Equilib Cooling Calculations

The ***Equilib*** module enables you to perform cooling calculations and display the phase transitions and compositions during

- **Equilibrium cooling**
- **Scheil-Gulliver cooling**
- **Annealing of casted alloys**

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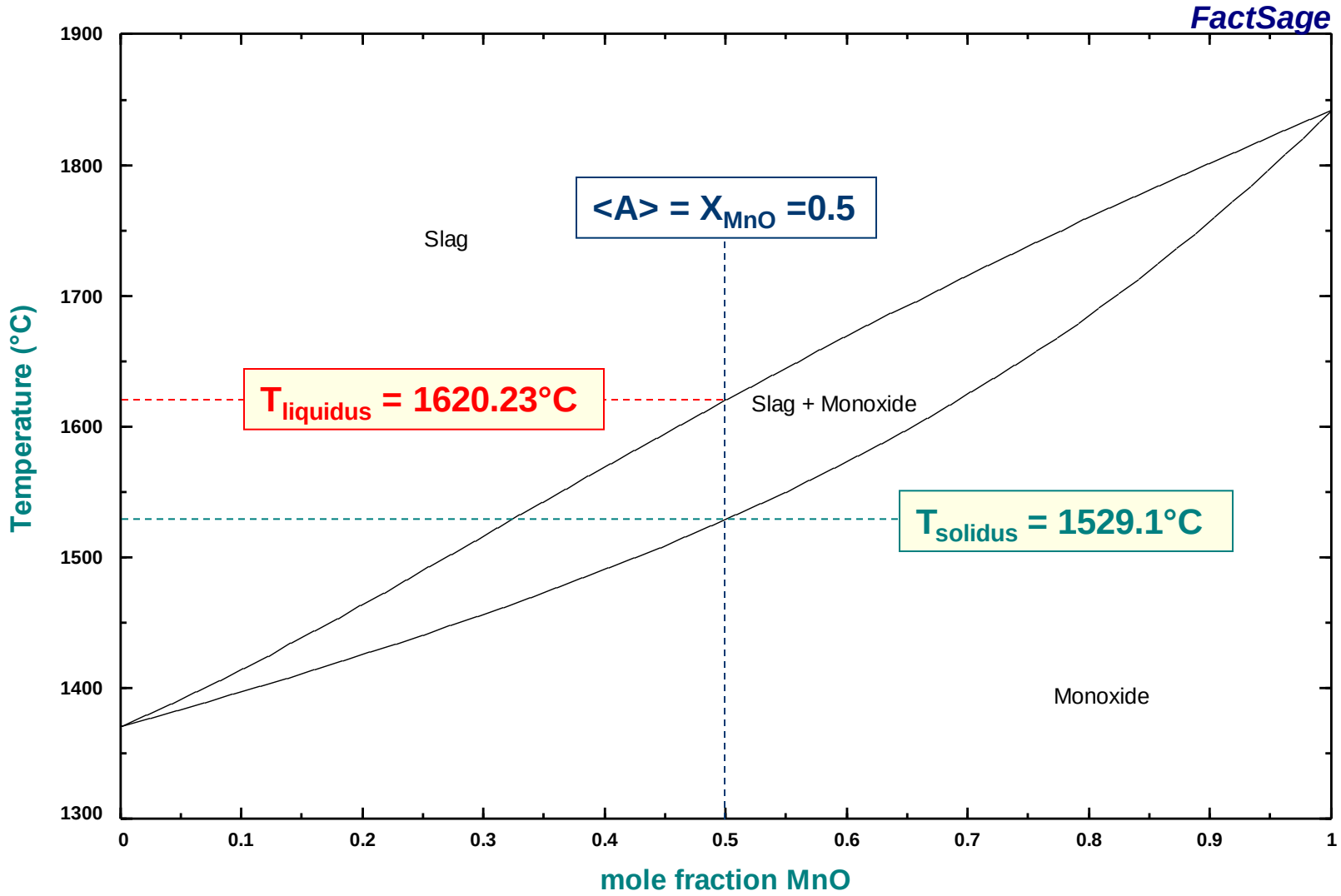
FeO-MnO : Phase transitions - binary phase diagram

FeO-MnO binary phase diagram calculated by ***Phase Diagram***



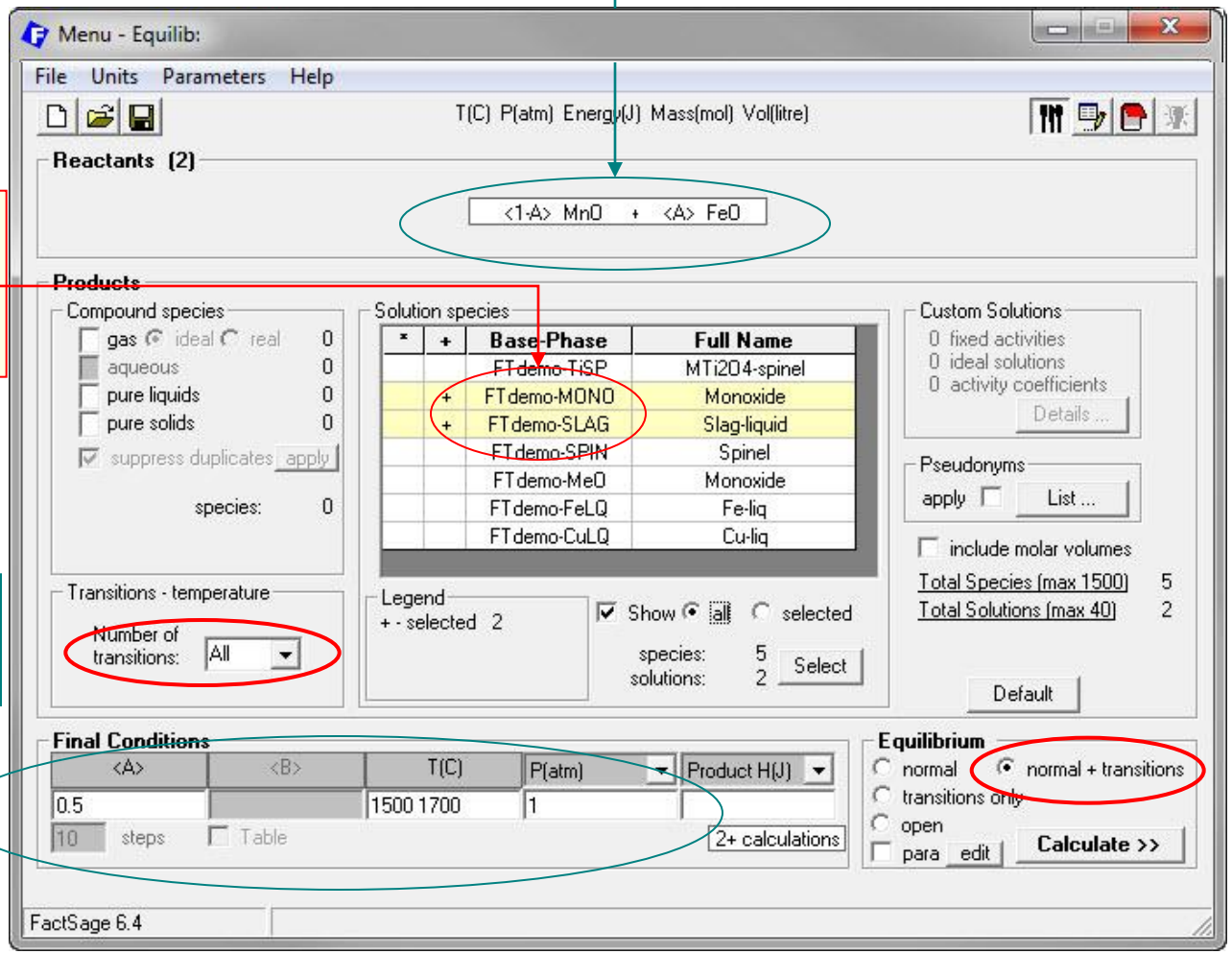
FeO-MnO : Equilibrium phase transitions at X_{FeO} = 0.5

1° Binary system <1-A> MnO + <A> FeO .

2° Possible products:

- solid solution (**MONO**)
- liquid Slag (**SLAG**)

3° <A> = **0.5**
T (°C) = **1500** and **1700**



Equilib will calculate the **equilibrium** at X_{FeO} **= 0.5** for temperatures varying from **1500°C** to **1700°C** and will search for **All** phase **transitions**.

FeO-MnO : Phase transitions showing liquidus and solidus

Results - Equilib 1620.23 C (page 3/4)

Output Edit Show Pages

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

1500 C | 1529.11 C | - 1620.23 C - | 1700 C

```
<1-A> MnO +  <A> FeO =

 1.0000      mol    Slag-liquid
 (71.392 gram, 1.0000 mol)
         (1620.23 C, 1 atm,      a=1.0000)
         ( 0.50000          FeO
         + 0.50000          MnO)

+ 0.00000     mol    Monoxide
         (1620.23 C, 1 atm,      a=1.(
         ( 0.30796          FeO
         + 0.69204          MnO)

where "A" on the reactant side is 0.5(

The cutoff concentration has been spe(

*************************************
      H            G            V
     (J)          (J)        (litre)
*************************************
-1.91102E+05 -5.49403E+05  0.00000E+0(
```

Equilibrium liquidus

Results - Equilib 1529.11 C (page 2/4)

Output Edit Show Pages

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

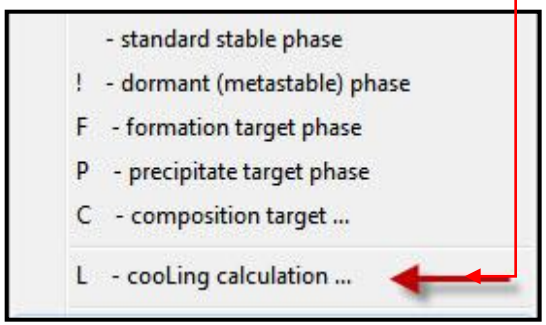
1500 C | - 1529.11 C - | 1620.23 C | 1700 C

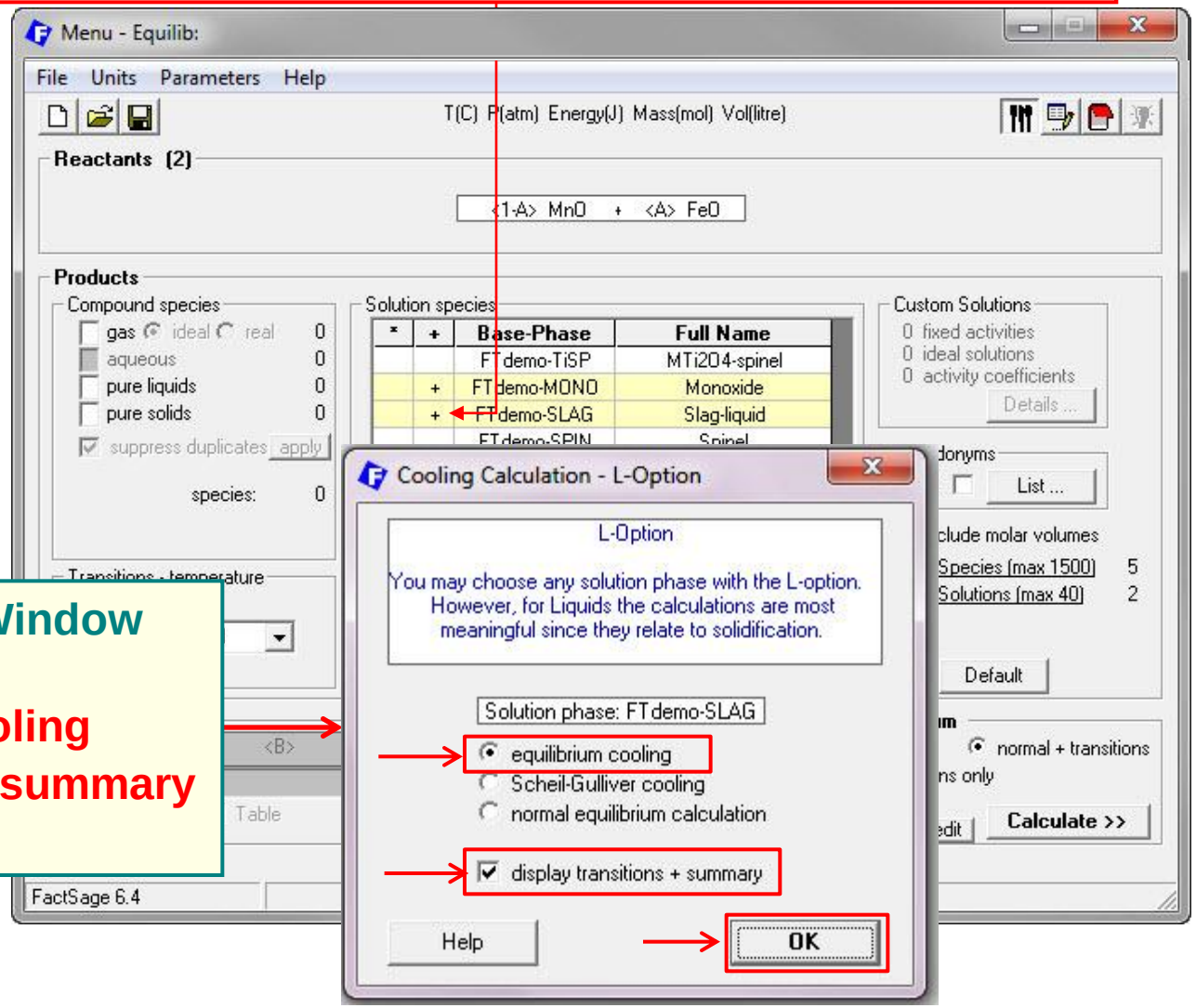
```
<1-A> MnO +  <A> FeO =

1.0000      mol    Monoxide
(71.392 gram, 1.0000 mol)
        (1529.11 C, 1 atm,      a=1.0000)
        ( 0.50000          FeO
        + 0.50000          MnO)

+ 0.00000     mol    Slag-liquid
        (1529.11 C, 1 atm,      a=1.0000)
        ( 0.67618          FeO
        + 0.32382          MnO)

where "A" on the reactant side is 0.50000

The cutoff concentration has been specified to 1.0000E-75

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
-2.38118E+05 -5.33297E+05  0.00000E+00  1.63783E+02  6.63565E+01
```

