MATGEN-IV
Cargèse, Corsica, France. September 27, 2007

Equilibrium Phase Diagrams

-Training Course-

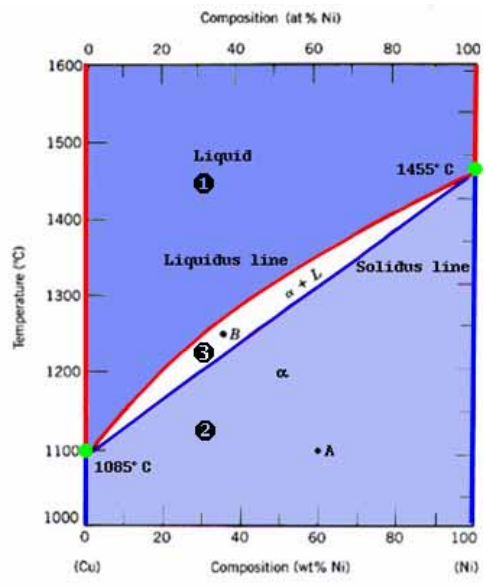
M.-N. de Noirfontaine, C. Girod Labianca, G.Inden

Part 3

Thermo-Calc software. Examples

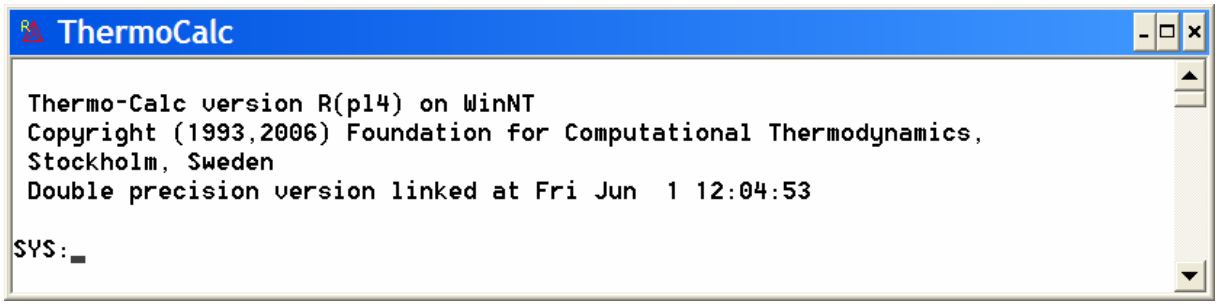
EXAMPLE 1

Calculation of the Cu-Ni phase diagram between 1000 and 1600°C

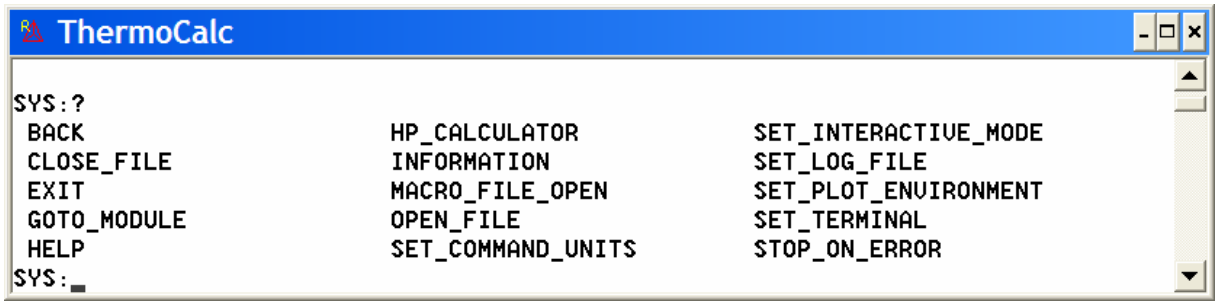


1. SELECTING THE THERMODYNAMIC FUNCTIONS OF THE SYSTEM

