

Alloy Design

- Solidification and Thermodynamics

1 – 30 **Solidification**

42 – 57 **Thermodynamic Properties**

Solidification

Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 3

Mass(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
80	Mg				1	
+ 15	Al				1	
+ 5	Zn				1	

Initial Conditions

Next >>

FactSage 6.2 bet Compound: 1/31 databases Solution: 1/31 databases

Solidification

Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 3

Mass(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
80	Mg				1	
+ 15	Al				1	
+ 5	Zn				1	

Initial Conditions

Next >>

FactSage 6.2 bet Compound: 1/31 databases Solution: 1/31 databases

Equilibrium cooling path

Al - Mg - Zn

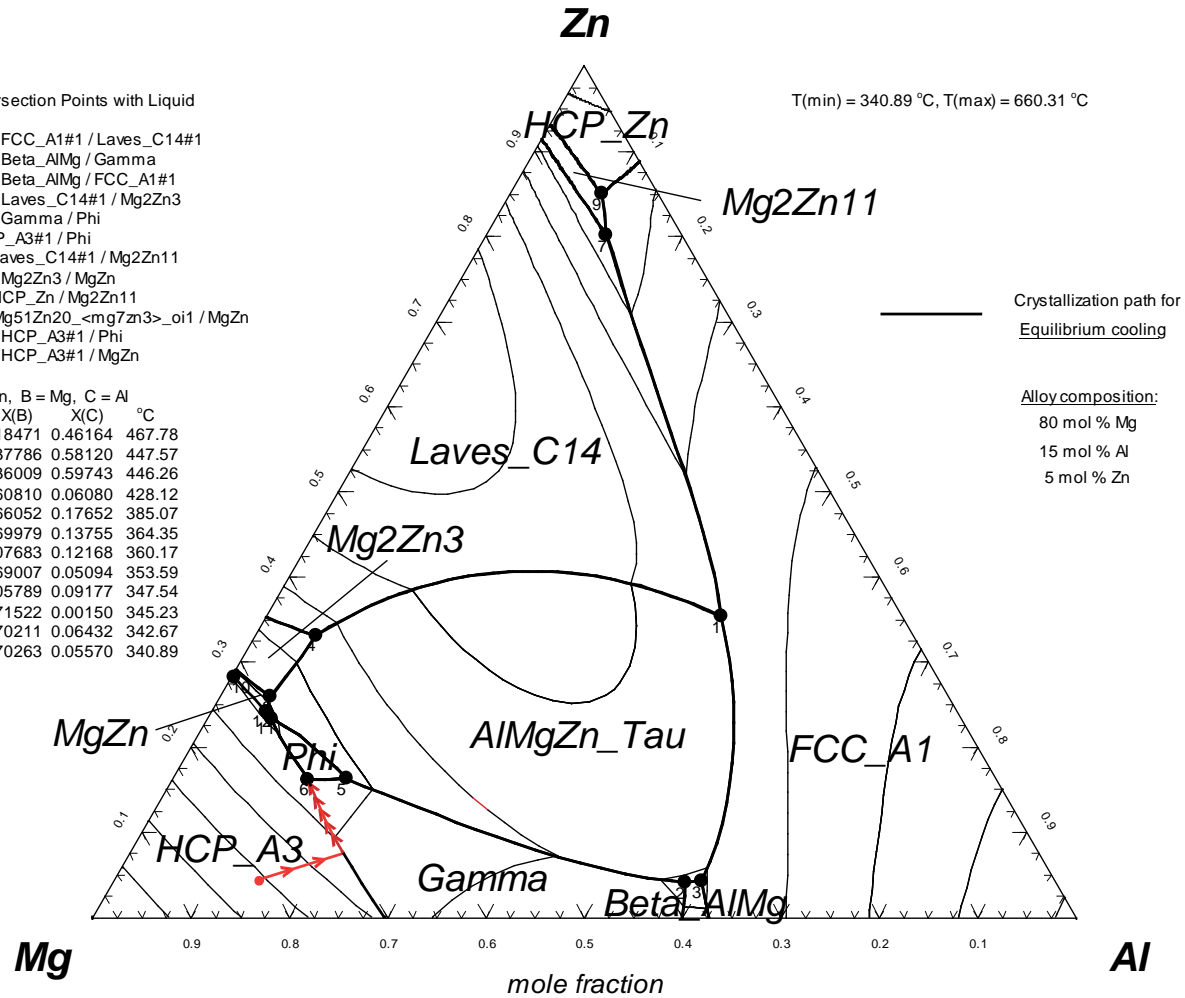
Data from FTlite - FACT light alloy databases



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



Select all solids and solutions

F Menu - Equilib: last system

File Units Parameters Help

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

Reactants (3)

80 Mg + 15 Al + 5 Zn

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 28
- suppress duplicates

species: 28

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

- | - immiscible 7
- + - selected 8

Show all selected

species: 98
solutions: 22

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 126
Total Solutions (max 40) 22