Equilibrium solidus

FeO-MnO : Simple equilibium cooling – L-Option

1° **Right-click** on the '+' column to open the **SLAG** extended menu and **select** **L– cooLing calculation**.to open the ***Cooling Calculation Window***





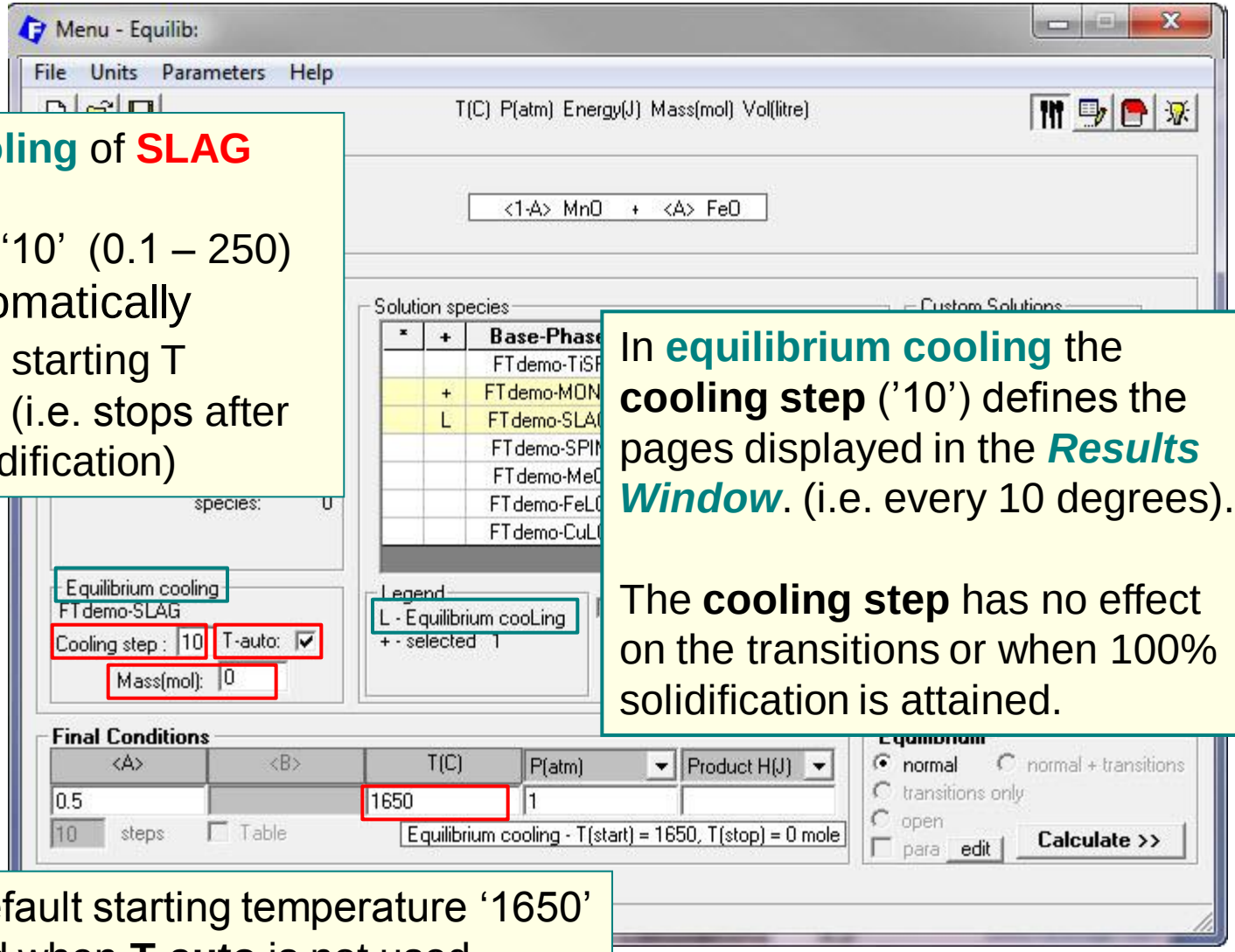
2° **Cooling Calculation Window**

- **select equilibrium cooling**
- **check √ transitions + summary**
- **click OK** to close.

FeO-MnO : Simple equilibium cooling – step, T-auto and stop

Equilibrium Cooling of **SLAG**

- **cooling step** '10' (0.1 – 250)
- **T-auto** √ automatically calculates the starting T
- **final mass** '0' (i.e. stops after complete solidification)



In **equilibrium cooling** the **cooling step** ('10') defines the pages displayed in the ***Results Window***. (i.e. every 10 degrees).

The **cooling step** has no effect on the transitions or when 100% solidification is attained.

Enter default starting temperature '1650' – applied when **T-auto** is not used

FeO-MnO : Equilibrium cooling – Summary and Transitions

Results - Equilib Summary (page-1/13)

Output Edit Show Pages

Summary

(mol) Vol(litre)

1550 C | 1540 C | 1530 C | 1529.11 C |

- Summary - | Transitions | 1630 C | 1620.23 C | 1620 C | 1610 C | 1600 C | 1590 C | 1580 C | 1570 C | 1560 C |

```
CONSTITUENTS AND PHASES AT 1529.11 C
(temperature of final disappearance of Slag-l
CONS.  PHASE                          TOTAL AMT/mol
  1    1 Monoxide                       2.0000E+00

('Double-Click' on any phase listed above to

SUMMARY OF REACTIONS

Cooling
1630 to 1620.23 C        (DELTA H = -6.3525E+02
Slag-liquid cooling

Constituent 1
1620.23 to 1529.11 C     (DELTA H = -4.7017E+04
Slag-liquid -> Monoxide

COMPOSITION OF PHASES IN CONSTITUENTS AT 1529
(temperature of final disappearance of Slag-l

Constituent 1
Monoxide
                                MOLE FRACTION  MA
Fe                                2.5000E-01
Mn                                2.5000E-01
O                                 5.0000E-01
                                TOTAL AMT/mol  TO
                                  2.0000E+00
```

Results - Equilib Transitions (page 0/13)

Output Edit Show Pages

Transitions

Vol(litre)

1550 C | 1540 C | 1530 C | 1529.11 C |

Summary | - Transitions - | 1630 C | 1620.23 C | 1620 C | 1610 C | 1600 C | 1590 C | 1580 C | 1570 C | 1560 C |

```
Temperature of transition -> 1620.23 C

EQUILIBRIUM COMPOSITION OF PHASES
Slag-liquid
                                MOLE FRACTION  MASS FRACTION
Fe                                2.5000E-01     3.9112E-01
Mn                                2.5000E-01     3.8477E-01
O                                 5.0000E-01     2.2411E-01
                                TOTAL AMT/mol  TOTAL AMT/gram
                                  2.0000E+00     7.1391E+01

-------------------------------------------------------------

Temperature of final disappearance of Slag-liquid -> 1529.11 C

EQUILIBRIUM COMPOSITION OF PHASES
Monoxide
                                MOLE FRACTION  MASS FRACTION
Fe                                2.5000E-01     3.9112E-01
Mn                                2.5000E-01     3.8477E-01
O                                 5.0000E-01     2.2411E-01
                                TOTAL AMT/mol  TOTAL AMT/gram
                                  2.0000E+00     7.1391E+01

AVERAGE COMPOSITION OF ALL PRODUCT PHASES TAKEN TOGETHER
                                MOLE FRACTION  MASS FRACTION
Fe                                2.5000E-01     3.9112E-01
Mn                                2.5000E-01     3.8477E-01
O                                 5.0000E-01     2.2411E-01
```

FeO-MnO : Equilibrium cooling - Liquidus and Solidus

Results - Equilib 1620.23 C (page 2/13)

Output Edit Show Pages

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

1550 C | 1540 C | 1530 C | 1529.11 C | Summary | Transitions | 1630 C | - 1620.23 C - | 1620 C | 1610 C | 1600 C | 1590 C | 1580 C | 1570 C | 1560 C

```
<1-A> MnO +  <A> FeO =                                  [Equilibrium Cooling]

 1.0000      mol    Slag-liquid
 (71.391 gram, 1.0000 mol)
          (1620.23 C, 1 atm,      a=1.0000)
          ( 0.50000          FeO
          + 0.50000          MnO)

          System component        Mole fracti
          Fe                        0.25000
          Mn                        0.25000
          O                         0.50000

+ 0          mol    Monoxide
          (1620.23 C, 1 atm,      a=1.0000)
          ( 0.30796          FeO
          + 0.69204          MnO)

          System component        Mole fracti
          Fe                        0.15398
          Mn                        0.34602
          O                         0.50000

where "A" on the reactant side is 0.50000
```

Liquidus

Results - Equilib 1529.11 C (page 13/13)

Output Edit Show Pages

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

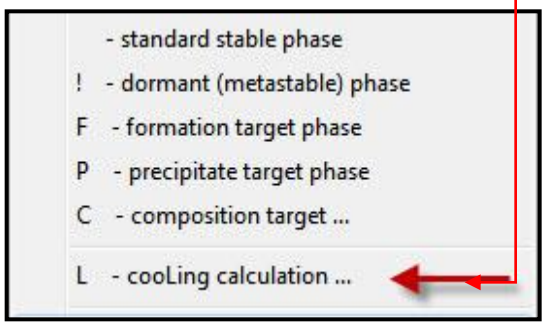
Summary | Transitions | 1630 C | 1620.23 C | 1620 C | 1610 C | 1600 C | 1590 C | 1580 C | 1570 C | 1560 C | 1550 C | 1540 C | 1530 C | - 1529.11 C -