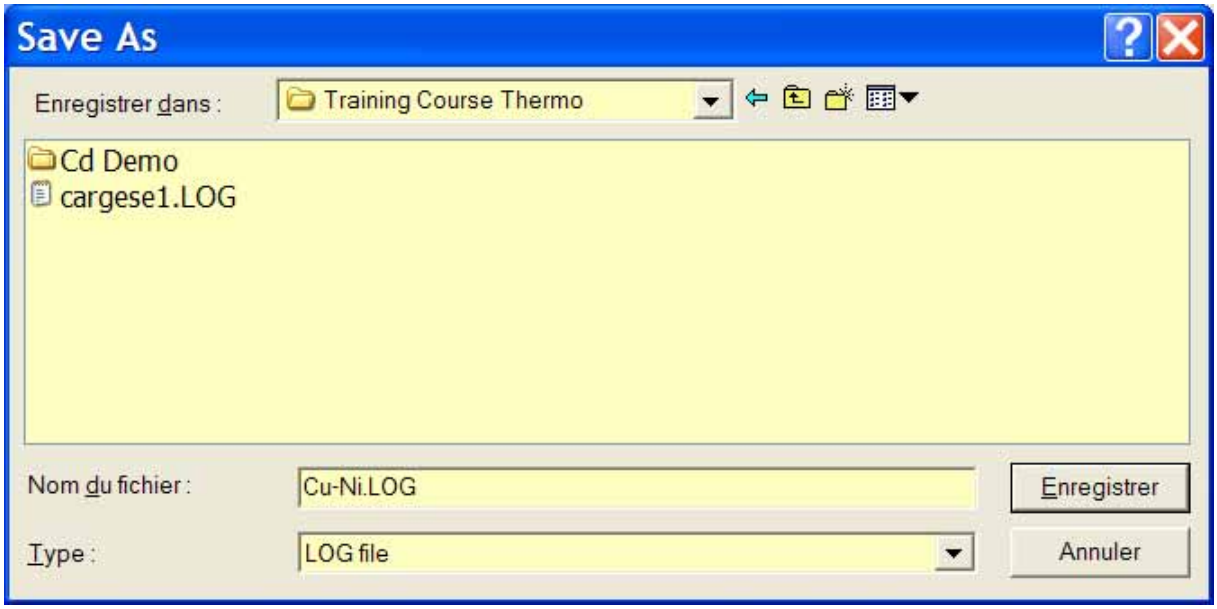
Running Thermo-Calc application: Execute “TCCR.exe”



SYS: ? (↵)
…This command lists the available commands

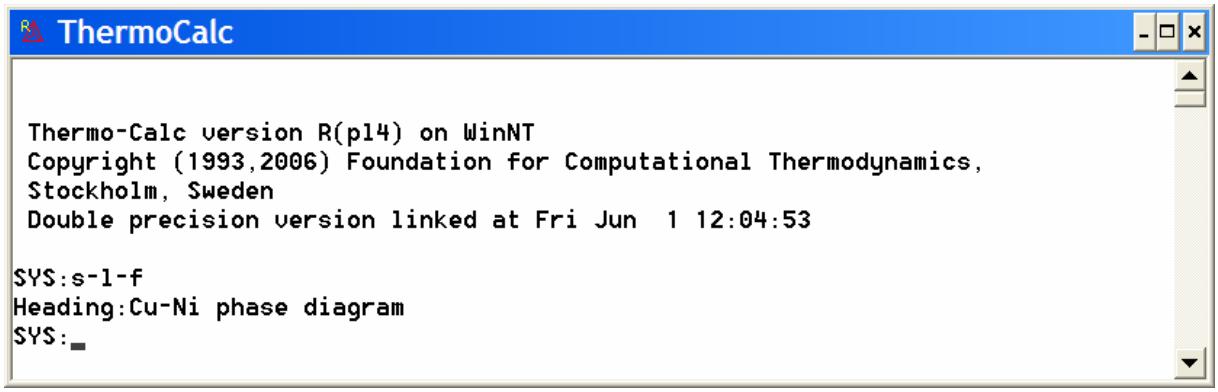


SYS: s-l-f
…This command in full is SET_LOG_FILE
…Choose the path and the name of the file



…The “Cu-Ni.LOG” file is created in the mentioned repertory.

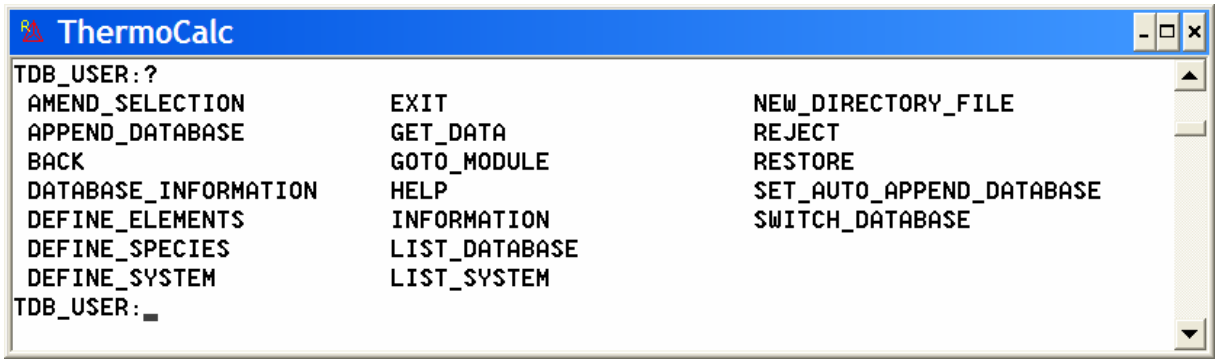
Heading: Cu-Ni phase diagram
…The heading for the Cu-Ni.LOG file