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		600 300 10	1	

10 steps Table 31 calculations

Equilibrium

- normal normal + transitions
- transitions only open
- predominant

FactSage 6.2 beta

F 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)

```

F 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 ...

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

390 C | 380 C | 370 C | 360 C | 350 C | 340 C | 330 C | 320 C | 310 C | 300 C | 290 C | 280 C | 270 C | 260 C | 250 C | 240 C | 230 C | 220 C | 210 C | 200 C | 190 C | 180 C | 170 C | 160 C | 150 C | 140 C | 130 C | 120 C | 110 C | 100 C | 90 C | 80 C | 70 C | 60 C | 50 C | 40 C | 30 C | 20 C | 10 C

+ 5 Zn =

Liquid#1
 100.00 mol, 1.4346 litre, 1.8654 g/ml
 600 C, 1 atm, a=1.0000)

0.000 Al V
 0.000 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

Results Processor: E:\FactSage\Workshop2010\Equi0.res

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 **Species** 0 selected
 Select Repeat

Graph
 Labels size: 12 no: 5
 chemical
 integer #
 none

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

FactSage 6.1 E:\FactSage\Workshop2010\Equi0.res 3May10 31 sets

Selection of axes

The screenshot displays the FactSage 6.2 beta Results Processor interface. The main window title is "Results - Equilib 600 C (page 1/31) FactSage 6.2 beta". The "Results Processor" window shows the chemical system "80 Mg + 15 Al + 5 Zn" at 600 C. A table of activity and mole fractions is visible in the background. A dialog box titled "Axes: gram vs T(C)" is open, allowing the user to select the Y-axis (gram) and X-axis (T(C)) and set their respective maximum, minimum, and tick every values. The dialog also includes buttons for "Cancel", "Refresh", and "OK".

Y-axis	X-axis
gram	T(C)
maximum: 3000	maximum: 600
minimum: 0	minimum: 300
tick every: 250	tick every: 25

Background Table Data:

Component	activity	mole
80 Mg	0	1.
15 Al	0	100.
5 Zn	0	100.

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

Results - Equilib 600 C (page 1/31) FactSage 6.2 beta

Species Selection - EQUILIB Results: gram vs T(C)

	#	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.

mole
 gram
 source

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

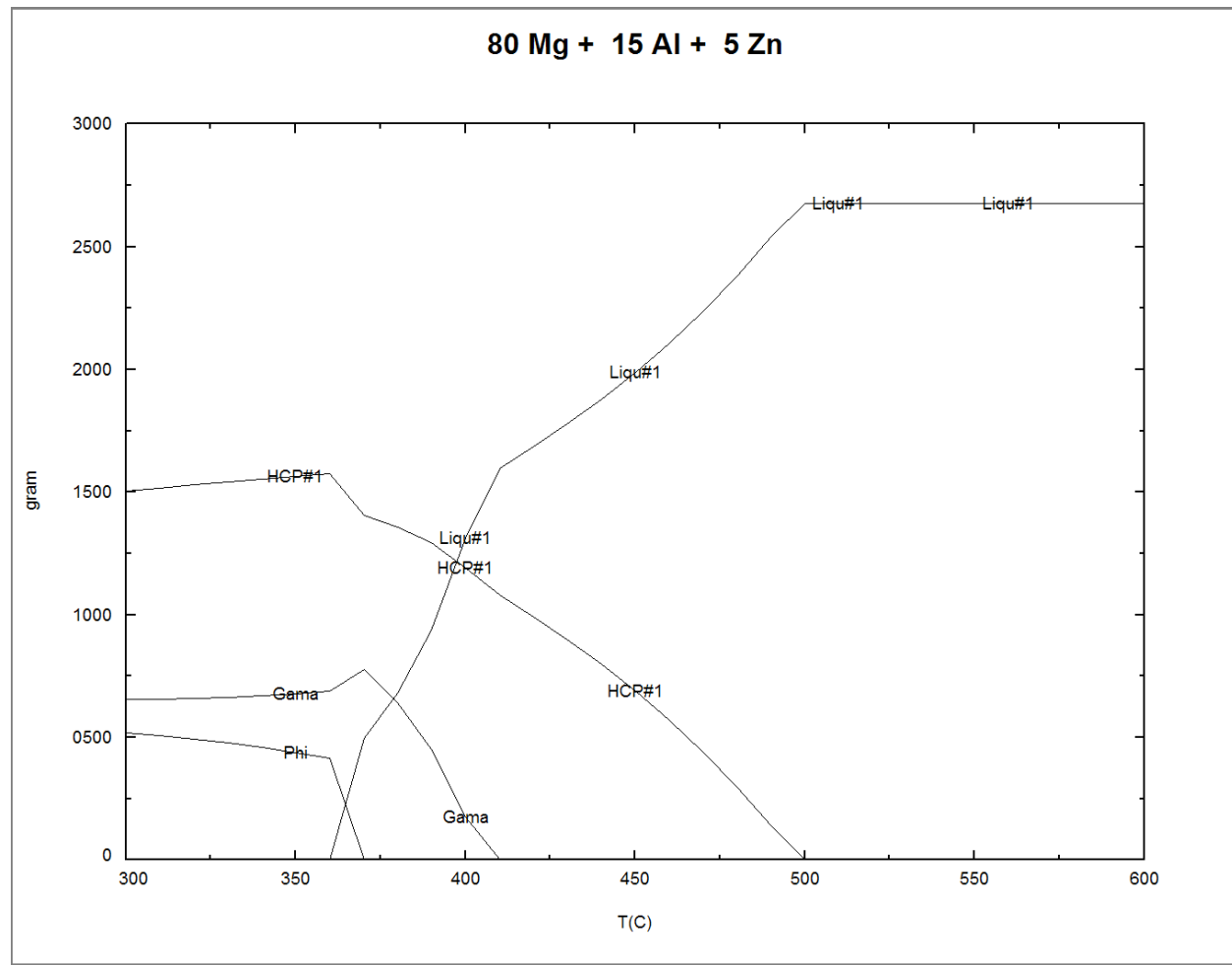
Select Top: 15
 4 species selected

Clear Refresh OK

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

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”

F Menu - Equilib: Mg80-Al15-Zn5-cooling

File Units Parameters Help

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

Reactants (3)

80 Mg + 15 Al + 5 Zn

Solution FTlite-Liqu

- clear
- ✓ - all species
- * - custom select species
- m - merge dilute solution from ...
- solution properties
- + - single phase
- ✓ I - possible 2-phase immiscibility
- J - possible 3-phase immiscibility
- ✓ - standard stable phase
- ! - dormant (metastable) phase
- F - formation target phase
- P - precipitate target phase
- S - Scheil cooling target phase
- D - solidification calculation ...**
- C - composition target ...
- Help ...

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
	I	FTlite-LC14	Laves_C14
	I	FTlite-LC15	Laves_C15
	I	FTlite-LC36A	ALaves_C36
	I	FTlite-LC36B	BLaves_C36

Legend
I - immiscible 7
+ - selected 8

Show all selected
 species: 98
 solutions: 22

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

Pseudonyms
 apply List ...

include molar volumes
 Total Species (max 1500) 126
 Total Solutions (max 40) 22
 Default

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

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

600 300 10 1

31 calculations

FactSage 6.2 beta E:\FactSage\Workshop2010\Equi1.DAT

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

The screenshot shows the FactSage software interface for an equilibrium solidification calculation. A dialog box titled "Solidification Calculation" is open, displaying an "IMPORTANT" message and three radio button options: "Equilibrium Solidification" (selected), "Scheil Solidification", and "regular equilibrium calculation". The "Solution phase" is set to "FTlite-Liqu".

The main interface shows the composition "80 Mg + 15 Al + 5 Zn" and a table of "Solution species":

ID	Base-Phase	Full Name
	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
I	FTlite-LC36B	BLaves_C36

Below the table, the "Legend" shows 7 immiscible phases (I) and 8 selected phases (D and +). The "Equilibrium" section has "include molar volumes" checked. The "Final Conditions" table shows a cooling step from 600°C to 0% liquid at 10 steps. The "Equilibrium" options are set to "normal".

Select starting temperature

F Menu - Equilib: Mg80-Al15-Zn5-cooling