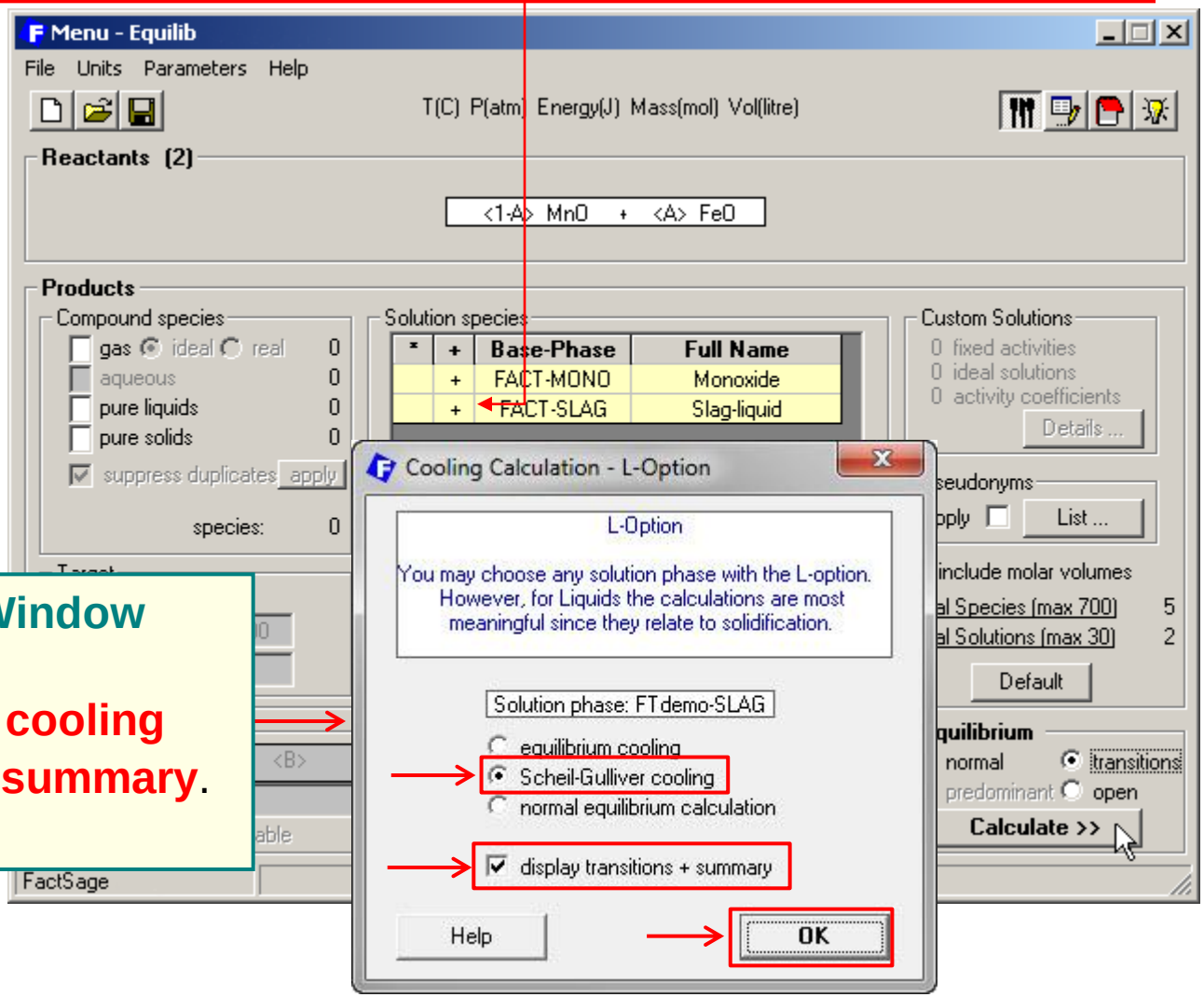
```
<1-A> MnO +  <A> FeO =                                  [Equilibrium Cooling]

 1.0000      mol    Monoxide
 (71.391 gram, 1.0000 mol)
          (1529.11 C, 1 atm,      a=1.0000)
          ( 0.50000          FeO
          + 0.50000          MnO)

          System component        Mole fraction  Mass fraction
          Fe                        0.25000        0.39112
          Mn                        0.25000        0.38477
          O                         0.50000        0.22411

+ 0          mol    Slag-liquid
          (1529.11 C, 1 atm,      a=1.0000)
          ( 0.67618          FeO
          + 0.32382          MnO)

          System component        Mole fraction  Mass fraction
          Fe                        0.33809        0.52776
          Mn                        0.16191        0.24863
          O                         0.50000        0.22361

where "A" on the reactant side is 0.50000
```

Solidus

FeO-MnO : Scheil-Gulliver cooling – L-Option

1° **Right-click** on the '+' column to open the **FACT-SLAG** extended menu and **select L– cooLing calculation**.to open the ***Cooling Calculation Window***





2° **Cooling Calculation Window**

- **select Scheil-Gulliver cooling**
- **check √ transitions + summary**.
- **click OK** to close.

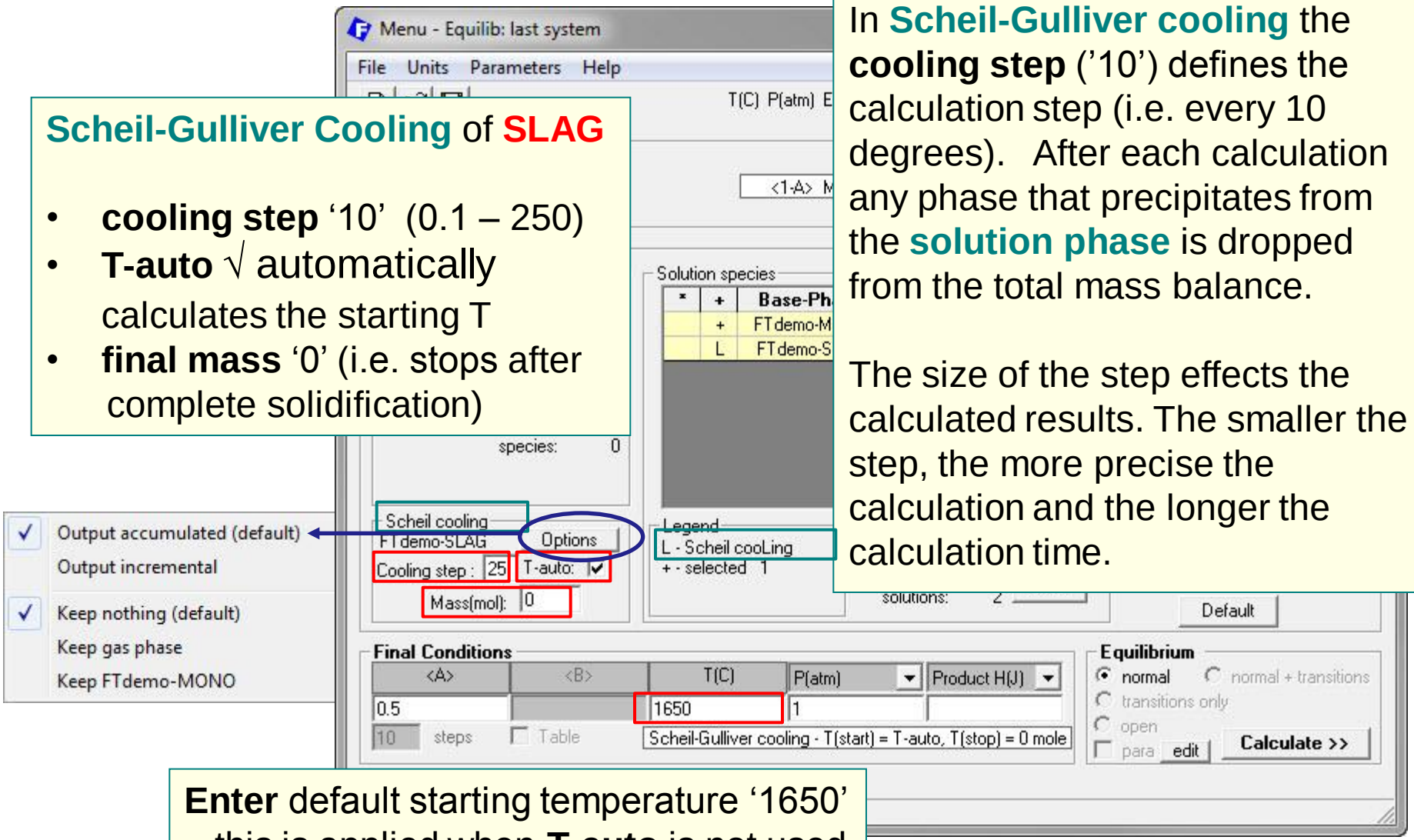
FeO-MnO : Scheil-Gulliver cooling – step, T-auto and stop

Scheil-Gulliver Cooling of SLAG

- **cooling step** '10' (0.1 – 250)
- **T-auto** √ automatically calculates the starting T
- **final mass** '0' (i.e. stops after complete solidification)

In **Scheil-Gulliver cooling** the **cooling step** ('10') defines the calculation step (i.e. every 10 degrees). After each calculation any phase that precipitates from the **solution phase** is dropped from the total mass balance.

The size of the step effects the calculated results. The smaller the step, the more precise the calculation and the longer the calculation time.



Enter default starting temperature '1650' – this is applied when **T-auto** is not used

FeO-MnO : Scheil cooling – Summary and Transitions

Results - Equilib Summary (page-1/11)

Output Edit Show Pages

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

1425 C | 1403.47 C

Summary | Transitions | 1625 C | 1620.23 C | 1600 C | 1575 C | 1550 C | 1525 C | 1500 C | 1475 C | 1450 C

```
SCHEIL-GULLIVER COOLING

CONSTITUENTS AND PHASES AT 1403.47 C
(temperature of final disappearance of Slag-liquid)
CONS.  PHASE                    TOTAL AMT/mol   TOTAL AMT
  1    1 Monoxide                 2.0000E+00      7.1391E

('Double-Click' on any phase listed above to recycle it

SUMMARY OF REACTIONS

Cooling
1625 to 1620.23 C       (DELTA H = -3.1022E+02 J)
Slag-liquid cooling

Constituent 1
1620.23 to 1403.47 C    (DELTA H = -8.5425E+03 J)
Slag-liquid -> Monoxide

COMPOSITION OF PHASES IN CONSTITUENTS AT 1403.47 C
(temperature of final disappearance of Slag-liquid)

Constituent 1
Monoxide
                            MOLE FRACTION   MASS FRACTIO
Fe                            2.5000E-01      3.9112E-01
Mn                            2.5000E-01      3.8477E-01
O                             5.0000E-01      2.2411E-01
                            TOTAL AMT/mol   TOTAL AMT/gr
```

Summary

Results - Equilib Transitions (page 0/11)

Output Edit Show Pages

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

1425 C | 1403.47 C

Summary | - Transitions - | 1625 C | 1620.23 C | 1600 C | 1575 C | 1550 C | 1525 C | 1500 C | 1475 C | 1450 C

```
Temperature of final disappearance of Slag-liquid -> 1403.47 C

AVERAGE COMPOSITION OF ALL PRODUCT PHASES TAKEN TOGETHER
                            MOLE FRACTION   MASS FRACTION
Fe                            2.5000E-01      3.9112E-01
Mn                            2.5000E-01      3.8477E-01
O                             5.0000E-01      2.2411E-01
                            TOTAL AMT/mol   TOTAL AMT/gram
                              2.0000E+00      7.1391E+01

REACTION BETWEEN 1620.23 C AND 1403.47 C

Slag-liquid -> Monoxide

Reactants
                            TOTAL AMT/mol   TOTAL AMT/gram
Slag-liquid                  -2.0000E+00     -7.1391E+01

Products (Constituent 1)
Monoxide
                            MOLE FRACTION   MASS FRACTION
Fe                            2.5000E-01      3.9112E-01
Mn                            2.5000E-01      3.8477E-01
O                             5.0000E-01      2.2411E-01
                            TOTAL AMT/mol   TOTAL AMT/gram
                              2.0000E+00      7.1391E+01

CONSTITUENTS AND PHASES AT 1403.47 C
```

Transitions

FeO-MnO : Scheil cooling – Start and Stop

Results - Equilib Summary (page-1/11)

Output Edit Show Pages

T(C) P(atm) Energy(J) Mass(mol) Vo

1425 C | 1403.47 C |

Summary | Transitions | 1625 C | 1620.23 C | 1600 C | 1575 C | 1550 C | 1525 C | 1500 C | 1475 C | 1450 C |

Start of solidification at 1620.23°C

```
SCHEIL-GULLIVER COOLING

CONSTITUENTS AND PHASES AT 1403.47 C
(temperature of final disappearance of Slag-liquid)
CONS.  PHASE                    TOTAL AMT/mol   TOTAL AMT
  1    1 Monoxide                 2.0000E+00      7.1391E

('Double-Click' on any phase listed above to recycle it

SUMMARY OF REACTIONS

Cooling
1625 to 1620.23 C       (DELTA H = -3.1022E+02 J)
Slag-liquid cooling

Constituent 1
1620.23 to 1403.47 C    (DELTA H = -8.5425E+03 J)
Slag-liquid -> Monoxide

COMPOSITION OF PHASES IN CONSTITUENTS AT 1403.47 C
(temperature of final disappearance of Slag-liquid)

Constituent 1
Monoxide
                              MOLE FRACTION   MASS FRACTIO
Fe                              2.5000E-01      3.9112E-01
Mn                              2.5000E-01      3.8477E-01
O                               5.0000E-01      2.2411E-01
                              TOTAL AMT/mol   TOTAL AMT/gr
```

Results - Equilib Transitions (page 0/11)

Output Edit Show Pages

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

1425 C | 1403.47 C |

Summary | Transitions | 1625 C | 1620.23 C | 1600 C | 1575 C | 1550 C | 1525 C | 1500 C | 1475 C | 1450 C |

```
Temperature of final disappearance of Slag-liquid -> 1403.47 C

AVERAGE COMPOSITION OF ALL PRODUCT PHASES TAKEN TOGETHER
                              MOLE FRACTION   MASS FRACTION
Fe                              2.5000E-01      3.9112E-01
Mn                              2.5000E-01      3.8477E-01
O                               5.0000E-01      2.2411E-01
                              TOTAL AMT/mol   TOTAL AMT/gram
                                2.0000E+00      7.1391E+01

REACTION BETWEEN 1620.23 C AND 1403.47 C

Slag-liquid -> Monoxide

Reactants
                              TOTAL AMT/mol   TOT
Slag-liquid                    -2.0000E+00    -7.1391E+01

Products (Constituent 1)
Monoxide
                              MOLE FRACTION   MASS FRACTION
Fe                              2.5000E-01      3.9112E-01
Mn                              2.5000E-01      3.8477E-01
O                               5.0000E-01      2.2411E-01
                              TOTAL AMT/mol   TOTAL AMT/gram
                                2.0000E+00      7.1391E+01

CONSTITUENTS AND PHASES AT 1403.47 C
```