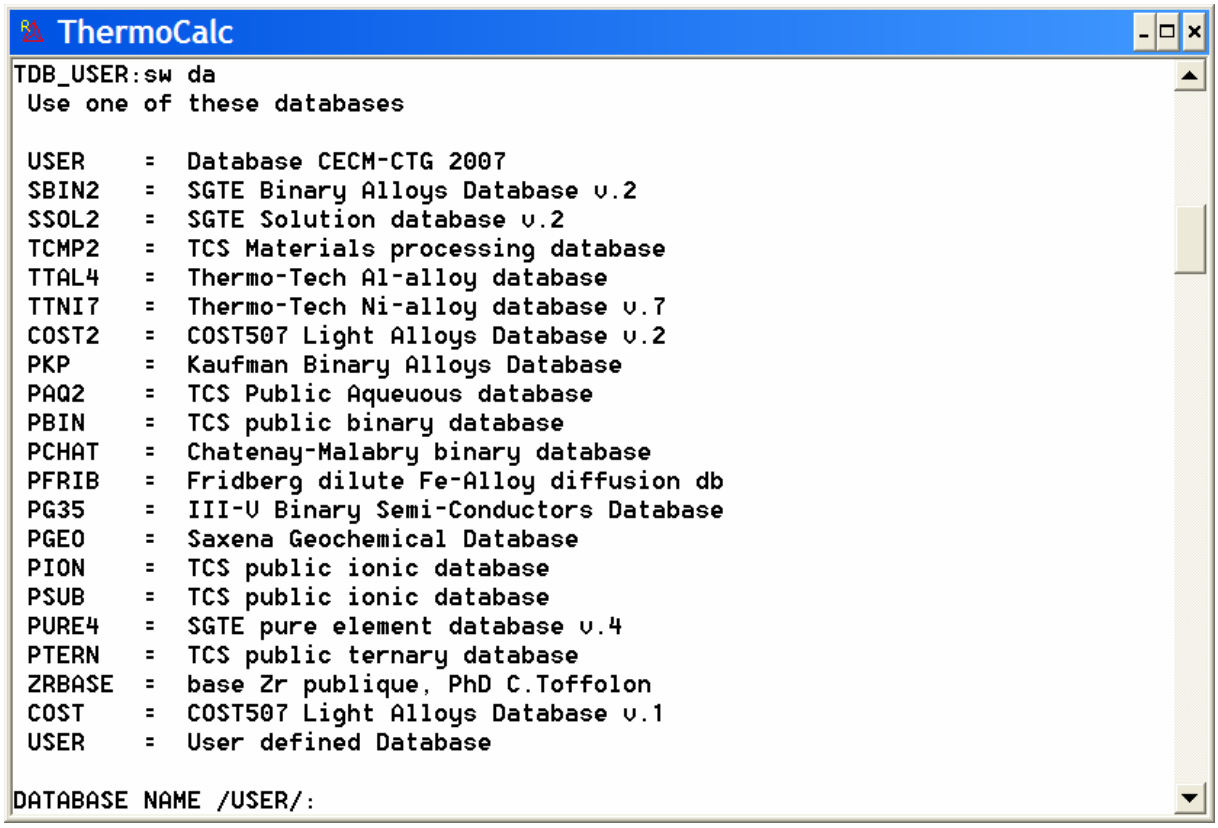
…Selection of the suitable database SSOL2:

SYS: go da
…This command in full is GOTO_MODULE DATABASE_RETRIEVAL
…Access to the **T**hermodynamic **D**ata**B**ase module (**TDB**)

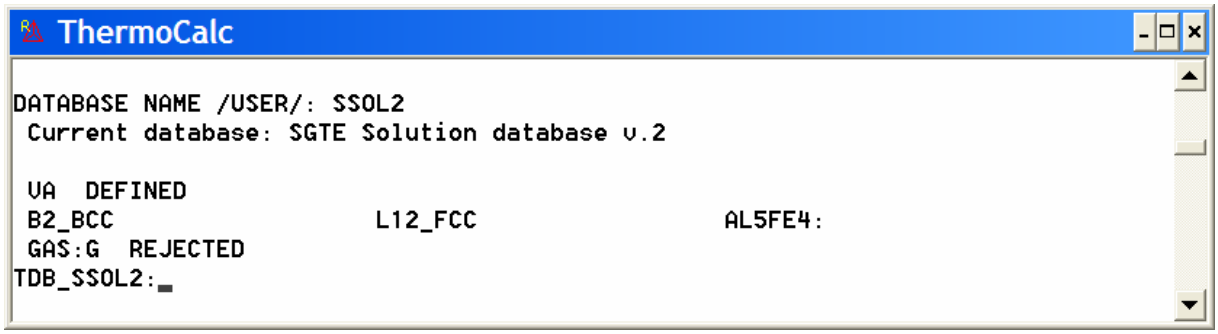
TDB-USER: ?