File Units Parameters Help

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

Reactants (3)

80 Mg + 15 Al + 5 Zn

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 28
- suppress duplicates

species: 28

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
	I	FTlite-LC36B	BLaves_C36

Legend

- I - immiscible 7
- D - Equilibrium solid'n
- + - selected 8

Show all selected

species: 98
solutions: 22

Custom Solutions

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

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 126
Total Solutions (max 40) 22

Equilibrium solidification

FTlite-Liqu

Cooling step T(C):

Mass(mol):

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		600	1	

10 steps Table

Equilibrium solidification - T(start) = 600, T(stop) = 0% liquid

Equilibrium

- normal normal + transitions
- transitions only open
- predominant

FactSage 6.2 beta E:\FactSage\Workshop2010\Equi1.DAT

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

F Results - Equilib Summary (page 1/54) FactSage 6.2 beta

Output Edit Show Pages

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

500 C | 497.61 C | 495 C |

555 C | 550 C | 545 C | 540 C | 535 C | 530 C | 525 C | 520 C | 515 C | 510 C | 505 C |

Summary | Transitions | 600 C | 595 C | 590 C | 585 C | 580 C | 575 C | 570 C | 565 C | 560 C |

SUMMARY OF REACTIONS

Cooling
600.00 to 497.61 C (DELTA H = -3.2631E+05 J, DELTA V = -2.3331E-02 dm3)
Liquid cooling

Constituent 1
497.61 to 404.48 C (DELTA H = -5.8386E+05 J, DELTA V = -4.0402E-02 dm3)
Liquid -> HCP_A3

Constituent 2
404.48 to 364.35 C (DELTA H = -4.2935E+05 J, DELTA V = -1.5773E-02 dm3)
Liquid -> HCP_A3 + Gamma

Constituent 3
364.35 C (isothermal) (DELTA H = -9.9409E+04 J, DELTA V = -9.4803E-04 dm3)
Liquid + Gamma -> HCP_A3 + Phi

COMPOSITION OF PHASES IN CONSTITUENTS AT 364.35 C
(temperature of final disappearance of Liquid)

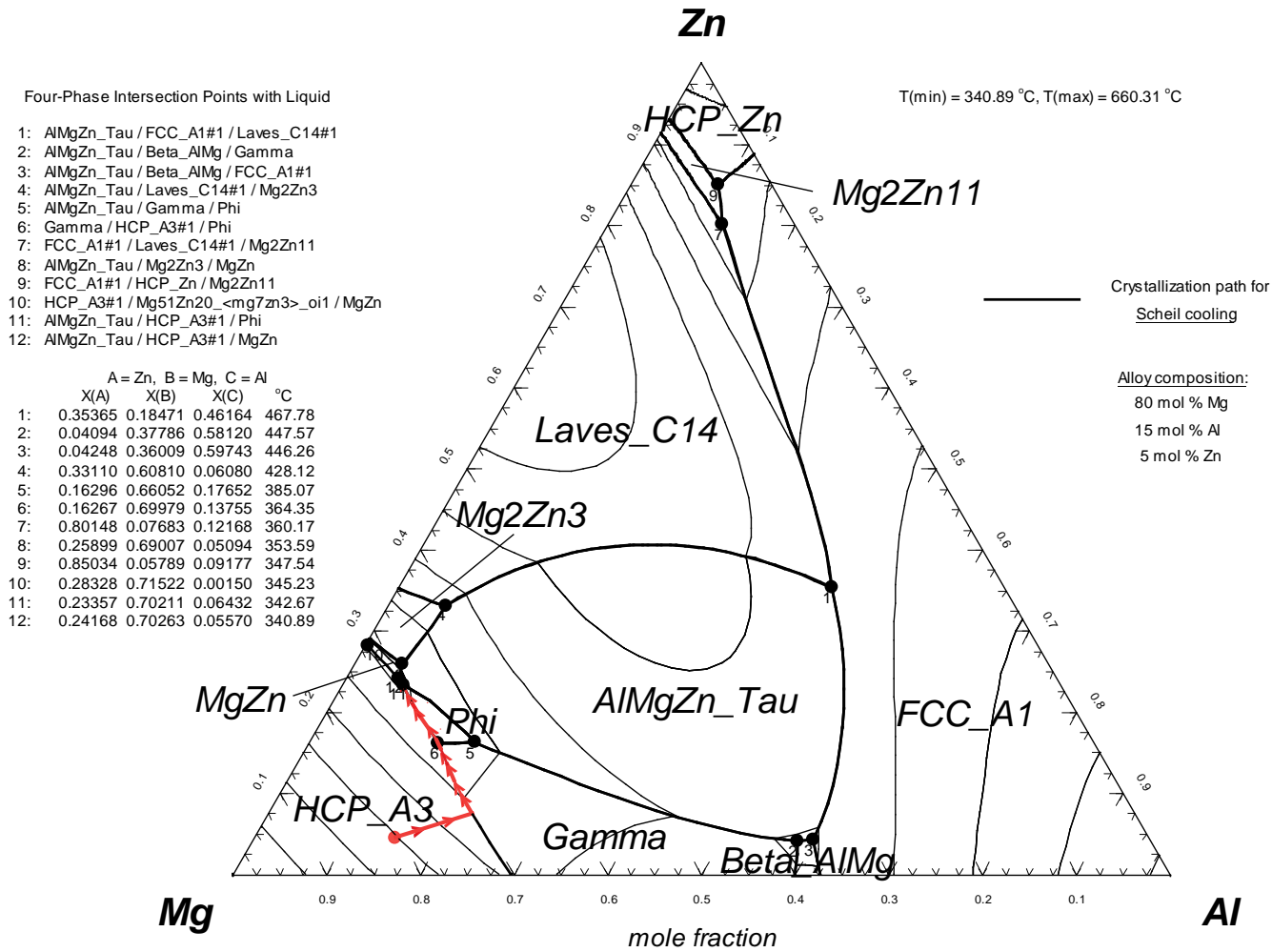
Constituent 1
HCP_A3

	MOLE FRACTION	MASS FRACTION
Zn	1.6532E-02	4.2994E-02
Al	5.9743E-02	6.4109E-02
Mg	9.2372E-01	8.9290E-01
	TOTAL AMT/mol	TOTAL AMT/gram

Scheil-Gulliver cooling path

Al - Mg - Zn

Data from FTlite - FACT light alloy databases



Scheil-Gulliver Target for liquid

(Set starting temperature at 600 °C)

(See Manual Equilib Advanced 2.3)

F Menu - Equilib: Mg80-Al15-Zn5-cooling

File Units Parameters Help

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

Reactants (3)

80 Mg + 15 Al + 5 Zn

Solution FTlite-Liqu

- clear
- ✓ - all species
- * - custom select species
- m - merge dilute solution from ...
- solution properties
- + - single phase
- ✓ I - possible 2-phase immiscibility
- J - possible 3-phase immiscibility
- ✓ - standard stable phase
- ! - dormant (metastable) phase
- F - formation target phase
- P - precipitate target phase
- S - Scheil cooling target phase**
- D - solidification calculation ...
- C - composition target ...

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
	I	FTlite-LC14	Laves_C14
	I	FTlite-LC15	Laves_C15
	I	FTlite-LC36A	ALaves_C36
	I	FTlite-LC36B	BLaves_C36

Legend
I - immiscible 7
+ - selected 8

Legend options: Show all selected

species: 98
solutions: 22

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

Default

Equilibrium
 normal normal + transitions
 transitions only open
 predominant

Calculate >>

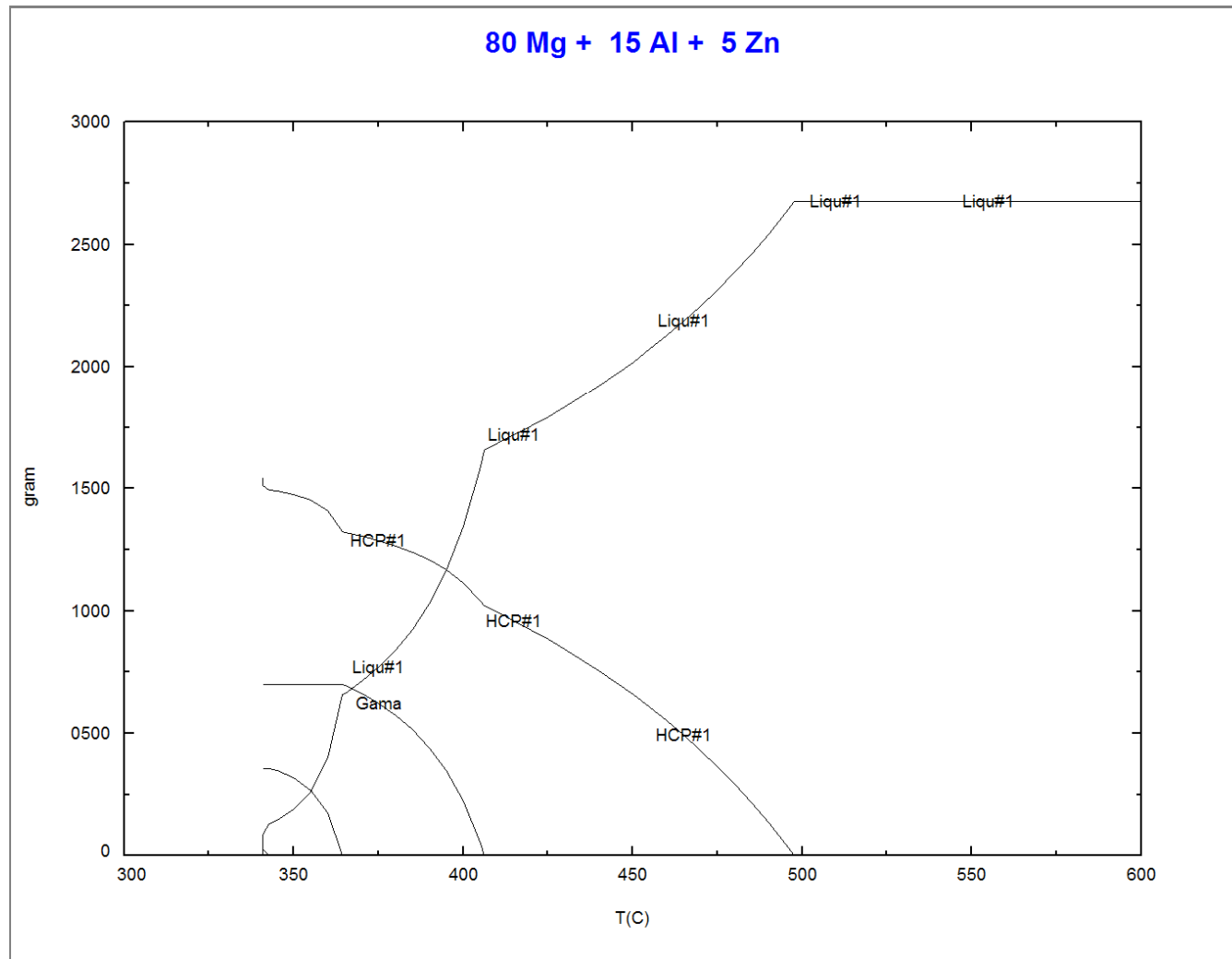
T(C) P(atm) Product H(J)

600 1

FactSage 6.2 beta E:\FactSage\Workshop2010\Equi1.DAT

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

F Menu - Equilib: Mg80-Al15-Zn5-cooling

File Units Parameters Help

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

Reactants (3)

80 Mg + 15 Al + 5 Zn

Solution FTlite-Liqu

- clear
- ✓ - all species
- * - custom select species
- m - merge dilute solution from ...
- solution properties

+ - single phase

- ✓ I - possible 2-phase immiscibility
- J - possible 3-phase immiscibility

- standard stable phase

- ! - dormant (metastable) phase
- F - formation target phase
- P - precipitate target phase
- S - Scheil cooling target phase
- ✓ D - solidification calculation ...
- C - composition target ...

Help ...

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

Legend

- I - immiscible 7
- D - Scheil solid'n.
- + - selected 8

Show all selected

species: 98
solutions: 22

Custom Solutions

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

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 126
Total Solutions (max 40) 22

Equilibrium

- normal normal + transitions
- transitions only open
- predominant

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

600 1

FactSage 6.2 beta E:\FactSage\Workshop2010\Equi1.DAT

F Menu - Equilib: Mg80-Al15-Zn5-cooling