End of solidification at 1403.47°C

FeO-MnO : Scheil cooling – incremental vs. accumulated

Incremental Scheil solidification at 1500°C

Summary | Transitions | 1625 C | 1620.23 C | 1600 C | 1575 C | 1550 C | 1525 C | - 1500 C - | 1475 C | 1450 C

[Incremental Scheil]

```
<1-A> MnO +  <A> FeO =

 0.22360    mol   Slag-liquid
 (16.010 gram, 0.22360 mol)
         (1500 C, 1 atm,      a=1.0000)
         ( 0.73123          FeO
         + 0.26877          MnO)

         System component        Mole fraction  Mass fr
         Fe                        0.36561        0.570
         Mn                        0.13439        0.206
         O                         0.50000        0.223

+ 9.6740E-02 mol   Monoxide
 (6.9129 gram, 9.6740E-02 mol)
         (1500 C, 1 atm,      a=1.0000
         ( 0.57467          FeO
         + 0.42533          MnO)

         System component        Mole fraction  Mass fr
         Fe                        0.28734        0.449
         Mn                        0.21266        0.327
         O                         0.50000        0.223

where "A" on the reactant side is 0.50000

The cutoff concentration has been specified to 1.0000E-

Mass fraction precipitated according to Scheil-Gulliver
```

- Output accumulated (default)
- Output incremental
- ✓ Keep nothing (default)
- Keep gas phase
- Keep FTdemo-MONO

- ✓ Output accumulated (default)
- Output incremental
- ✓ Keep nothing (default)
- Keep gas phase
- Keep FTdemo-MONO

Results - Equilib 1500 C (page 7/11)

Output Edit Show Pages

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

1425 C | 1403.47 C

Summary | Transitions | 1625 C | 1620.23 C | 1600 C | 1575 C | 1550 C | 1525 C | - 1500 C - | 1475 C | 1450 C

[Accumulated Scheil]

Accumulated Scheil solidification at 1500°C

```
<1-A> MnO +  <A> FeO =

 0.77640    mol   Monoxide
 (55.381 gram, 0.77640 mol)
         (1500 C, 1 atm,      a=1.0000)
         ( 0.43341          FeO
         + 0.56659          MnO)

         System component        Mole fraction  Mass fraction
         Fe                        0.21670        0.33932
         Mn                        0.28330        0.43638
         O                         0.50000        0.22430

+ 0.22360    mol   Slag-liquid
 (16.010 gram, 0.22360 mol)
         (1500 C, 1 atm,      a=1.0000)
         ( 0.73123          FeO
         + 0.26877          MnO)

         System component        Mole fraction  Mass fraction
         Fe                        0.36561        0.57032
         Mn                        0.13439        0.20623
         O                         0.50000        0.22345

where "A" on the reactant side is 0.50000

The cutoff concentration has been specified to 1.0000E-70

Mass fraction precipitated according to Scheil-Gulliver = 0.77574
```

Al-Mg-Zn : Equilibrium cooling X_{Mg}=0.8,X_{Al}=0.15,X_{Zn}=0.05

Al-Mg-Zn polythermal liquidus projection calculated by ***Phase Diagram*** with data taken from **FTlite – FACT light alloy databases**

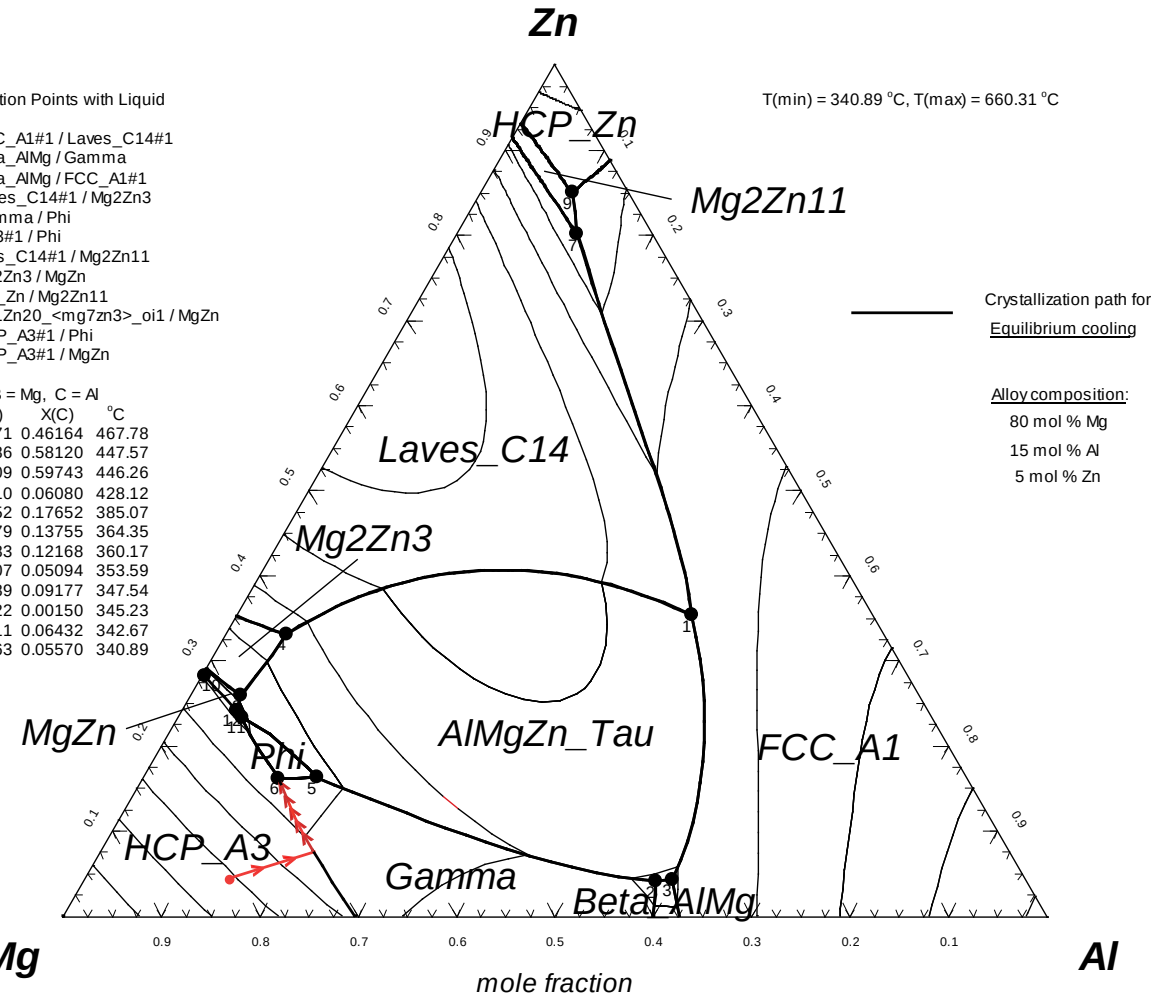
Four-Phase Intersection Points with Liquid

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

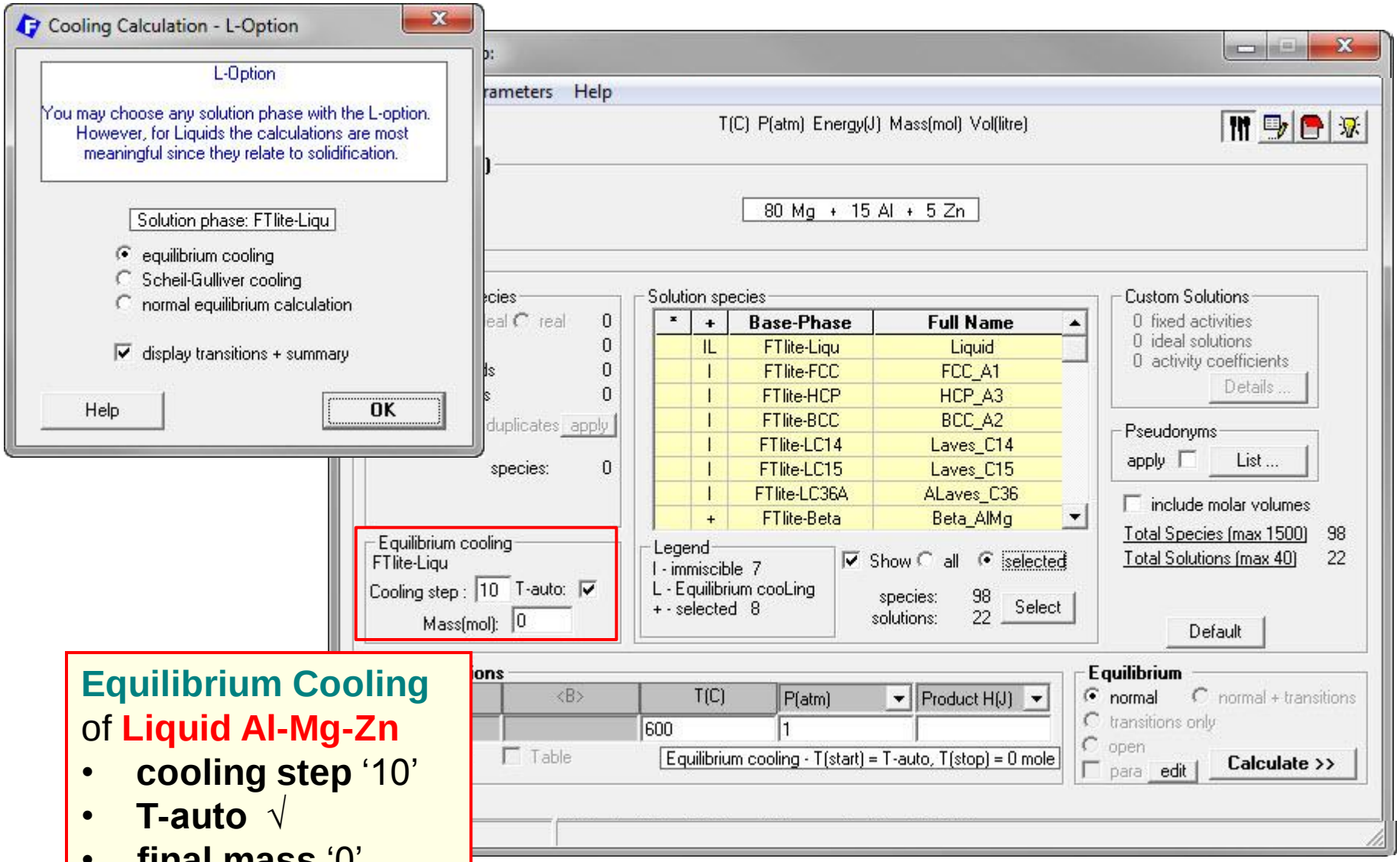
T(min) = 340.89 °C, T(max) = 660.31 °C



Crystallization path for Equilibrium cooling

Alloy composition:
80 mol % Mg
15 mol % Al
5 mol % Zn

Al-Mg-Zn : Equilibium cooling – L-Option



Equilibrium Cooling
of **Liquid Al-Mg-Zn**

- **cooling step** '10'
- **T-auto** √
- **final mass** '0'

Al-Mg-Zn : Equilibium cooling – Summary of Results

Results - Equilib Summary (page-1/18)

Output Edit Show Pages

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

420 C | 410 C | 404.48 C | 400 C | 390 C | 380 C | 370 C | 364.35 C | 364.35 C

Summary | Transitions | 500 C | 497.61 C | 490 C | 480 C | 470 C | 460 C | 450 C | 440 C | 430 C

```
SUMMARY OF REACTIONS

Cooling
500 to 497.61 C        (DELTA H = -7.4229E+03 J)
Liquid cooling

Constituent 1
497.61 to 404.48 C     (DELTA H = -5.8385E+05 J)
Liquid -> HCP_A3

Constituent 2
404.48 to 364.35 C     (DELTA H = -4.2933E+05 J)
Liquid -> HCP_A3 + Gamma

Constituent 3
364.35 C (isothermal)  (DELTA H = -9.9422E+04 J)
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                            1.6531E-02     4.2984E-02
Al                            5.9743E-02     6.4109E-02
Mg                            9.2373E-01     8.9291E-01
                            TOTAL AMT/mol  TOTAL AMT/gram
```

Al-Mg-Zn : Equilibium cooling – Plot Results

Results - Equilib Summary (page-1/18)

Output Edit Show Pages

Save or Print
Plot
Equilib Results file
Stream File
Format
Fact-XML
Fact-Optimal
Fact-Function-Builder
Refresh ...

Plot Results ...
Repeat Plot - gram vs T(C) ...

