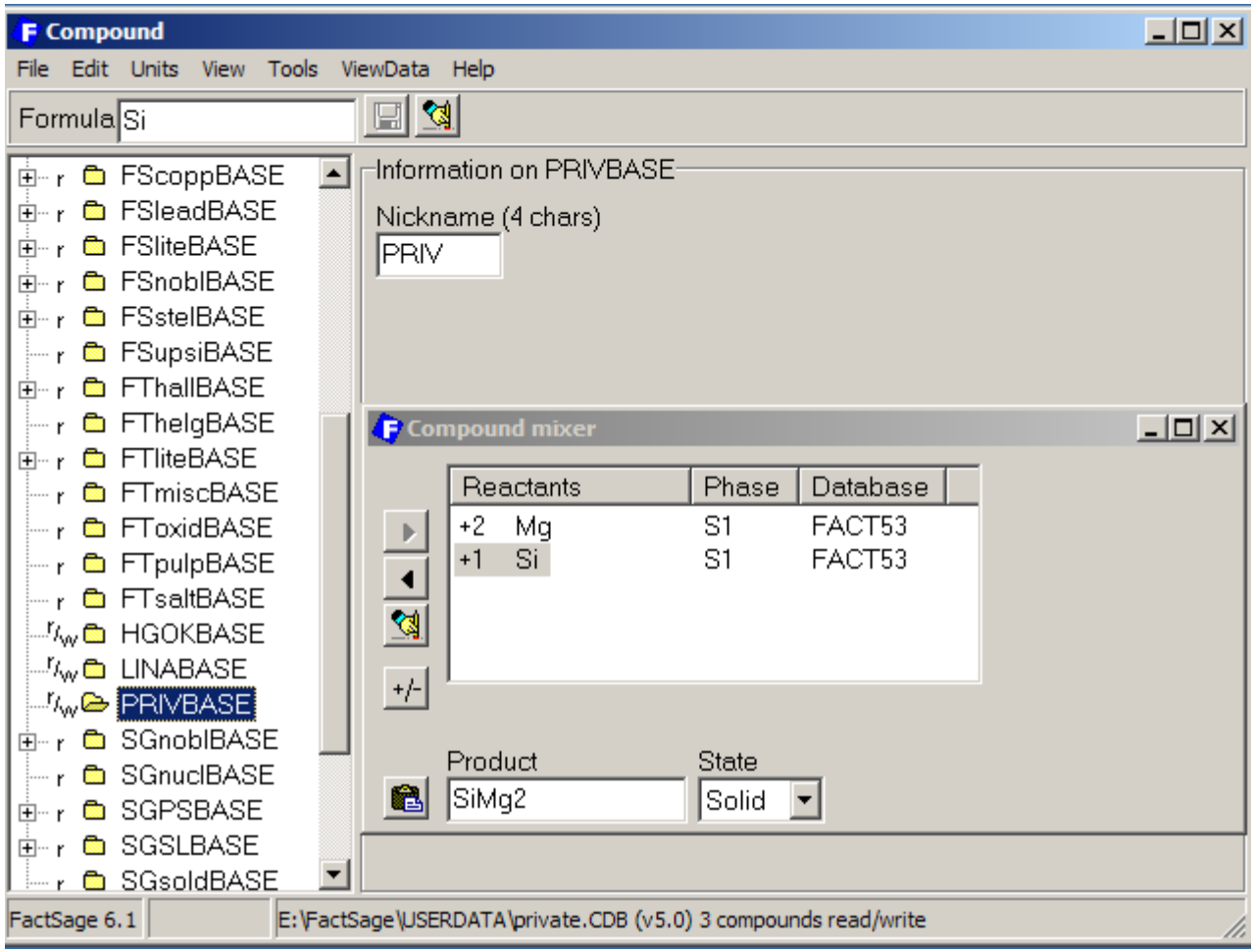
(see Manual COMPOUND, particularly section 14)