 File Units Parameters Help

F 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
	I	FTlite-LC36B	BLaves_C36

fixed activities
 ideal solutions
 activity coefficients
 Details ...

Pseudonyms
 apply List ...

include molar volumes
 Total Species (max 1500) 126
 Total Solutions (max 40) 22
 Default

Legend
 I - immiscible 7
 D - Scheil solid'n.
 + - selected 8
 Show all selected
 species: 98
 solutions: 22
 Select

Final Conditions

<A>		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\Equil.DAT

Output for Scheil-Gulliver Solidification

F Results - Equilib Summary (page 1/60) FactSage 6.2 beta

Output Edit Show Pages

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

500 C	497.61 C	495 C								
555 C	550 C	545 C	540 C	535 C	530 C	525 C	520 C	515 C	510 C	505 C
Summary	Transitions	600 C	595 C	590 C	585 C	580 C	575 C	570 C	565 C	560 C

SUMMARY OF REACTIONS

Cooling
600.00 to 497.61 C (DELTA H = -3.2631E+05 J, DELTA V = -2.3338E-02 dm3)
Liquid cooling

Constituent 1
497.61 to 406.12 C (DELTA H = -5.5476E+05 J, DELTA V = -4.2376E-02 dm3)
Liquid -> HCP_A3

Constituent 2
406.12 to 364.35 C (DELTA H = -4.1656E+05 J, DELTA V = -1.3422E-02 dm3)
Liquid -> HCP_A3 + Gamma

Constituent 3
364.35 to 342.67 C (DELTA H = -2.0728E+05 J, DELTA V = 3.7122E-03 dm3)
Liquid -> HCP_A3 + Phi

Constituent 4
342.67 to 340.89 C (DELTA H = -1.7047E+04 J, DELTA V = 5.3375E-04 dm3)
Liquid -> HCP_A3 + AlMgZn_Tau

Constituent 5
340.89 C (isothermal) (DELTA H = -1.7309E+04 J, DELTA V = -9.7359E-04 dm3)
Liquid -> HCP_A3 + MgZn + AlMgZn_Tau

COMPOSITION OF PHASES IN CONSTITUENTS AT 340.89 C
(temperature of final disappearance of Liquid)

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

Input for Scheil Solidification AZ91 + 0.25% Mn

F Menu - Equilib: AZ91+0.25MnScheil solidif-anneal

File Units Parameters Help

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

Reactants (4) Menu Window

(gram) 89.75 Mg + 9 Al + Zn + 0.25 Mn

Products

Compound species
 gas ideal real 0
 aqueous 0
 pure liquids 0
 pure solids 42
 suppress duplicates
 species: 42

Scheil solidification
 FTlite-Liqu
 Cooling step T(C):
 Mass(g):

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
	+	FTlite-CBCC	CBCC_A12
	+	FTlite-CUB1	CUB_A13
	I	FTlite-LC14	Laves_C14
	I	FTlite-LC15	Laves_C15

Legend
 I - immiscible 7
 D - Scheil solid'n.
 + - selected 12
 Show all selected
 species: 144
 solutions: 26

Custom Solutions
 fixed activities
 ideal solutions
 activity coefficients

Pseudonyms
 apply

include molar volumes
 Total Species (max 1500) 186
 Total Solutions (max 40) 26

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		600	1	

10 steps Table
 Scheil solidification - T(start) = 600, T(stop) = 0% liquid

Equilibrium
 normal normal + transitions
 transitions only open
 predominant

FactSage 6.2 beta E:\FactSage\Workshop2010\Equi2.DAT

- 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

Results - Equilib Summary (page 1/63) FactSage 6.2 beta

Output Edit Show Pages

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

515 C | 510 C | 505 C | 565 C | 560 C | 555 C | 550 C | 545 C | 540 C | 535 C | 530 C | 525 C | 524.13 C | 520 C | Summary | Transitions | 600 C | 595 C | 594.16 C | 594.07 C | 590 C | 585 C | 580 C | 575 C | 570 C

CONSTITUENTS AND PHASES AT 340.89 C
(temperature of final disappearance of Liquid)

CONS.	PHASE	TOTAL AMT/mol	TOTAL AMT/gram	TOTAL VOL/dm3
1	1 Al8Mn5_D810	1.3000E-05	5.0016E-04	0.0000E+00
2	1 HCP_A3	2.6553E+00	6.4835E+01	3.7348E-02
2	2 Al8Mn5_D810	7.5208E-03	2.8466E-01	0.0000E+00
3	1 HCP_A3	6.3501E-01	1.5580E+01	8.9318E-03
3	2 Mn4Al11_s1 (s)	4.2236E-03	1.4545E-01	3.9104E-05
4	1 HCP_A3	6.8848E-02	1.6956E+00	9.6840E-04
4	2 MnAl4_s1 (s)	5.4348E-04	1.7703E-02	5.1307E-06
5	1 HCP_A3	1.9793E-01	4.8919E+00	2.7840E-03
5	2 Gamma	4.5374E-01	1.1829E+01	5.8585E-03
5	3 MnAl4_s1 (s)	8.0664E-04	2.6275E-02	7.6150E-06
6	1 HCP_A3	7.1854E-03	1.8145E-01	1.0107E-04
6	2 Phi	1.0937E-02	3.7590E-01	1.3948E-04
6	3 Mn4Al11_s1 (s)	1.3737E-06	4.7306E-05	1.2719E-08
7	1 HCP_A3	7.7230E-04	1.9634E-02	1.0863E-05
7	2 AlMgZn_Tau	6.7930E-04	2.9033E-02	7.6764E-06
7	3 Mn4Al11_s1 (s)	3.4940E-08	1.2032E-06	3.2350E-10
8	1 HCP_A3	1.2674E-03	3.2220E-02	1.7826E-05
8	2 MnZn	9.0952E-04	3.9431E-02	1.0890E-05

FactSage: Equilib

Do you wish to recycle Phase 1 of Constituent 2?

HCP_A3

	MOLE FRACTION	MASS FRACTION
Zn	4.7645E-04	1.2760E-03
Mn	8.3198E-05	1.8719E-04
Al	3.3684E-02	3.7222E-02
Mg	9.6576E-01	9.6132E-01
TOTAL AMT/mol		TOTAL AMT/gram
2.6553E+00		6.4835E+01

OK Cancel

Imported automatically into Equilib (change mass to 100 g)

Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 1