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

430 C

```
Liquid -> HCP_A3 + Gamma

Constituent 3
364.35 C (isothermal)   (DELT
Liquid + Gamma -> HCP_A3 + P

COMPOSITION OF PHASES IN CON
(temperature of final disapp

Constituent 1
HCP_A3

Zn
Al
Mg
```

Plot: gram vs T(C)

File Help

80 Mg + 15 Al + 5 Zn

Axes	Variables	Minimum	Maximum
	activity	0	1.
	mole	0	
	mole fract.	0	
Y-axis	gram	0	
	weight %	0	
	Alpha	0	
X-axis	T(C)	364.35	
	P(atm)	1.	
	Cp(J)	3098.2	
	G(J)	-3.5780E	
	Vol(litre)	0	
	H(J)	8.3791E	
	V(litre)	0	
	S(J)	5542.8	
	- page -	1.	

Axes: gram vs T(C)

Y-variable X-variable Swap Axes

Y-axis		X-axis	
gram		T(C)	
maximum	2000	maximum	500
minimum	0	minimum	360
tick every	250	tick every	10

Cancel Refresh OK

Axes: gram vs T(C) | Species: 0 selected | Select | Repeat | Axes

Graph: Labels size: 9 no: 9 — chemical / integer # / none

color / reactants / file name — full screen / Viewer / Figure

Plot >>

Al-Mg-Zn : Equilibium cooling – Plot Results

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)

File Show

+	#	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.

Mass: mole / gram

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

source

Select Top 15

4 species selected

Clear

Refresh

OK

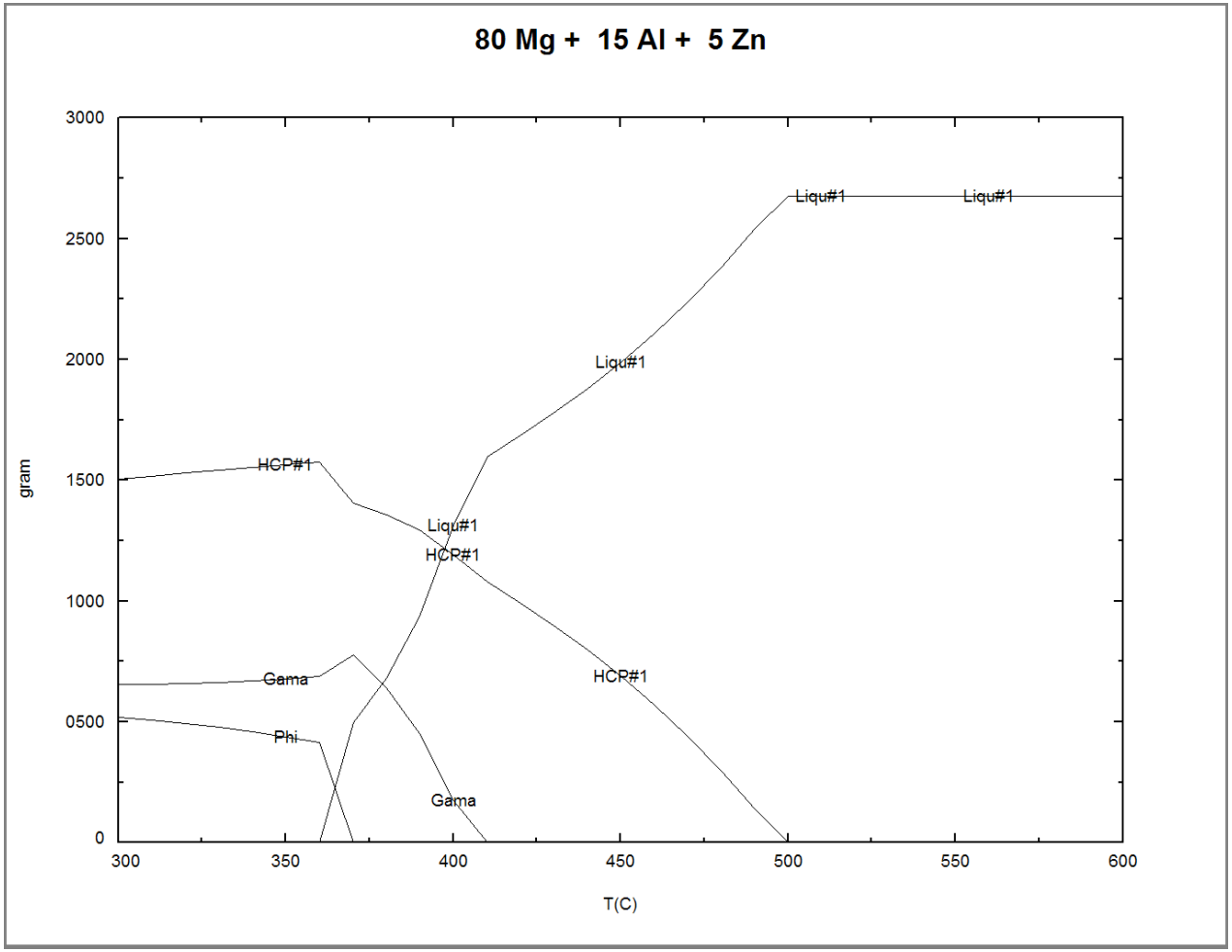
Click on the "+" column to add or remove species.

Al-Mg-Zn : Equilibium cooling – Plot Results

Liquidus at about 500 °C

Univariant at about 400 °C

??? reaction at about 300 °C



Al-Mg-Zn : Scheil cooling X_{Mg}=0.8,X_{Al}=0.15,X_{Zn}=0.05

Al-Mg-Zn polythermal liquidus projection calculated by ***Phase Diagram*** with data taken from **FTlite – FACT light alloy databases**

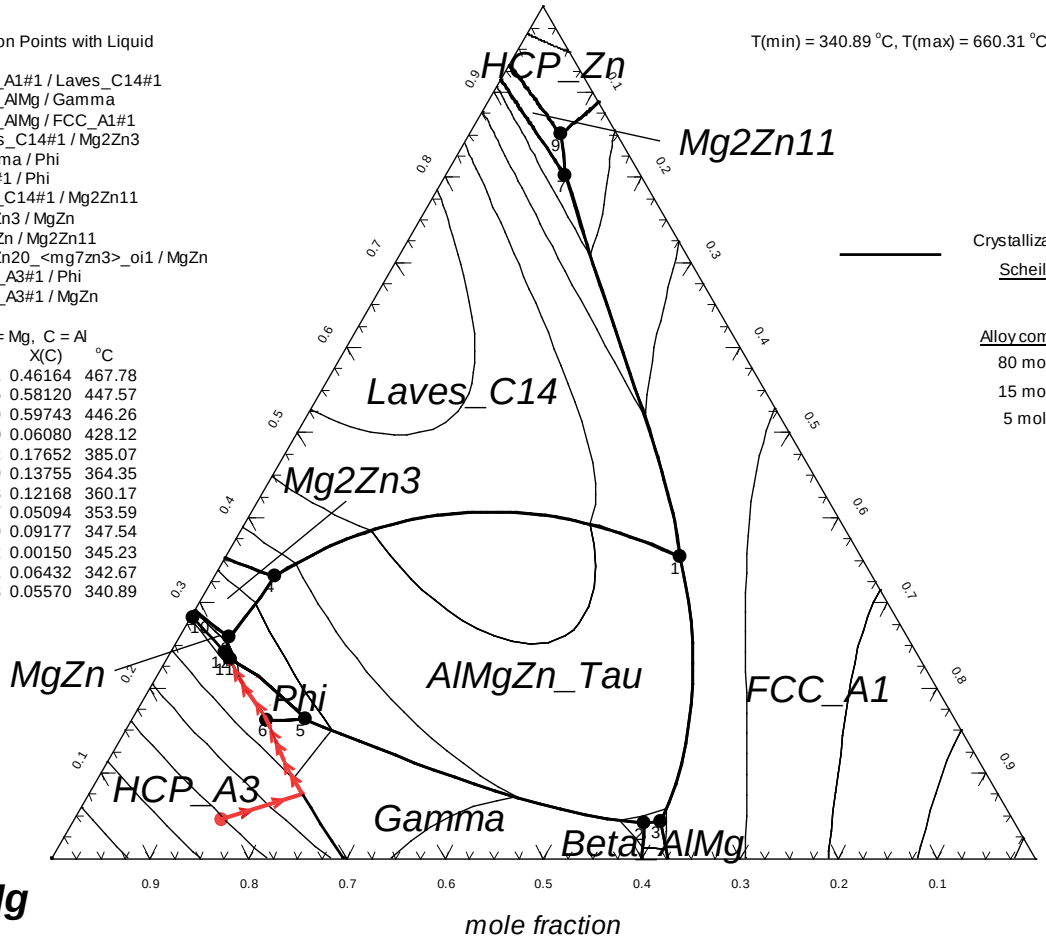
Four-Phase Intersection Points with Liquid