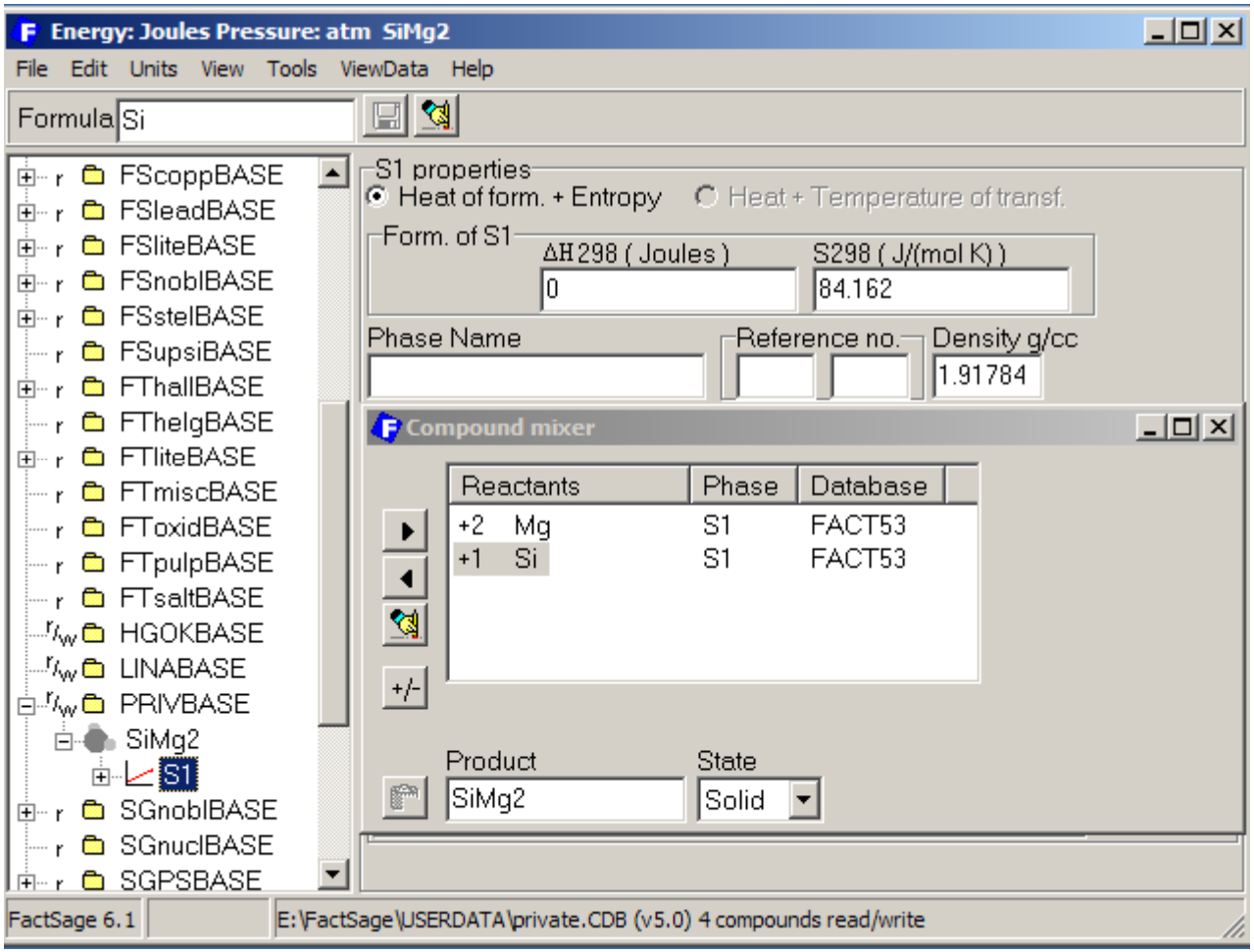
- Drag and drop Mg(s1) and Si(s1) into reactants box



- Click on “PRIVBASE” and then paste compound into PRIVBASE



- Data for Mg_2Si in PRIVBASE ($\Delta H = 0$, $\Delta S = 0$)



- Add ΔH = -68000, ΔS = -13.0