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100	[Rc C2 P1] HCP_A3 Constituent-2 Weight %: 1.0000E+02 Total 1.2760E-01 Zn 1.8719E-02 Mn 3.7222E+00 Al 9.6132E+01 Mg				2	

Initial Conditions

Next >>

FactSage 6.2 bet. Compound: 1/31 databases Solution: 1/31 databases

Anneal at 150 to 500 °C

F Menu - Equilib: AZ91+0.25MnScheil solidif-anneal

File Units Parameters Help

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

Reactants (1)

(gram) 100 [Rc_C2_P1]

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 42
- suppress duplicates

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	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

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 186
Total Solutions (max 40) 26

Target

- none -

Estimate T(K):

Mass(g):

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		150 500 5	1	

10 steps Table

Equilibrium

- normal normal + transitions
- transitions only open
- predominant

FactSage 6.2 beta E:\FactSage\Workshop2010\Equi2.DAT

Plot equilibrium products in HCP phase of constituent 2 after annealing

F Results - Equilib 150 C (page 3/73) FactSage 6.2 beta

Output Edit Show Pages

Save or Print ▶ T(C) P(atm) Energy(J) Mass(g) Vol(litre)

Plot ▶ Plot Results ...

Equilib Results file ▶ Repeat Plot - gram vs T(C) ...

Stream File ▶

Format ▶

Fact-XML ▶

Fact-Optimal ▶

Refresh ...

245 C | 250 C | 255 C | 260 C |

170 C | 175 C | 180 C | 185 C | 190 C | 195 C | 200 C | 205 C |

2_P1] =

1 mol HCP_A3#1
 (3.9086 mol, 5.4908E-02 litre, 1.7342 g/ml)
 (150.00 C, 1 atm, a=1.0000)

100 wt.% Al V
 34 wt.% Mg V
 + 4.3044E-11 wt.% Mn V
 + 9.6336E-02 wt.% Zn V)

System component	Mole fraction	Mass fraction
Zn	3.5892E-04	9.6336E-04
Mn	1.9088E-13	4.3044E-13
Al	1.5982E-02	1.7700E-02
Mg	0.98366	0.98134

Lattice parameter a/nm = 0.32137
 Lattice parameter c/nm = 0.52162
 c/a = 1.6231

+ 4.7194 gram Gamma
 (4.7194 gram, 3.1913E-03 mol, 2.3172E-03 litre, 2.0367 g/ml)
 (150.00 C, 1 atm, a=1.0000)

(0.57494 wt.% Mg10Al24Al24 V
 + 1.9462E-02 wt.% Mg10Al24Mg24 V
 + 95.028 wt.% Mg10Mg24Al24 V
 + 3.2107 wt.% Mg10Mg24Mg24 V
 + 0.27666 wt.% Mg10Zn24Al24 V
 + 9.5182E-03 wt.% Mg10Zn24Mg24 V
 + 5.1964E-03 wt.% Mg10Al24Zn24 V)

- Select axes

The screenshot shows the FactSage 6.2 beta interface. The main window is titled "Results - Equilib 150 C (page 3/73) FactSage 6.2 beta". A plot window titled "Plot: log10(gram) vs T(C)" is open, displaying a table of data. The table has columns for "activity" and "mole" and rows for "log10(gram)" and "T(C)".

	activity		
log10(gram)	0		1.
T(C)	0		4.0947

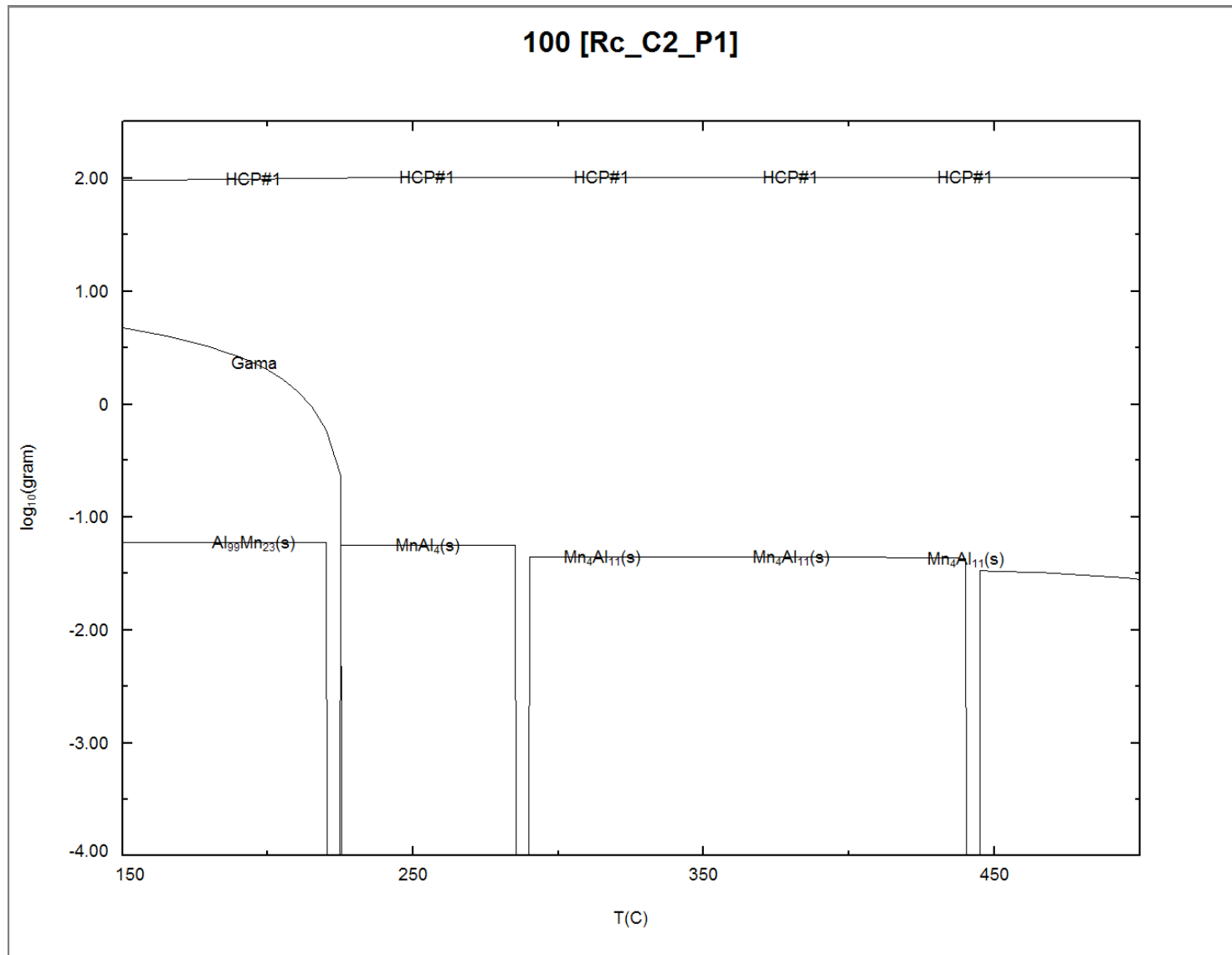
An "Axes: log10(gram) vs T(C)" dialog box is open, allowing the user to select the Y-axis variable (log10(gram)) and the X-axis variable (T(C)). The dialog box also includes fields for "maximum", "minimum", and "tick every" for both axes.

Y-axis: log10(gram)
maximum: 2.5
minimum: -4
tick every: 0.5

X-axis: T(C)
maximum: 500
minimum: 150
tick every: 50

Buttons: Cancel, Refresh, OK

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



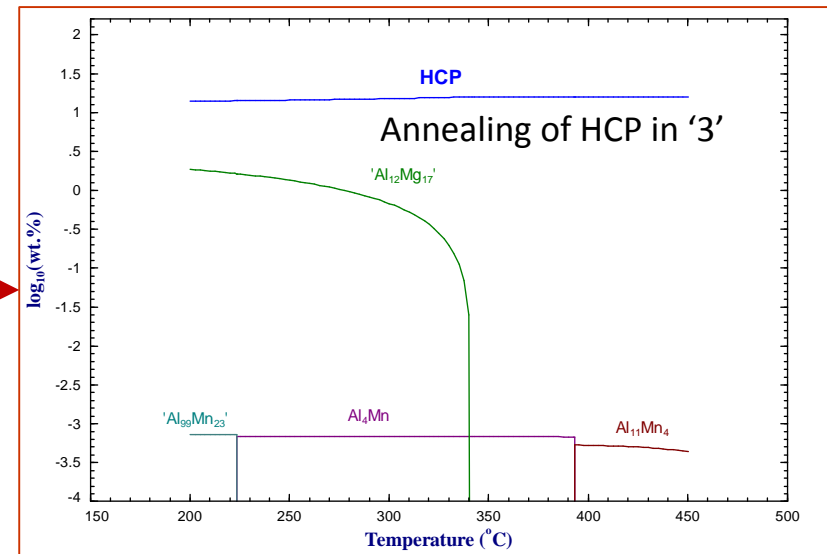
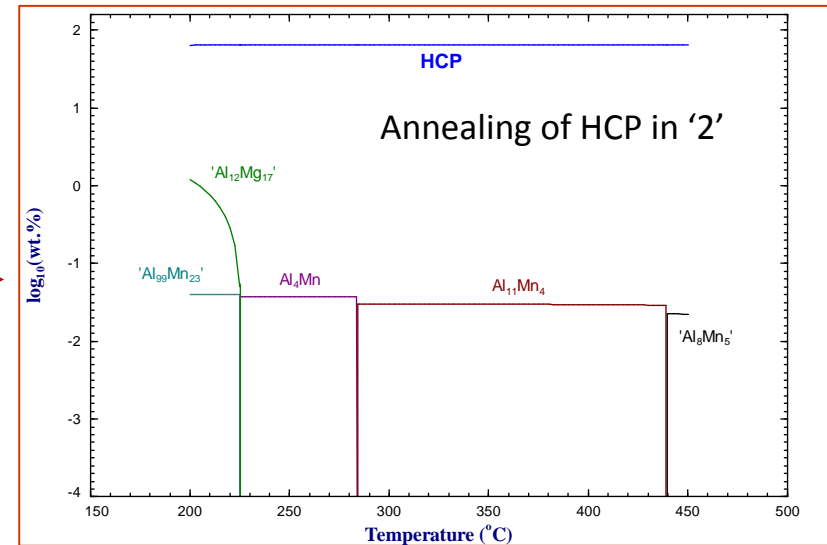
- Solidification software (extended Scheil cooling)
 - Scheil cooling + post equilibration of Scheil microstructure
- AZ91 alloy + 0.25 wt.% Mn

Tracking microstructure constituents

Annealing Phases vs T for HCP in the different microstructural constituents

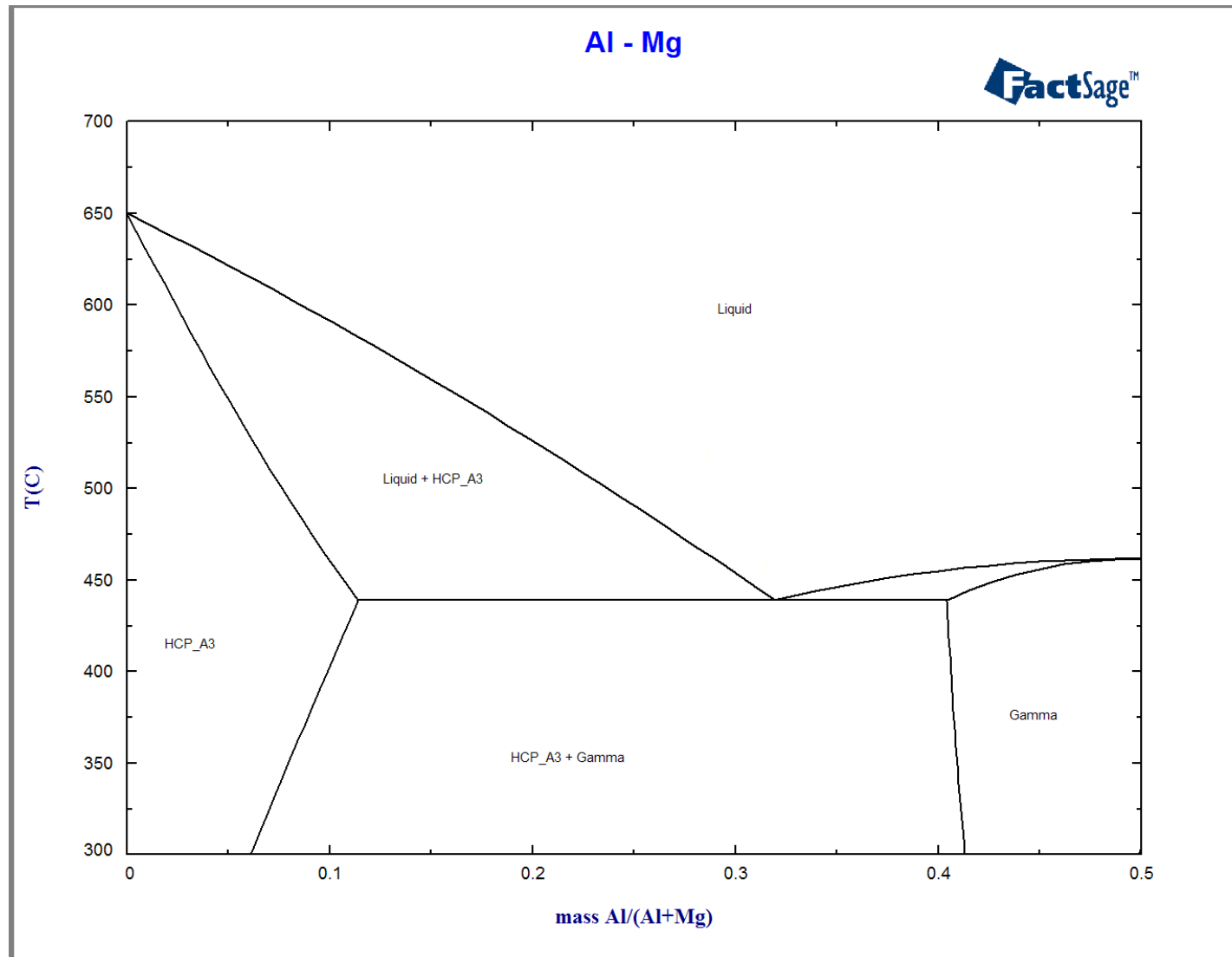
Amount & Average Composition of the HCP phase at 340.89°C

	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



F 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

species: 0

Solution species

*	+	Base-Phase	Full Name
		FTlite-Liqu	Liquid
		FTlite-HCP	HCP_A3
	+	FTlite-Gama	Gamma

Legend

- | - immiscible 2
- + - selected 1

Show all selected

species: 12
solutions: 5

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 12
Total Solutions (max 40) 5

Target

- none -

Estimate T(K):

Mass(g):

Variables

T(min)	H(max)	Al/(Al+Mg)			
300	30000	0.5			

H - H300 C / (Al+Mg) (J) vs Al/(Al+Mg)

Phase Diagram

Y
X

FactSage 6.2 beta E:\FactSage\Workshop2010\Phas11.DAT

Selecting variables for H-X diagram

The screenshot shows the FactSage software interface for creating a phase diagram. The main window is titled "Menu - Phase Diagram: Mg-Al for H-X". A dialog box titled "Variables: Al-Mg H - H300 C (J) vs composition #1." is open, allowing the user to select variables and parameters for the plot.

Variables: The "Variables" section shows a graph icon and a radio button selected for "compositions" (value 1). A "log10(a)" dropdown is set to 0. A "Next >>" button is visible.

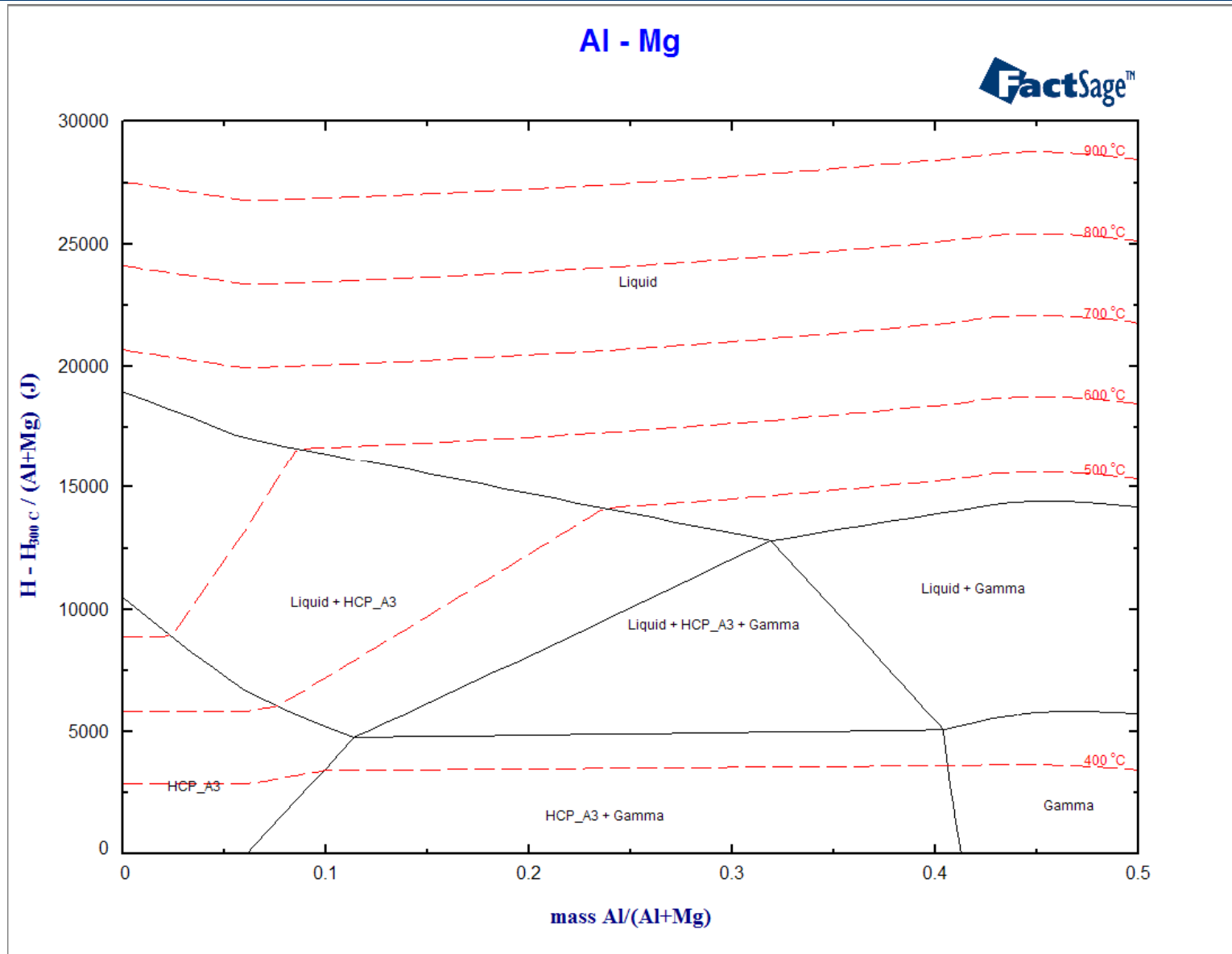