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

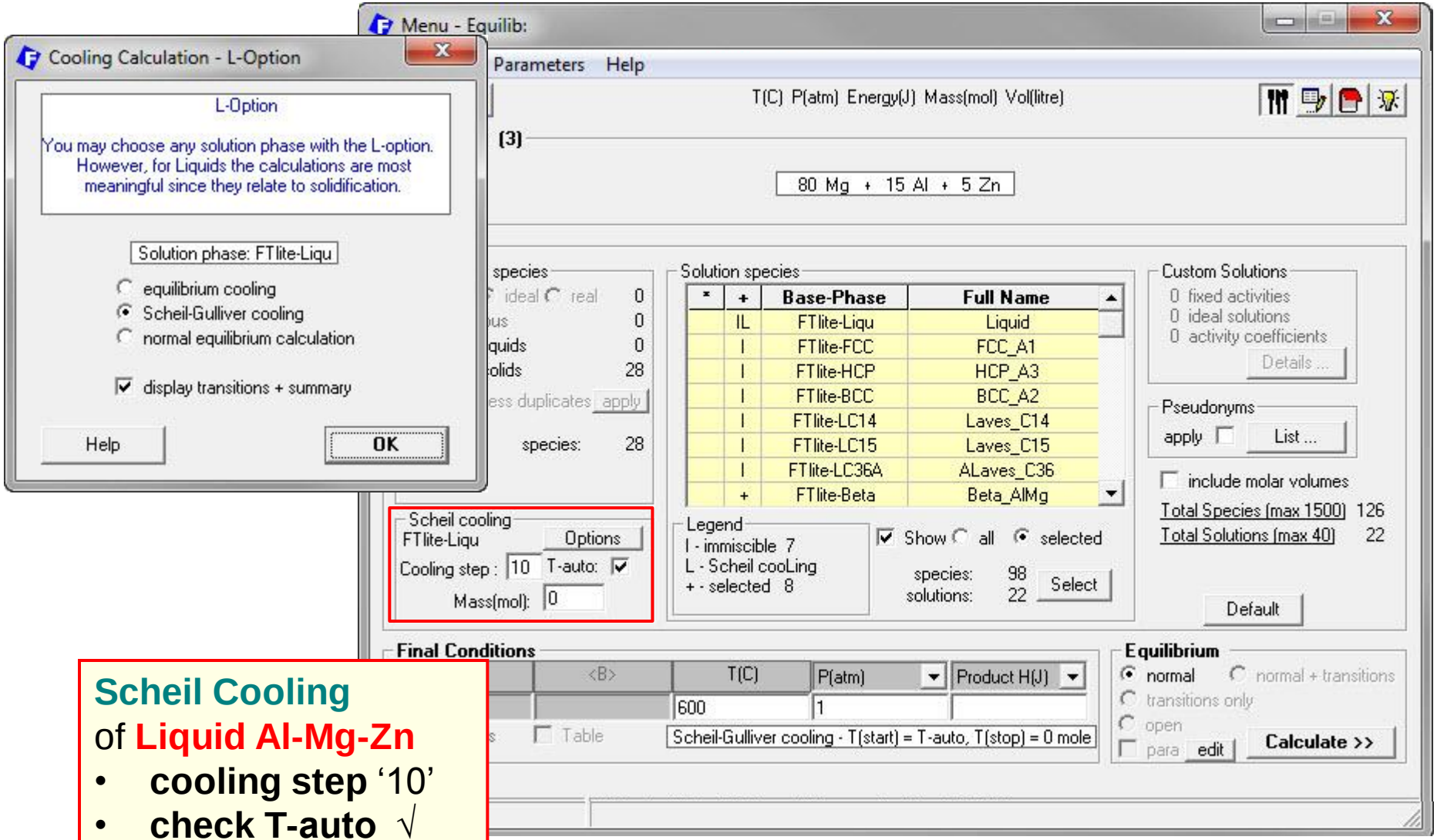
T(min) = 340.89 °C, T(max) = 660.31 °C



Crystallization path for Scheil cooling

Alloy composition:
80 mol % Mg
15 mol % Al
5 mol % Zn

Al-Mg-Zn : Scheil-Gulliver cooling – L-Option

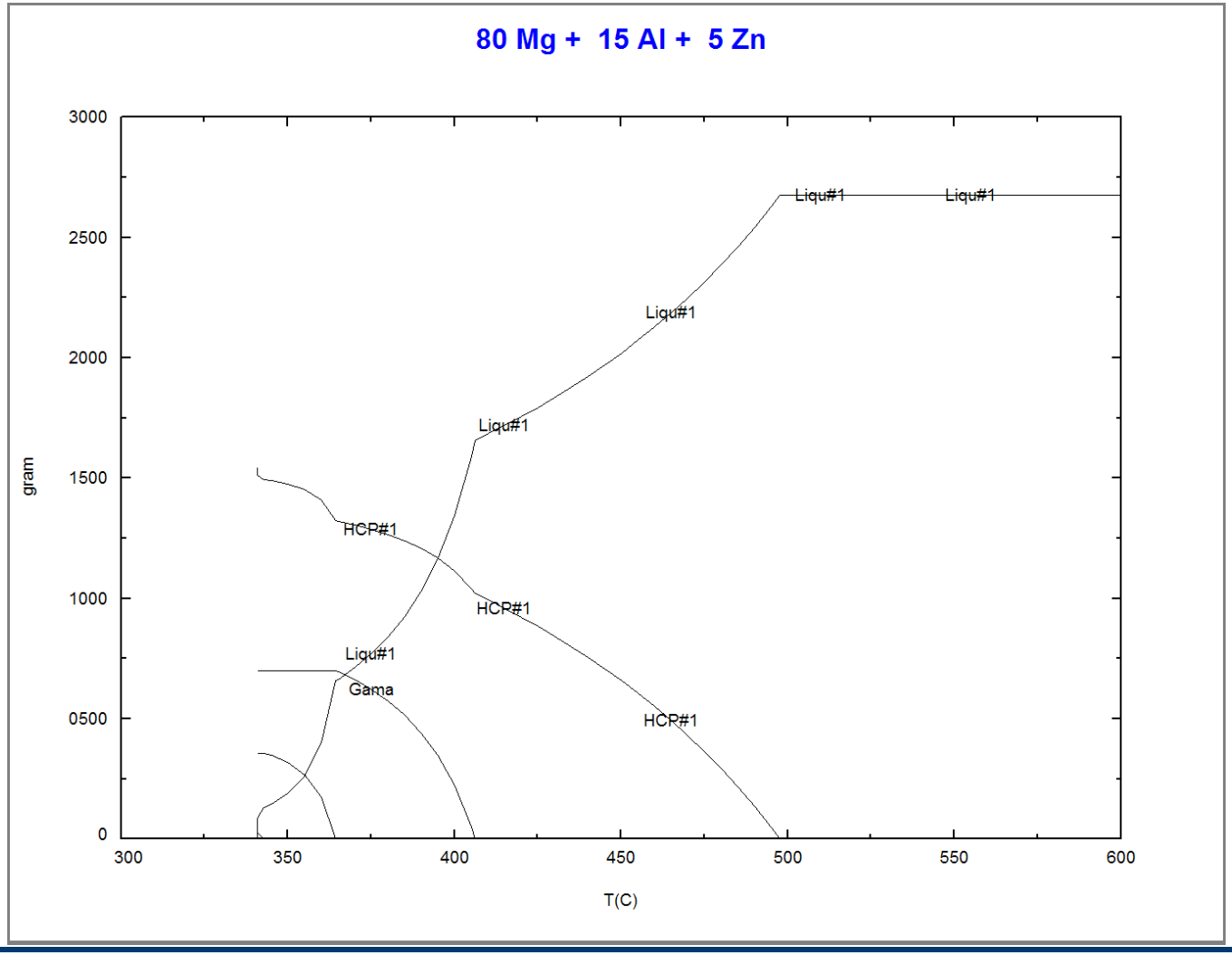


Scheil Cooling
of **Liquid Al-Mg-Zn**

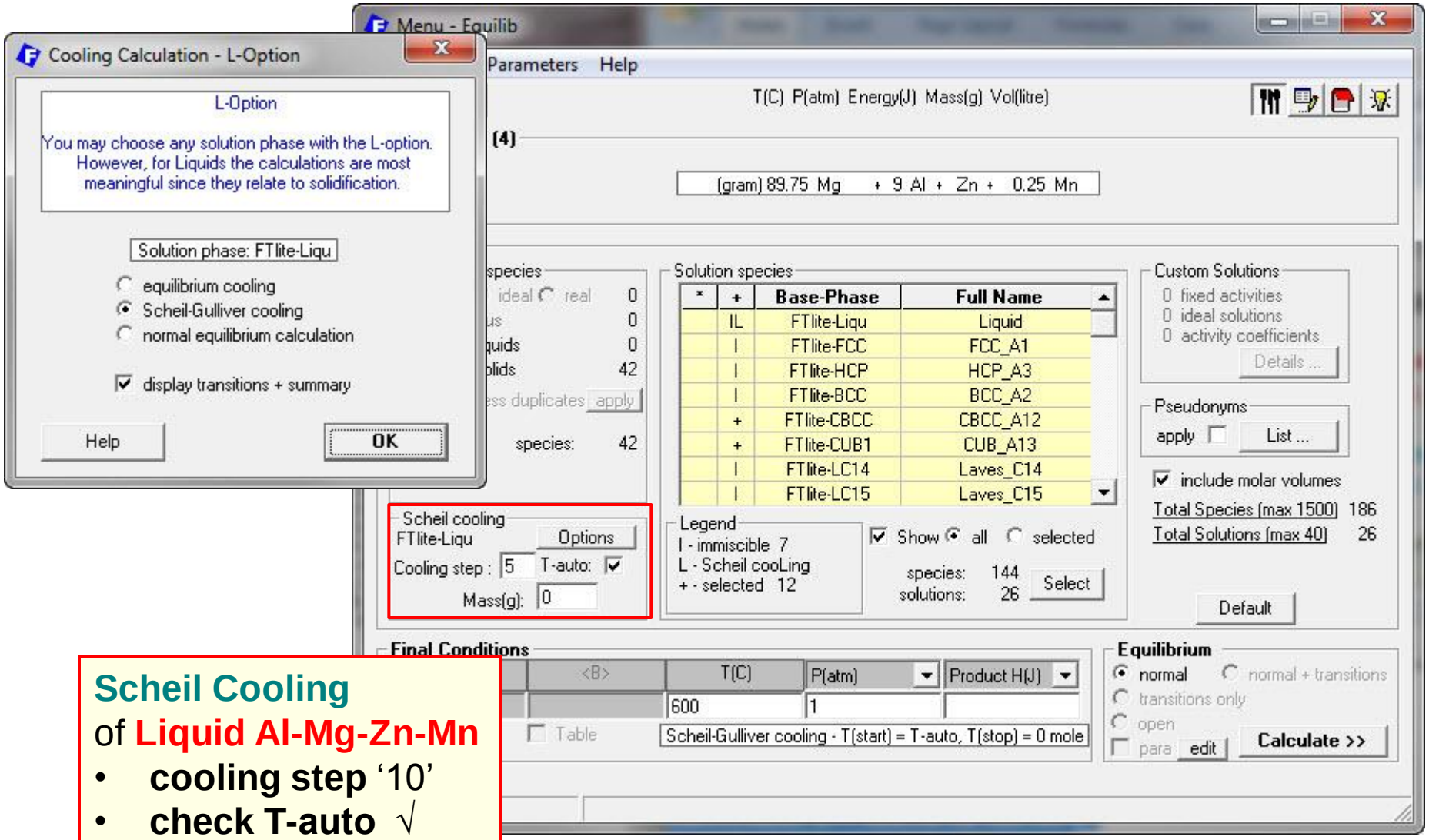
- **cooling step** '10'
- **check T-auto** √
- **enter final mass** '0'

Graphical output of Scheil target calculation

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



Al-Mg-Zn-Mn : Scheil cooling AZ91 + 0.25 wt.% Mn alloy



Scheil Cooling
of **Liquid Al-Mg-Zn-Mn**

- **cooling step** '10'
- **check T-auto** √
- **enter final mass** '0'

Al-Mg-Zn-Mn : Scheil cooling – Summary and Transitions

AZ91 + 0.25 wt.% Mn alloy:

89.75Al-9Mg-Zn-0.25Mg (wt%)

Results - Equilib Summary (page-1/60)

Output Edit Show Pages

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

510 C | 505 C | 500 C |

560 C | 555 C | 550 C | 545 C | 540 C | 535 C | 530 C | 525 C | 524.12 C | 520 C | 515 C |

- Summary - | Transitions | 595 C | 594.16 C | 594.07 C | 590 C | 585 C | 580 C | 575 C | 570 C | 565 C |

Summary

```
SCHEIL-GULLIVER COOLING

CONSTITUENTS AND PHASES AT 340.89 C
(temperature of final disappearance of Liquid)
CONS.  PHASE                          TOTAL AMT/mol   TOTAL AMT/gram
  1    1 Al8Mn5_D810                   1.3055E-05      5.0230E-04

  2    1 HCP_A3                        2.6553E+00      6.4835E+01
  2    2 Al8Mn5_D810                   7.5208E-03      2.8466E-01

  3    1 HCP_A3                        6.3501E-01      1.5580E+01
  3    2 Mn4Al11_s1(s)                 4.2235E-03      1.4544E-01

  4    1 HCP_A3                        6.8848E-02      1.6956E+00
  4    2 MnAl4_s1(s)                   5.4346E-04      1.7702E-02

  5    1 HCP_A3                        1.9793E-01      4.8919E+00
  5    2 Gamma                         4.5374E-01      1.1829E+01
  5    3 MnAl4_s1(s)                   8.0662E-04      2.6274E-02

  6    1 HCP_A3                        7.1873E-03      1.8150E-01
  6    2 Phi                           1.0940E-02      3.7598E-01
  6    3 Mn4Al11_s1(s)                 1.3741E-06      4.7318E-05

  7    1 HCP_A3                        7.7250E-04      1.9639E-02
  7    2 AlMgZn_Tau                    6.7948E-04      2.9038E-02
  7    3 Mn4Al11_s1(s)                 3.4950E-08      1.2035E-06

  8    1 HCP_A3                        1.2677E-03      3.2228E-02
  8    2 MgZn                          9.0976E-04      3.9438E-02
```

Results - Equilib Transitions (page 0/60)

Output Edit Show Pages

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

510 C | 505 C | 500 C |

560 C | 555 C | 550 C | 545 C | 540 C | 535 C | 530 C | 525 C | 524.12 C | 520 C | 515 C |

Summary | - Transitions - | 595 C | 594.16 C | 594.07 C | 590 C | 585 C | 580 C | 575 C | 570 C | 565 C |

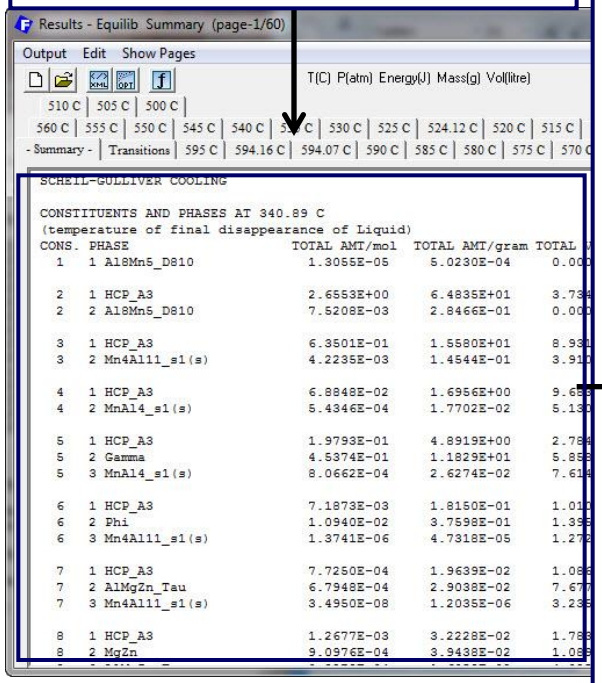
Transitions

```
SCHEIL-GULLIVER COOLING

Starting temperature -> 595 C
Cooling step -> 5 C

COMPOSITION OF Liquid
                              MOLE FRACTION   MASS FRACTION
Zn                              3.7803E-03      1.0000E-02
Mn                              1.1247E-03      2.5000E-03
Al                              8.2441E-02      9.0000E-02
Mg                              9.1265E-01      8.9750E-01
                              TOTAL AMT/mol   TOTAL AMT/gram
                                4.0461E+00      1.0000E+02

-------------------------------------------------------------

Temperature of transition -> 594.16 C

COMPOSITION OF Liquid
                              MOLE FRACTION   MASS FRACTION
Zn                              3.7803E-03      1.0000E-02
Mn                              1.1247E-03      2.5000E-03
Al                              8.2441E-02      9.0000E-02
Mg                              9.1265E-01      8.9750E-01
                              TOTAL AMT/mol   TOTAL AMT/gram
                                4.0461E+00      1.0000E+02

-------------------------------------------------------------

Temperature of transition -> 594.07 C
```

Al-Mg-Zn-Mn : Scheil cooling - Microstructure Constituents

Summary & Transitions

Microstructure constituents of AZ91 + 0.25 wt.% Mn alloy after Scheil cooling.