T and P: The "T and P" section has a "Temperature" dropdown set to "enthalpy". The "Pressure" section has a radio button selected for "P(bar)" and a dropdown set to "constant". The "log P" section has a value of 1. The "Temperature" section has input fields for "H(J) max" (30000), "T(C) min" (300), and "Iso-T step" (100). A checkbox for "plot iso-thermal lines" is checked. The Y-axis label is "Y-axis: H-H(Tmin)/(Al+Mg)".

Compositions (mass): The "Compositions (mass)" section shows the composition of the system. The X-axis is set to "Al/(Al+Mg)". The composition is defined as 1 Al + 0 Mg (X-axis) and 1 Al + 1 Mg (Y-axis). The X-axis range is from 0 (min) to 0.5 (max).

Buttons: "Cancel" and "OK" buttons are at the bottom of the dialog. A "Calculate >>" button is at the bottom right of the main window.

Status Bar: The status bar at the bottom shows "FactSage 6.2 beta" and the file path "E:\FactSage\Workshop2010\Phas11.DAT".

Calculated Mg-Al H-X diagram



Al - Mg - Zn

Data from FTlite - FACT light alloy databases

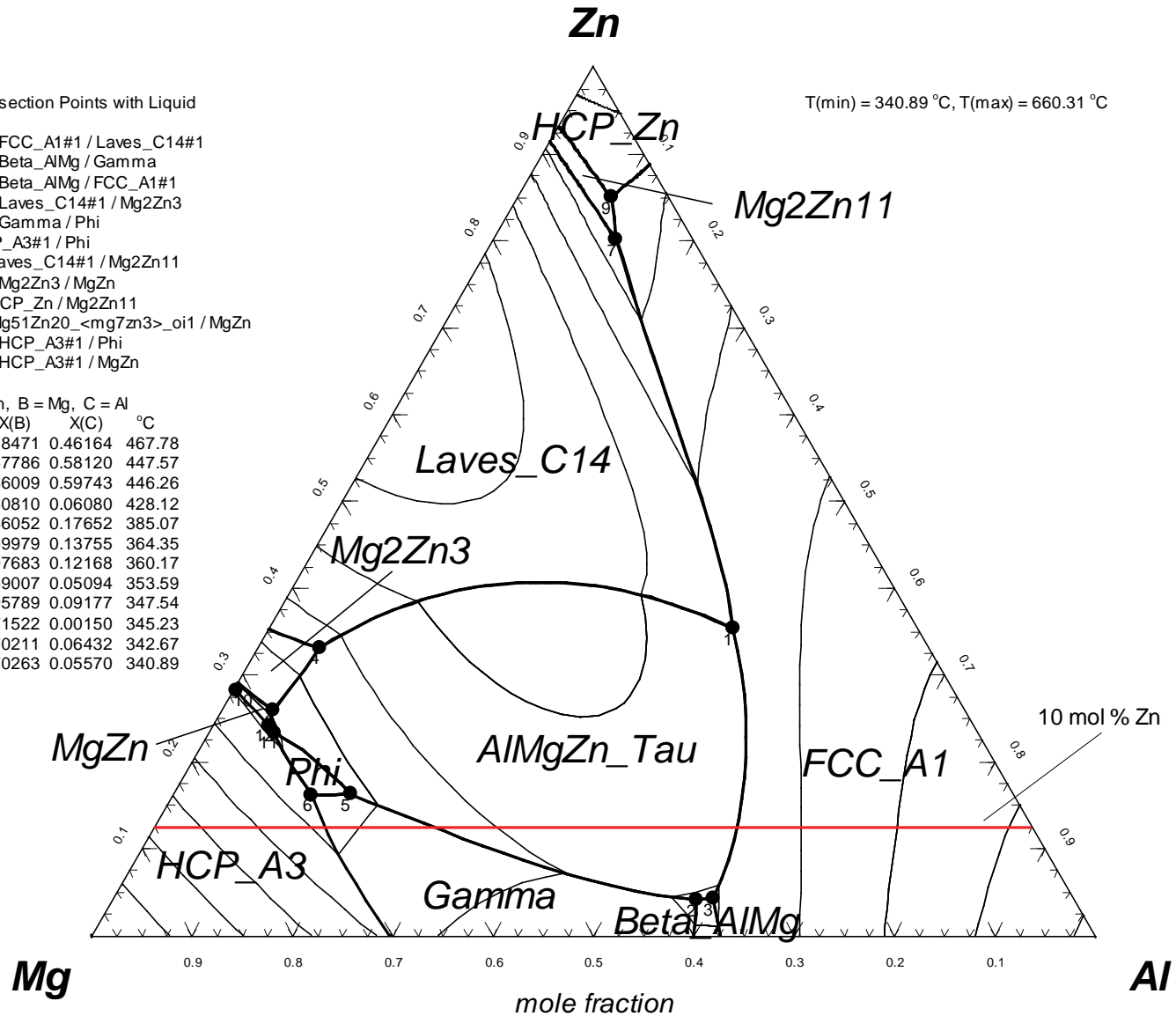


Four-Phase Intersection Points with Liquid

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

- 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



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

F Menu - Phase Diagram: Mg-Al-10%Zn T-X.fig

File Units Parameters Variables Help

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

Components (3)

Mg + Al + Zn

Products

Compound species
 gas ideal real 0
 aqueous 0
 pure liquids 0
 pure solids 28
 suppress duplicates apply
 species: 28

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-Beta	Beta_ALMg

Legend
 | - immiscible 7
 + - selected 8

Show all selected
 species: 98
 solutions: 22

Custom Solutions
 0 fixed activities
 0 ideal solutions
 0 activity coefficients

Pseudonyms
 apply

include molar volumes
 Total Species (max 1500) 126
 Total Solutions (max 40) 22

Variables

T(C)	Al/(Mg+Al+Zn)	Zn/(Mg+Al+Zn)		
25 725	0 0.9	0.1		

T(C) vs Al/(Mg+Al+Zn)

Phase Diagram

Y
X

FactSage 6.2 beta E:\FactSage\Workshop2010\Phas1.DAT

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

- Selection of variables

Menu - Phase Diagram: Mg-Al-10%Zn T-X.fig

File Units Parameters Variables Help

F Variables: Mg-Al-Zn T(C) vs composition #1.

Variables

compositions 2

log10(a) 0

Y steps: 10

X steps: 10

Next >>

T and P

Temperature

T(C) Y-axis

Max: 725

Min: 25

1/TK

Pressure

P(atm) constant

log P 1

Compositions (mole)

#1. 0 Mg + 1 Al + 0 Zn = X-axis

1 Mg + 1 Al + 1 Zn = 0.9 (max)

0 (min)

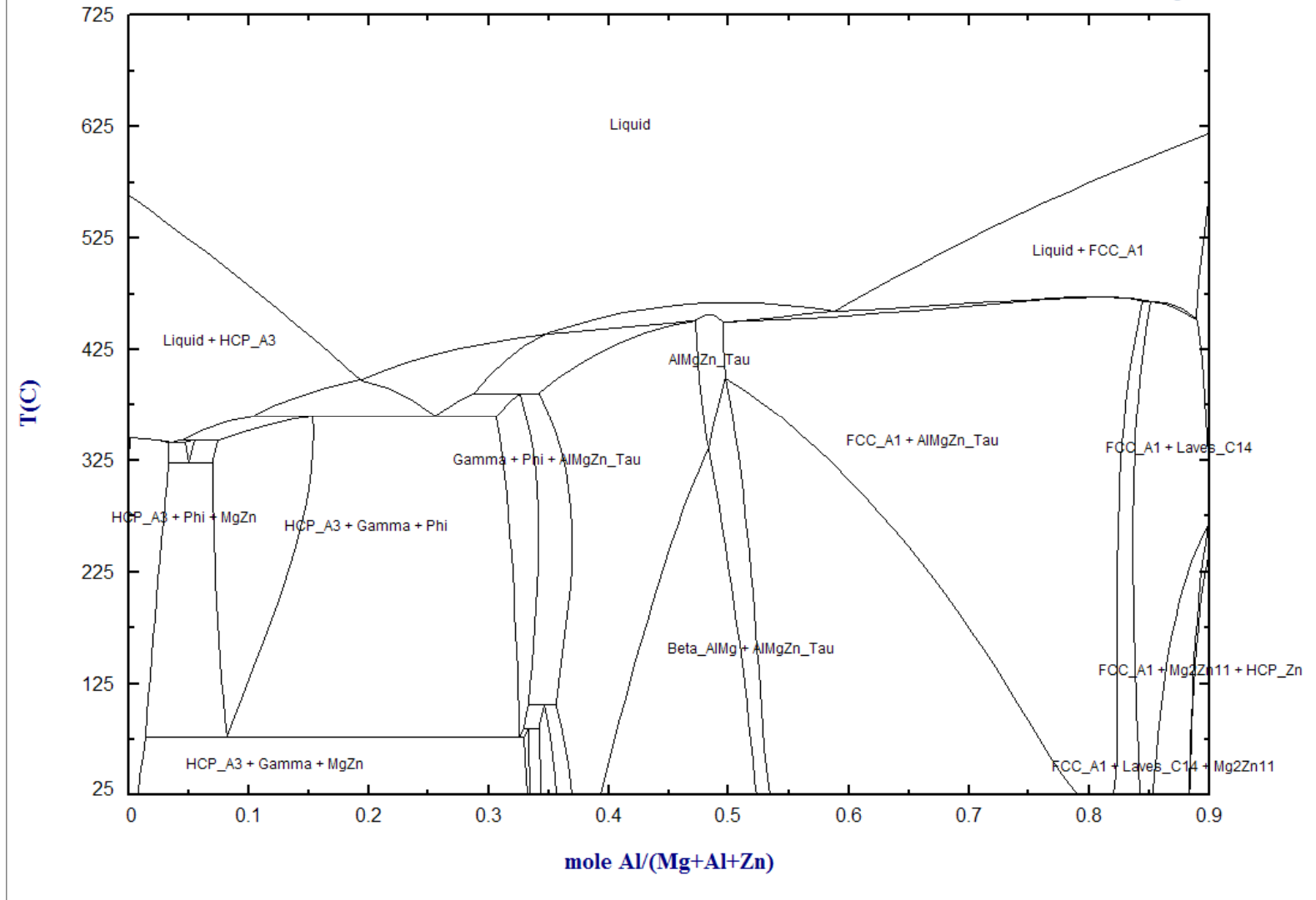
#2. 0 Mg + 0 Al + 1 Zn = constant

1 Mg + 1 Al + 1 Zn = 0.1

Cancel OK

FactSage 6.2 beta E:\FactSage\Workshop2010\Phas1.DAT

Mg - Al - Zn
mole Zn/(Mg+Al+Zn) = 0.1



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

F Menu - Phase Diagram: Mg-Al-10%Zn for H-X

File Units Parameters Variables Help

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

Components (3)
Mg + Al + Zn

Products

Compound species
 gas ideal real 0
 aqueous 0
 pure liquids 0
 pure solids 1
 suppress duplicates apply
 * - custom selection species: 1

Solution species

*	+	Base-Phase	Full Name
	+	FTlite-Liqu	Liquid
	+	FTlite-FCC	FCC_A1
	+	FTlite-HCP	HCP_A3
	+	FTlite-LC14	Laves_C14
	+	FTlite-Beta	Beta_AIMg
	+	FTlite-Gama	Gamma
	+	FTlite-Phi	Phi
	+	FTlite-MgZn	MgZn

Legend
+ - selected 9
 Show all selected
species: 41
solutions: 9

Custom Solutions
 fixed activities
 ideal solutions
 activity coefficients

Pseudonyms
 apply

include molar volumes
 Total Species (max 1500) 42
 Total Solutions (max 40) 9

Variables

T(min)	H(max)	Al/(Mg+Al+Zn)	Zn/(Mg+Al+Zn)
25	30000	0.9	0.1

H - H25 C / (Mg+Al+Zn) (J) vs Al/(Mg+Al+Zn)

Phase Diagram
Y
X

FactSage 6.2 beta E:\FactSage\Workshop2010\Phas15.DAT

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

Variables: Mg-Al-Zn H - H25 C (J) vs composition #1.

Variables
 compositions 2
 log10(a) 0
 Y steps: 10
 X steps: 10
 Next >>

T and P
 Temperature: enthalpy vs X
 H(J) max: 30000
 T(C) min: 25
 Iso-T step: 100
 plot iso-thermal lines
 Y-axis: H-H(Tmin)/(Mg+Al+Zn)
 Pressure: P(atm) constant 1
 log P 1

Compositions (mole)

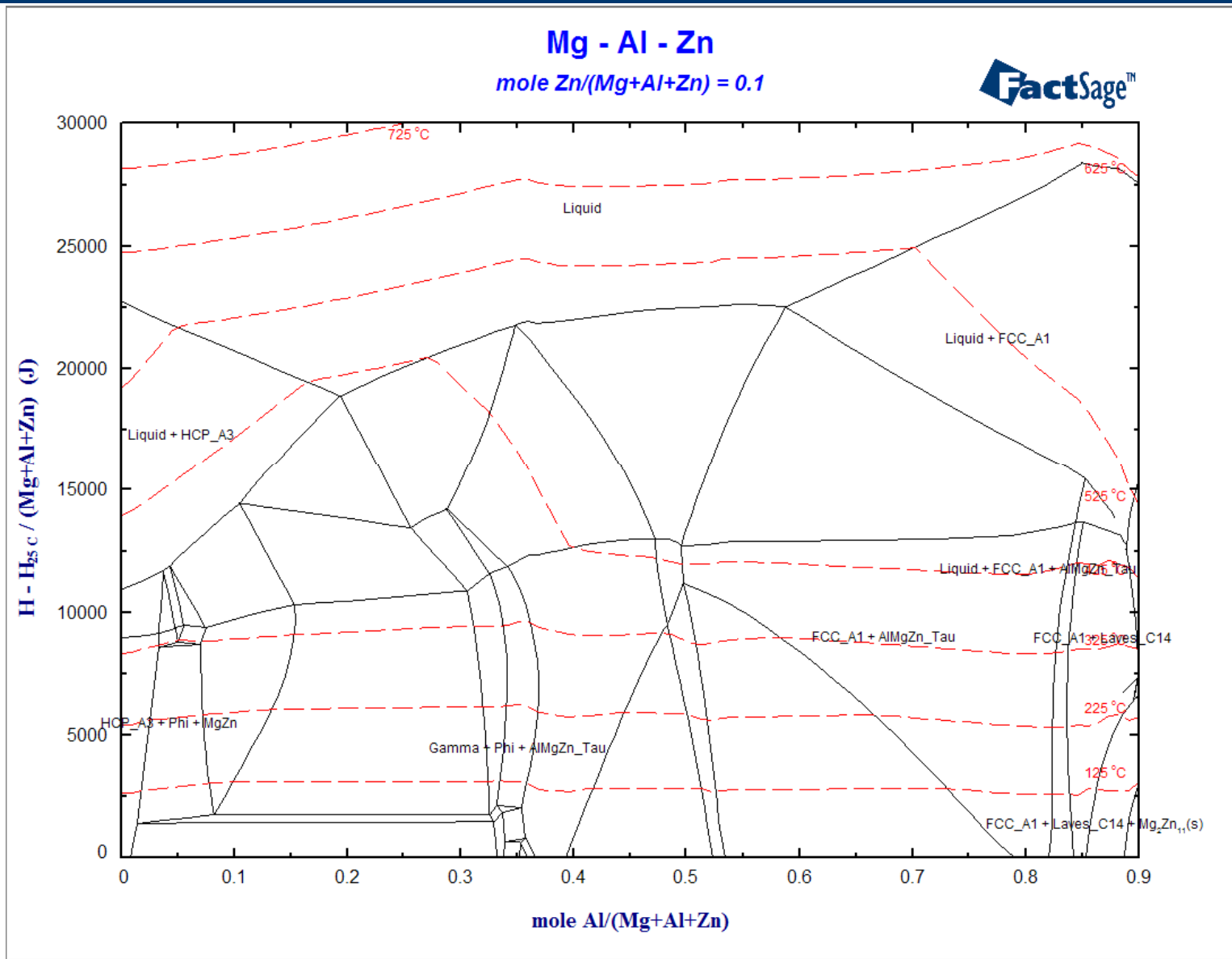
#1. 0 Mg + 1 Al + 0 Zn = X-axis
 1 Mg + 1 Al + 1 Zn = 0.9 (max)
 0 (min)

#2. 0 Mg + 0 Al + 1 Zn = constant
 1 Mg + 1 Al + 1 Zn = 0.1

Cancel OK

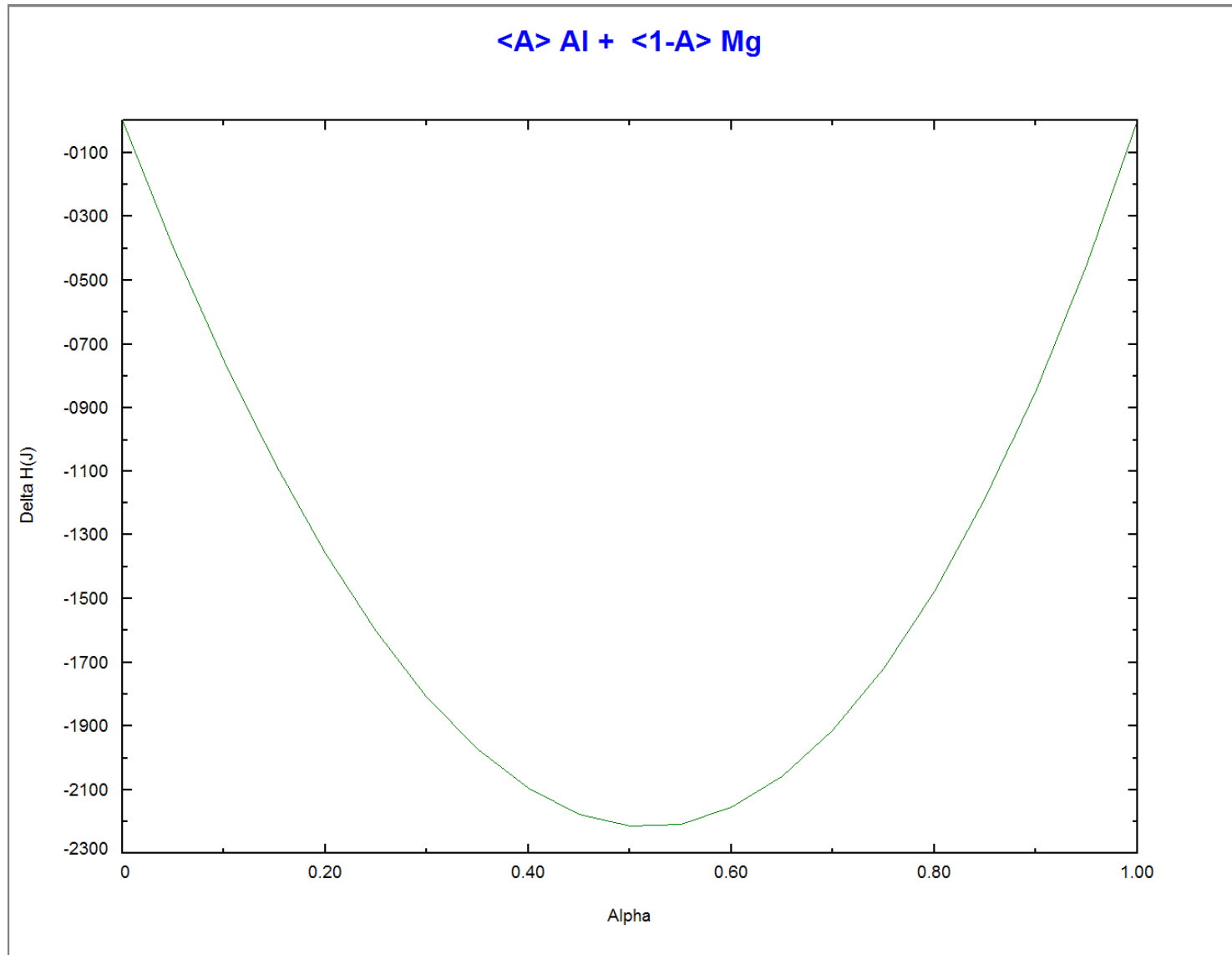
FactSage 6.2 beta E:\FactSage\Workshop2010\Phas15.DAT

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 °C

1 - 2

Mass(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
<A>	Al	liquid	800	1	1	
+ <1-A>	Mg	liquid	800	1	1	

Initial Conditions

Next >>

FactSage 6.2 bet. Compound: 1/31 databases Solution: 1/31 databases