CONS		PHASE	TOTAL AMT/Wt.%	DESCRIPTION
1	1	Al8Mn5_D810	0.05%	Constituent 1 594.16 to 594.07 C
				Liquid -> Al8Mn5_D810
2	1	HCP_A3	6483.50%	Constituent 2 594.07 to 524.12 C
2	2	Al8Mn5_D810	28.47%	Liquid -> HCP_A3 + Al8Mn5_D810
3	1	HCP_A3	1558.00%	Constituent 3 524.12 to 447.41 C
3	2	Mn4Al11_s1(s)	14.54%	Liquid -> HCP_A3 + Mn4Al11_s1(s)
4	1	HCP_A3	169.56%	Constituent 4 447.41 to 431.70 C
4	2	MnAl4_s1(s)	1.77%	Liquid -> HCP_A3 + MnAl4_s1(s)
5	1	HCP_A3	489.19%	Constituent 5 431.70 to 364.34 C
5	2	Gamma	1182.90%	Liquid -> HCP_A3 + Gamma + MnAl4_s1(s)
5	3	MnAl4_s1(s)	2.63%	
6	1	HCP_A3	18.15%	Constituent 6 364.34 to 342.67 C
6	2	Phi	37.60%	Liquid -> HCP_A3 + Phi + Mn4Al11_s1(s)
6	3	Mn4Al11_s1(s)	0.00%	
7	1	HCP_A3	1.96%	Constituent 7 342.67 to 340.89 C
7	2	AlMgZn_Tau	2.90%	Liquid -> HCP_A3 + AlMgZn_Tau + Mn4Al11_s1(s)
7	3	Mn4Al11_s1(s)	0.00%	
8	1	HCP_A3	3.22%	
8	2	MgZn	3.94%	Constituent 8 340.89 C (isothermal)
8	3	AlMgZn_Tau	1.64%	Liquid -> HCP_A3 + MgZn + AlMgZn_Tau + Mn4Al11_s1(s)
8	4	Mn4Al11_s1(s)	0.00%	

Final disappearance of liquid at 340.89°C

- 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

Al-Mg-Zn-Mn : Selecting constituent 2 HCP phase for annealing

Results - Equilib Summary (page-1/60)

Output Edit Show Pages

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

510 C | 505 C | 500 C |

560 C | 555 C | 550 C | 545 C | 540 C | 535 C | 530 C | 525 C | 524.12 C | 520 C | 515 C |

- Summary - | Transitions | 595 C | 594.16 C | 594.07 C | 590 C | 585 C | 580 C | 575 C | 570 C | 565 C |

SCHEIL-GULLIVER COOLING

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	1.3055E-05	5.0230E-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)	4.2235E-03	1.4544E-01	3.9104E-05
				9.6839E-04
				5.1305E-06
				2.7840E-03
5	2 Gamma	4.5374E-01	1.1829E+01	5.8586E-03
5	3 MnAl4_s1(s)	8.0662E-04	2.6274E-02	7.6148E-06
6	1 HCP_A3	7.1873E-03	1.8150E-01	1.0109E-04
6	2 Phi	1.0940E-02	3.7598E-01	1.3952E-04
6	3			1.2722E-08
7	1			1.0866E-05
7	2 AlMgZn_Tau	6.7948E-04	2.9038E-02	7.6777E-06
7	3 Mn4Al11_s1(s)	3.4950E-08	1.2035E-06	3.2358E-10
8	1 HCP_A3	1.2677E-03	3.2228E-02	1.7831E-05
8	2 MgZn	9.0976E-04	3.9438E-02	1.0892E-05

1° **Point mouse** to **constituent 2 HCP_A3** and **double-click**

2° Click **OK** to recycle **HCP_A3**

FactSage 6.3: Equilib

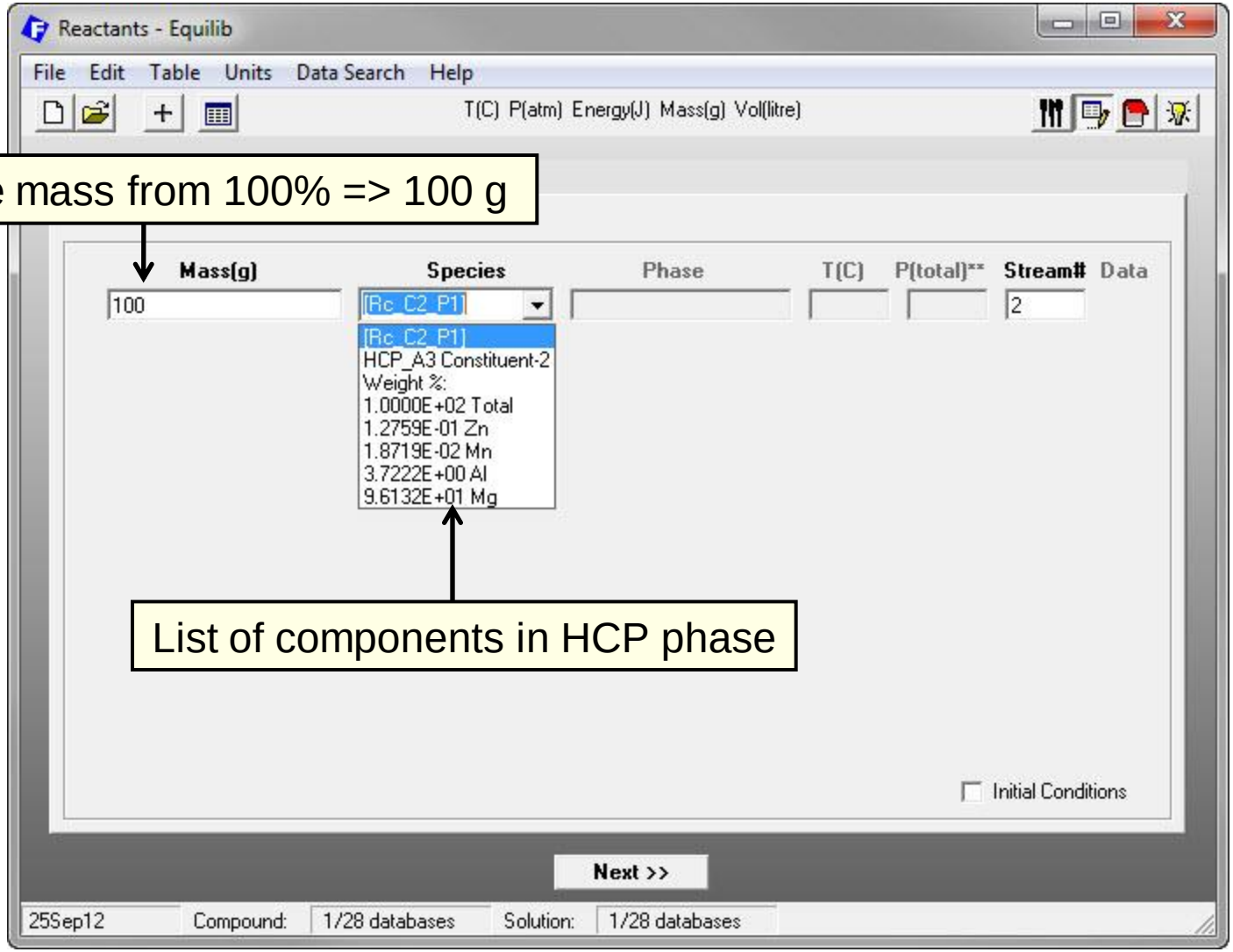
Do you wish to recycle Phase 1 of Constituent 2?

HCP_A3

	MOLE FRACTION	MASS FRACTION
Zn	4.7652E-04	1.2759E-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

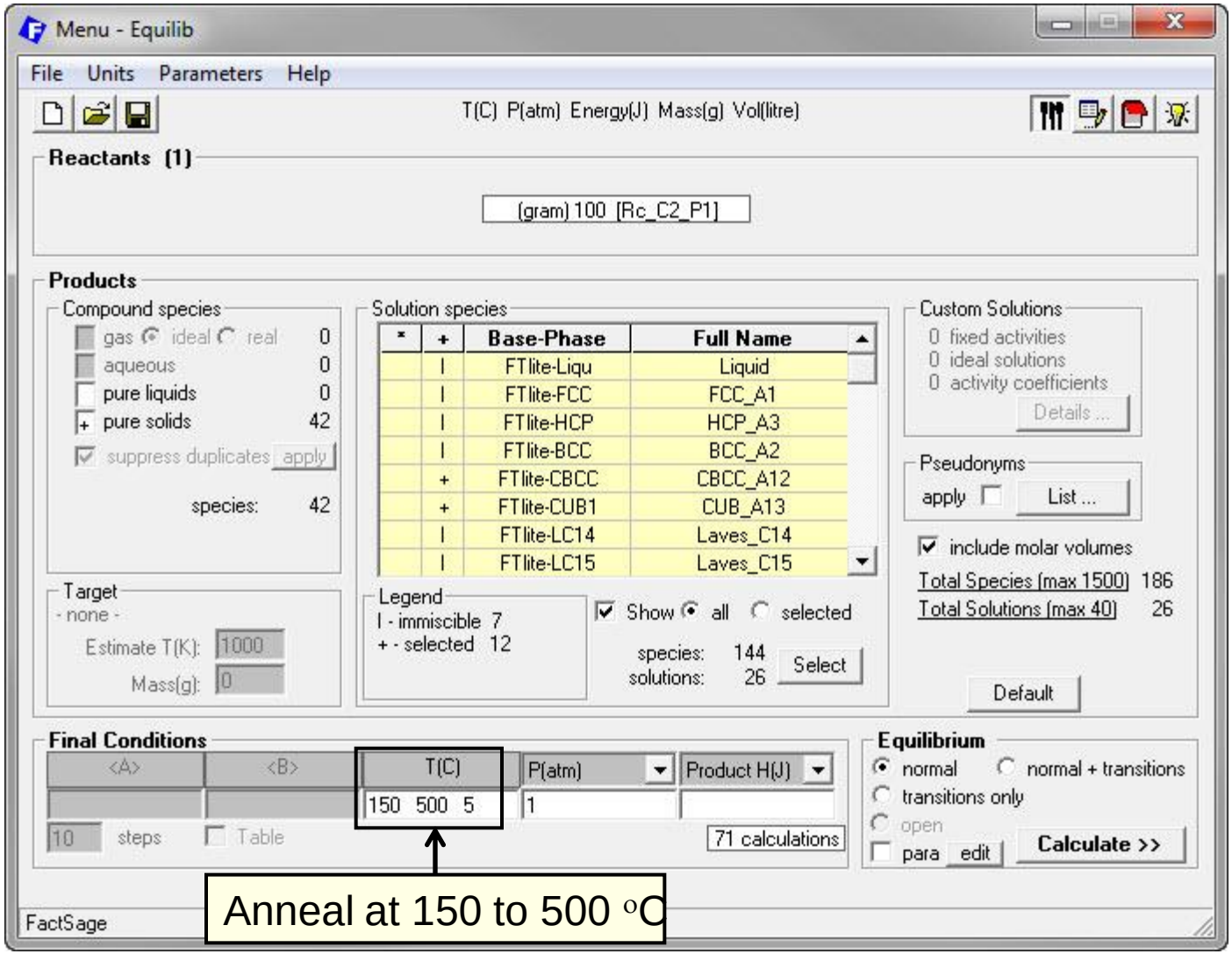
Al-Mg-Zn-Mn : HCP phase imported into *Reactant Window*



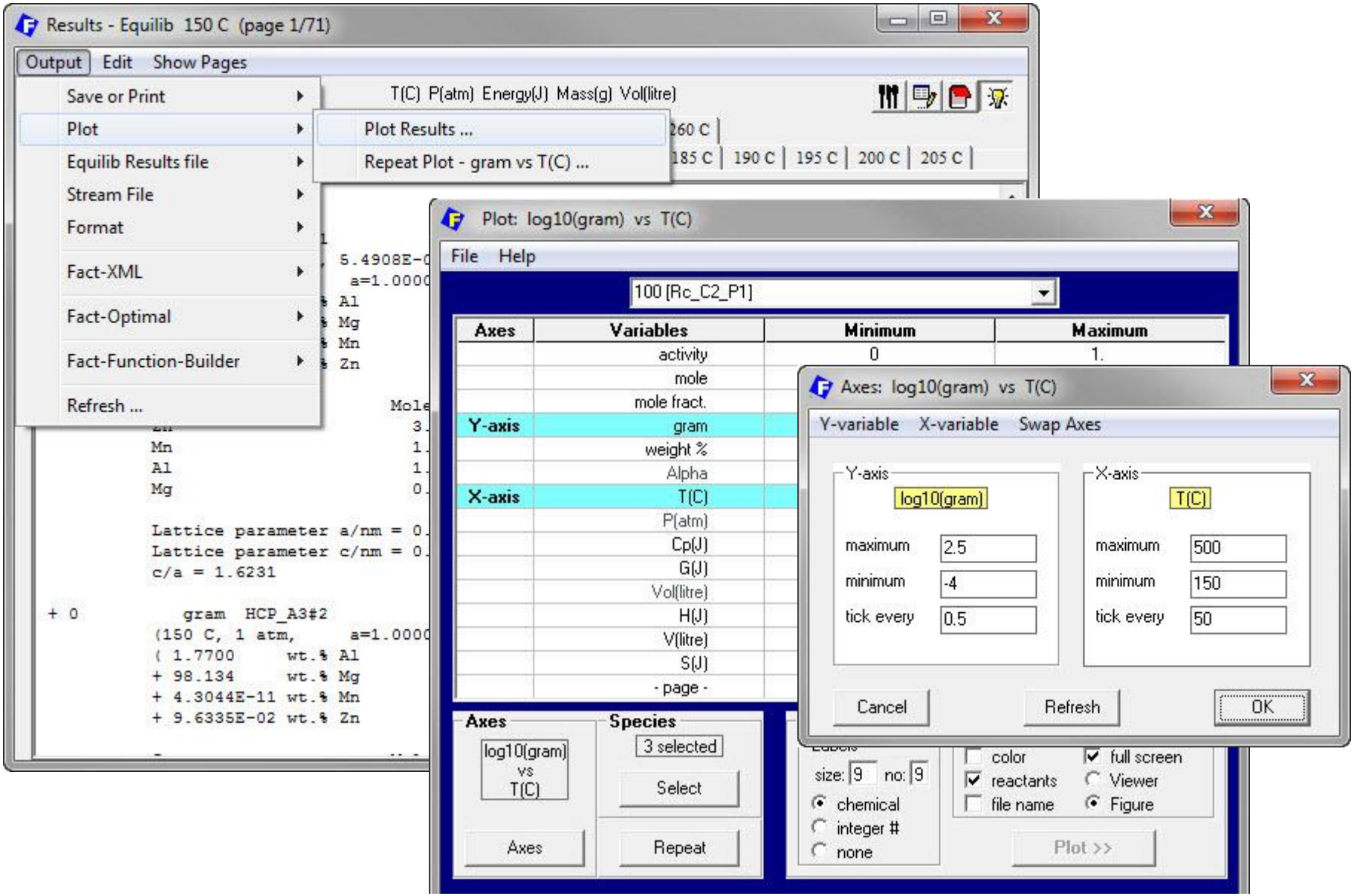
Change mass from 100% => 100 g

List of components in HCP phase

Al-Mg-Zn-Mn : Equilibrium calculation – annealing HCP phase

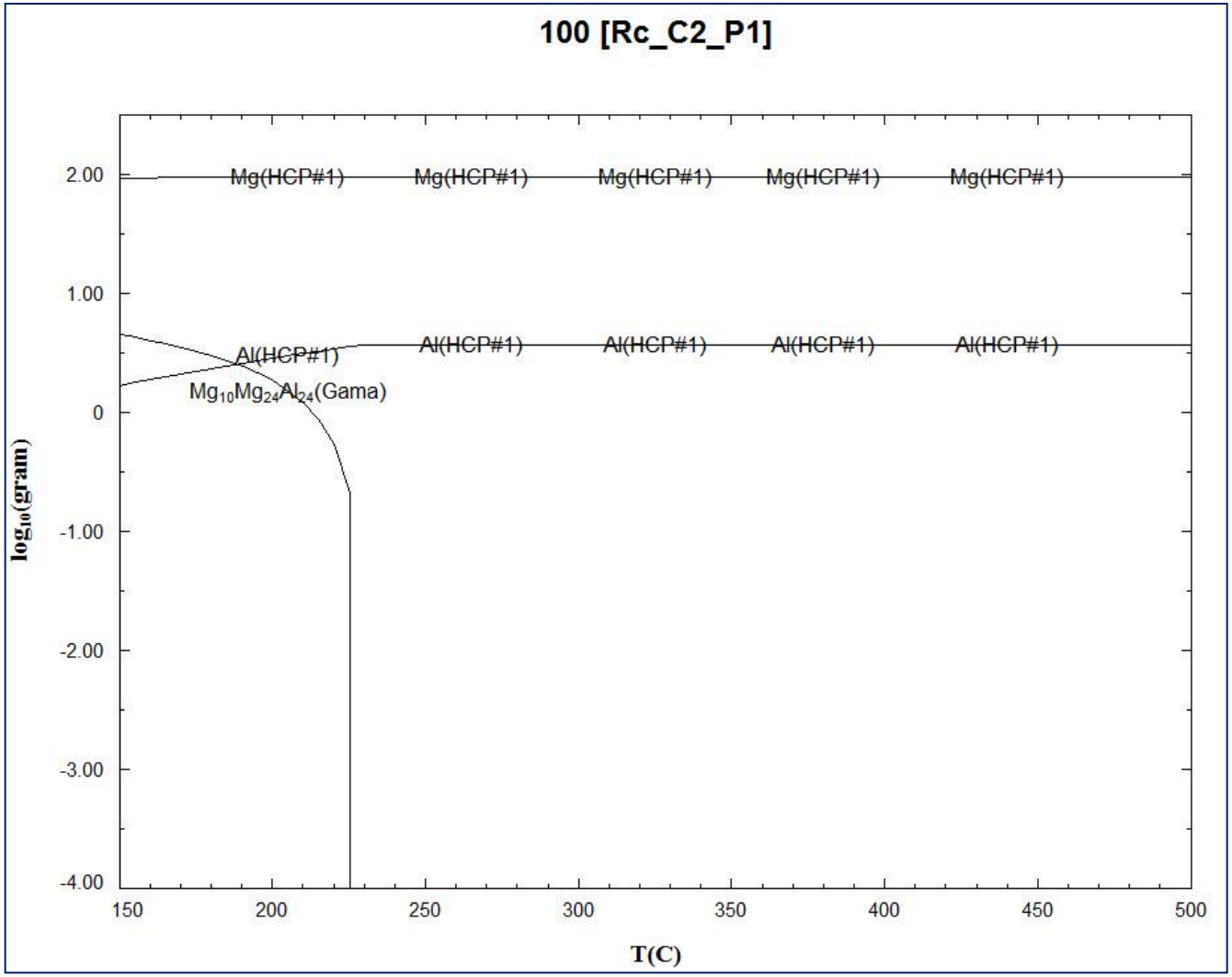


Al-Mg-Zn-Mn : Plotting annealed HCP phase

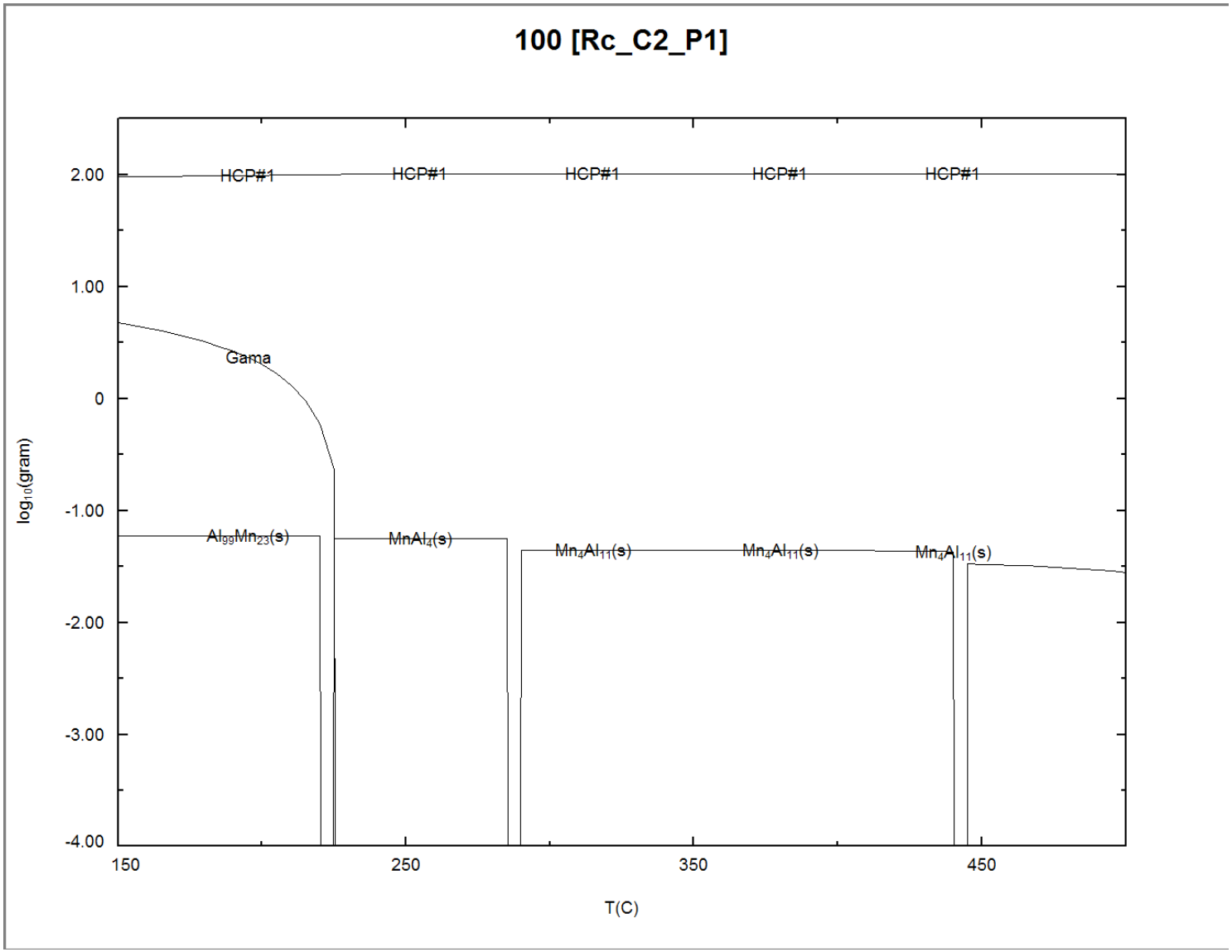


Al-Mg-Zn-Mn : Graph of annealed HCP phase

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



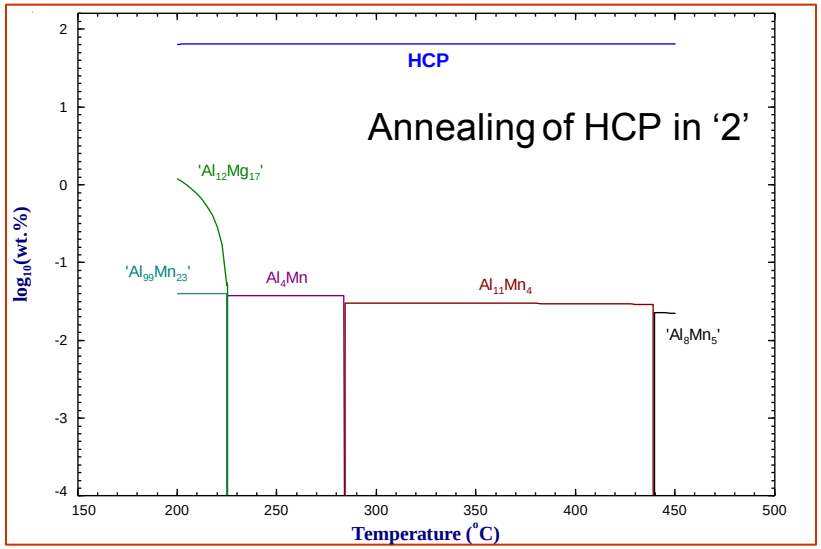
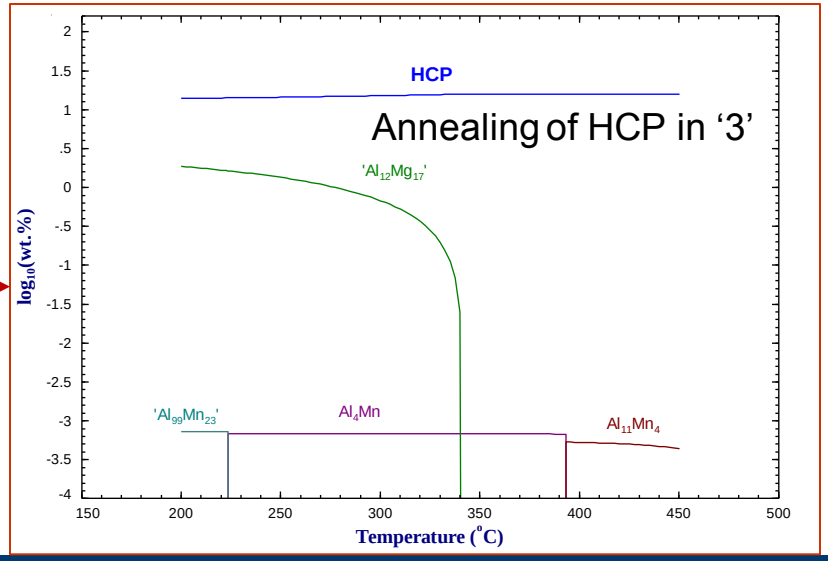
Equilibrium phase distribution in HCP phase of constituent 2 after annealing (HCP + precipitates)



- 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