F 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 + <1-A> Mg
(800C,liq,#1) (800C,liq,#1)

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
	+	FTlite-Liqu	Liquid

Legend
+- selected 1

Show all selected

species: 2

solutions: 1

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 2

Total Solutions (max 40) 1

Final Conditions

<A>		T(C)	P(atm)	Delta H(J)
0	1	800	1	

10 steps Table

Equilibrium

- normal normal + transitions
- transitions only open
- predominant

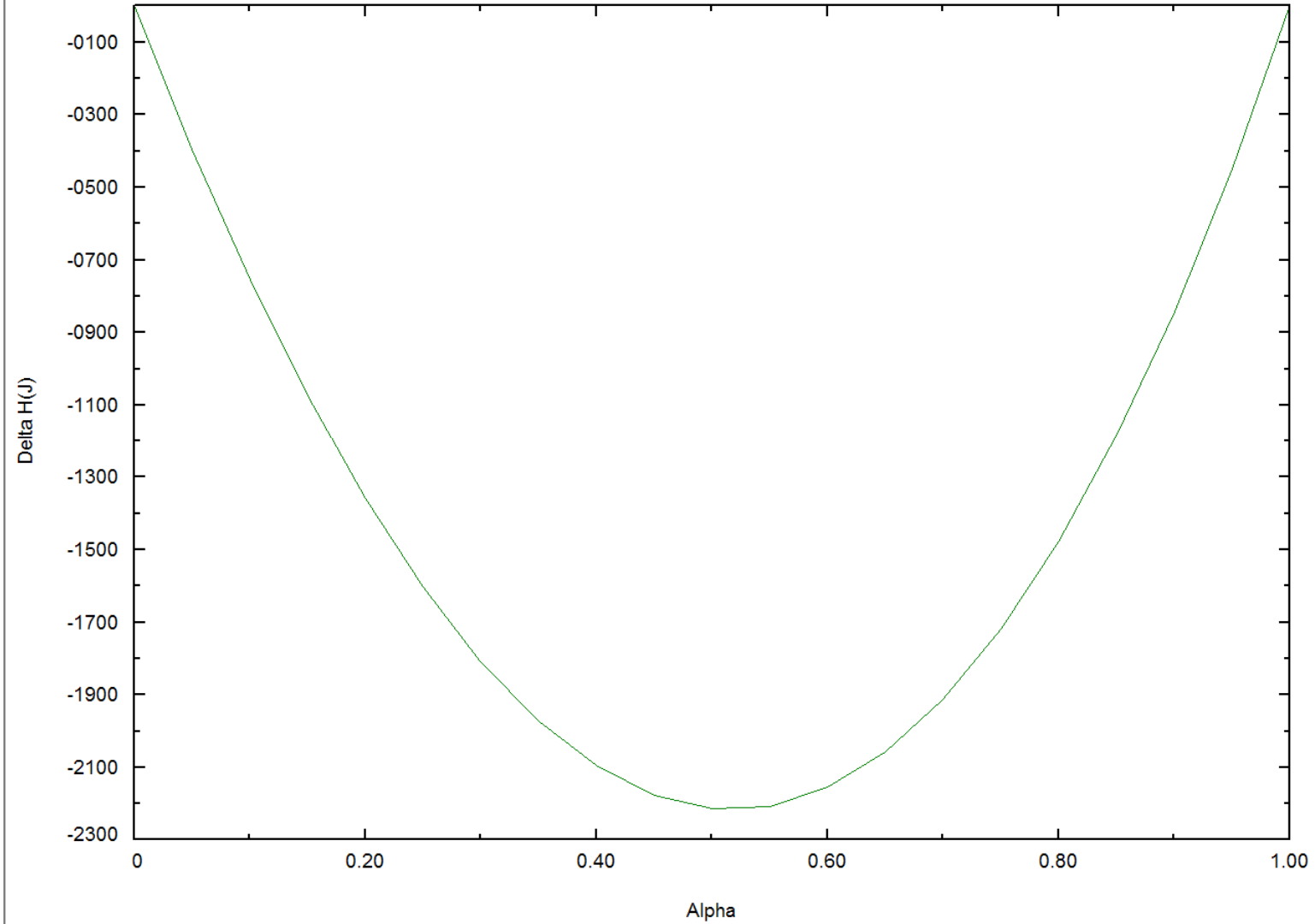
FactSage 6.2 beta E:\FactSage\Workshop2010\Equi3.DAT

Plot results – selection of axes

The screenshot shows the FactSage 6.2 beta Results Processor interface. The main window displays a table of thermodynamic data for the reaction $\langle A \rangle \text{Al} + \langle 1-A \rangle \text{Mg}$. The table includes columns for activity and mole fractions. A dialog box titled "Axes: Delta H(J) vs Alpha" is open, allowing the user to select the Y and X variables and set their ranges and tick marks. The Y-axis is set to "Delta H(J)" with a maximum of 0 and a minimum of -2300, with a tick every 100. The X-axis is set to "Alpha" with a maximum of 1 and a minimum of 0, with a tick every 0.1. The dialog also includes options for "Reactants", "File name", "Viewer", and "Figure".

Component	Activity	Mole
$\langle A \rangle \text{Al}$	0	1.
$\langle 1-A \rangle \text{Mg}$	0	1.

<A> Al + <1-A> Mg



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)

F 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 + <1-A> Mg
(800C.liq.#1) (800C.liq.#1)

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
	+	FTlite-Liqu	Liquid
		FTlite-FCC	FCC_A1
		FTlite-HCP	HCP_A3
		FTlite-BCC	BCC_A2
		FTlite-LC14	Laves_C14
		FTlite-LC15	Laves_C15
		FTlite-Beta	Beta_ALMg
		FTlite-Gama	Gamma

Legend
+ - selected 1

Show all selected

species: 2

solutions: 1

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 2
Total Solutions (max 40) 1

Target

- none -

Estimate T(K):

Mass(mol):

Final Conditions

<A>		T(C)	P(atm)	Delta H(J)
0.05	0.95	0.05		

steps Table

Equilibrium

- normal normal + transitions
- transitions only open
- predominant

FactSage 6.2 beta E:\FactSage\Workshop2010\Equi3.DAT

Solution Properties

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

The screenshot shows the FactSage 6.2 beta software interface. The main window is titled 'F Menu - Equilib: last system'. The 'Reactants (2)' field contains '<A> Al + <1-A> Mg'. A context menu is open over the 'Solution FTlite-Liqu' phase, listing various options such as '- clear', '- all species', '- custom select species ...', '- merge dilute solution from', '- solution properties ...', '+ - single phase', '- possible 2-phase immiscibility', '- possible 3-phase immiscibility', '- standard stable phase', '- dormant (metastable) phase', '- formation target phase', '- precipitate target phase', '- Scheil cooling target phase', '- solidification calculation ...', and '- composition target ...'. The 'Solution species' table is visible, showing the following data:

*	+	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-Beta	Beta_AlMg
		FTlite-Gama	Gamma

The 'Legend' section shows '+ - selected 1' and 'Show all selected' options. The 'Equilibrium' section has radio buttons for 'normal', 'normal + transitions', 'transitions only', and 'predominant'. The 'Calculate >>' button is visible at the bottom right. The status bar at the bottom left shows 'FactSage 6.2 beta' and the bottom center shows '19 calculations'.

- Select properties to be calculated

Menu - Equilib: last system

File Units Parameters Help

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

Reactants (2)

Products

Compound species

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

Target

- none -

Estimate T(K): 1000

Mass(mol): 0

Final Conditions

<A>

0.05 0.95 0.05

10 steps Table

FactSage 6.2 beta

F Molar Partial Properties FTLite-Liqu - Liquid

Output Species Standard States

Units: T(C), P(atm), Energy(J), Mass(mol), Vol(litre)

2/2 species partial properties integral properties 2/17 properties

+	Property	Description of Partial Property
	a(i)	activity of species i
+	gamma(i)	activity coefficient of species i = a(i)/a_ideal(i)
	Delta_g(i)	= g(i) - go(i) = RT ln a(i)
+	Delta_h(i)	= h(i) - ho(i) = h(excess)(i)
	Delta_s(i)	= s(i) - so(i)
	g(i)	= h(i) - T.s(i)
	h(i)	absolute h of species i with respect to elements at 25 C
	s(i)	absolute s of species i
	go(i)	g of species i in standard state
	ho(i)	h of species i in standard state
	so(i)	s of species i in standard state
	a_ideal(i)	ideal activity of species i = mole fraction X(i)
	Delta_g_ideal(i)	= RT ln a_ideal(i)
	Delta_s_ideal(i)	= -R ln a_ideal(i)
	g_excess(i)	= Delta_g(i) - Delta_g_ideal(i)
	s_exc	Select All
	s(i)	Clear
	cp(i)	Close
		heat capacity of species i = d(h(i))/dT

Calculate >>

- Open spreadsheet

The screenshot shows the FactSage 6.2 beta interface. The main window is titled 'Menu - Equilib: last system'. A dialog box titled 'Molar Partial Properties FTlite-Liqu - Liquid' is open, showing a list of properties and their descriptions. The 'Open Spreadsheet' option is selected in the 'Output' tab. The 'Description of Partial Property' table is visible, listing various thermodynamic properties and their definitions.

Molar Partial Properties FTlite-Liqu - Liquid

Output: Energy(J), Mass(mol), Vol(litre)

Species: properties integral properties

2/17 properties

Description of Partial Property	
a(i)	activity of species i
+ gamma(i)	activity coefficient of species i = a(i)/a_ideal(i)
Delta_g(i)	= g(i) - go(i) = RT ln a(i)
+ Delta_h(i)	= h(i) - ho(i) = h(excess)(i)
Delta_s(i)	= s(i) - so(i)
g(i)	= h(i) - T.s(i)
h(i)	absolute h of species i with respect to elements at 25 C
s(i)	absolute s of species i
go(i)	g of species i in standard state
ho(i)	h of species i in standard state
so(i)	s of species i in standard state
a_ideal(i)	ideal activity of species i = mole fraction X(i)
Delta_g_ideal(i)	= RT ln a_ideal(i)
Delta_s_ideal(i)	= -R ln a_ideal(i)
g_excess(i)	= Delta_g(i) - Delta_g_ideal(i)
s_exc	= s(i) - s_ideal(i)
cp(i)	heat capacity of species i = d(h(i))/dT

Buttons: Select All, Clear, Close

Calculate >>

- Spreadsheet showing calculated solution properties

Menu - Equilib: last system

File Units Parameters Help

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

Reactants (2)

Molar Partial Properties FTlite-Liqu - Liquid

Molar Partial Properties FTlite-Liqu - Liquid - Energy(J), (mol)

File Edit Swap rows and columns

Component i	Page	<Alpha>	T(C)	P(atm)	X(Al)	X(Mg)	gamma(i)	Delta_h(i)
	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

Al_Liqu

0.05 0.050000

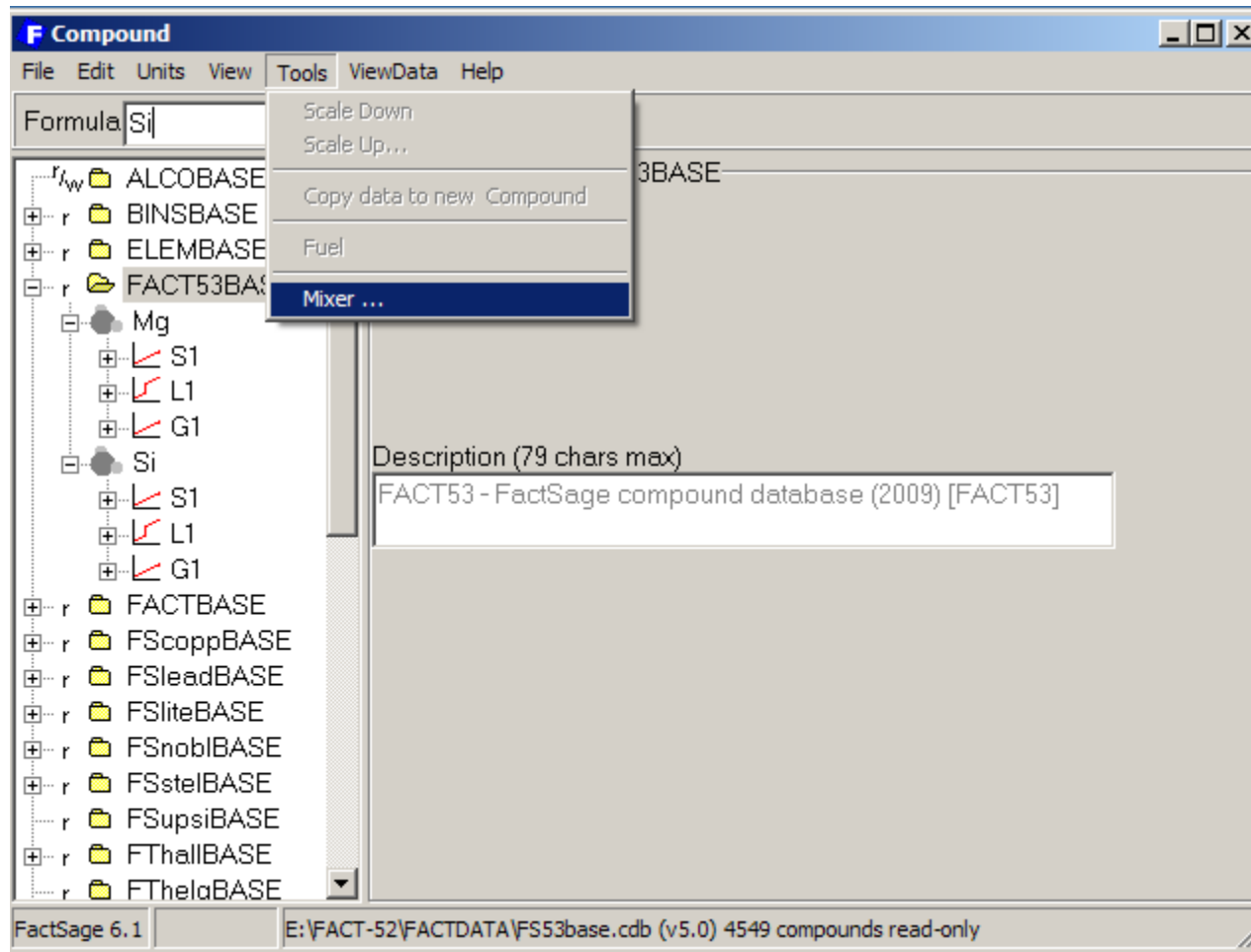
10 steps Table

cp(i) heat capacity of species i = d[h(i)]/dT

Calculate >>

FactSage 6.2 beta

- Using COMPOUND module to create compound Mg_2Si in a private database with
 $2\text{Mg} + \text{Si} = \text{Mg}_2\text{Si} \quad \Delta H = -68000 \text{ J/mol} \quad \Delta S = -13.0 \text{ J/mol}^{-1}$
 relative to $\text{Mg}(\text{s1})$ and $\text{Si}(\text{s1})$ from FS53 database
 (see Manual COMPOUND, particularly section 14)



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

The screenshot shows the FactSage software interface. The main window title is "Energy: Joules Pressure: atm Si". The "Formula" field contains "Si". The left sidebar shows a tree view of databases, with "Mg" and "Si" expanded. Under "Si", the "S1" entry is selected. The "S1 properties" window is open, showing "Heat of form. + Entropy" selected. The "Form. of S1" section has "ΔH298 (Joules)" set to 0 and "S298 (J/(mol K))" set to 18.82. The "Phase Name" is "Solid", "Reference no." is 128, and "Density g/cc" is 2.33. The "Compound mixer" window is also open, showing a table of reactants:

Reactants	Phase	Database
+2 Mg	S1	FACT53
+1 Si	S1	FACT53

Below the table, the "Product" is "SiMg2" and the "State" is "Solid". The status bar at the bottom indicates "FactSage 6.1" and the file path "E:\FACT-52\FACTDATA\F553base.cdb (v5.0) 4549 compounds read-only".

- Click on "PRIVBASE" and then paste compound into PRIVBASE

FactSage 6.1

File Edit Units View Tools ViewData Help

Formula

Information on PRIVBASE

Nickname (4 chars)

Compound mixer

Reactants	Phase	Database
+2 Mg	S1	FACT53
+1 Si	S1	FACT53

Product State

E:\FactSage\USERDATA\private.CDB (v5.0) 3 compounds read/write

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

Energy: Joules Pressure: atm SiMg2

File Edit Units View Tools ViewData Help

Formula

S1 properties

Heat of form. + Entropy Heat + Temperature of transf.

Form. of S1	ΔH_{298} (Joules)	S_{298} (J/(mol K))
	0	84.162

Phase Name Reference no. Density g/cc

Compound mixer

Reactants	Phase	Database
+2 Mg	S1	FACT53
+1 Si	S1	FACT53

Product State

FactSage 6.1 E:\FactSage\USERDATA\private.CDB (v5.0) 4 compounds read/write

- Add $\Delta H = -68000$, $\Delta S = -13.0$

Energy: Joules Pressure: atm SiMg2

File Edit Units View Tools ViewData Help

Formula: Si

S1 properties

Heat of form. + Entropy Heat + Temperature of transf.

Form. of S1

ΔH_{298} (Joules)	S_{298} (J/(mol K))
-68000	71.162

Phase Name: Reference no.: Density g/cc: 1.91784

Compound mixer

Reactants	Phase	Database
+2 Mg	S1	FACT53
+1 Si	S1	FACT53

Product: SiMg2 State: Solid

FactSage 6.1 Modified E:\FactSage\USERDATA\private.CDB (v5.0) 4 compounds read/write