TDB-USER: sw da
…This command in full is SWITCH_DATABASE
…All the available databases are listed

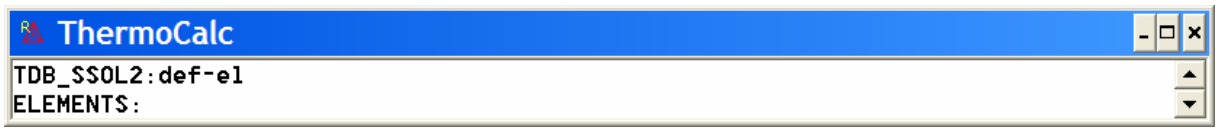


TDB-USER: SSOL2

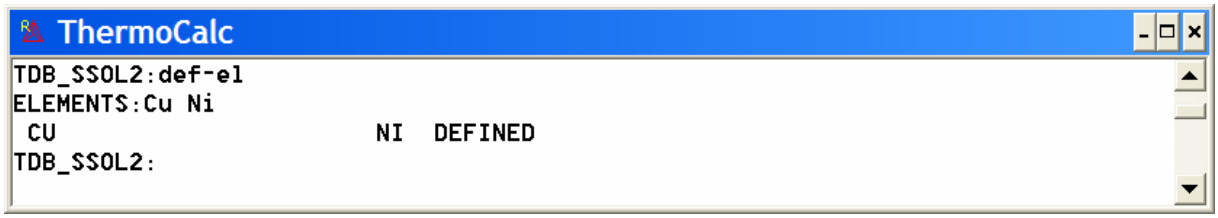


…Define the system in terms of elements: selection of Cu and Ni

TDB-SSOL2: def-el
…This command in full is DEFINE_ELEMENTS

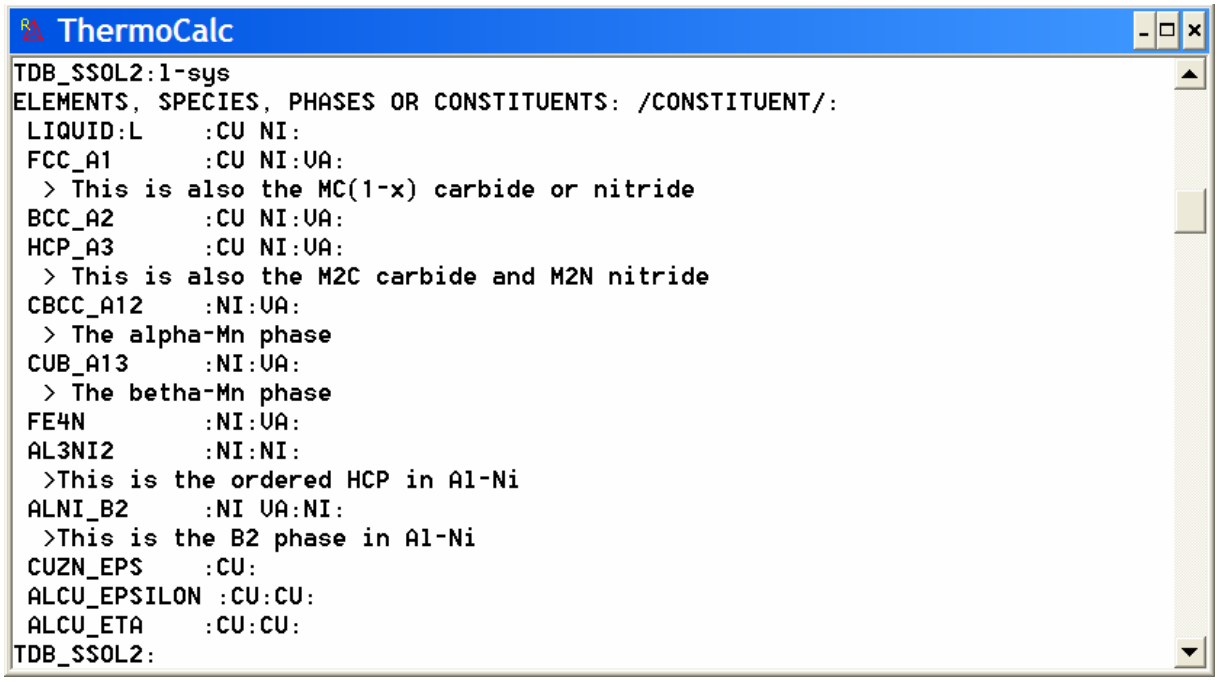


ELEMENTS: Cu Ni



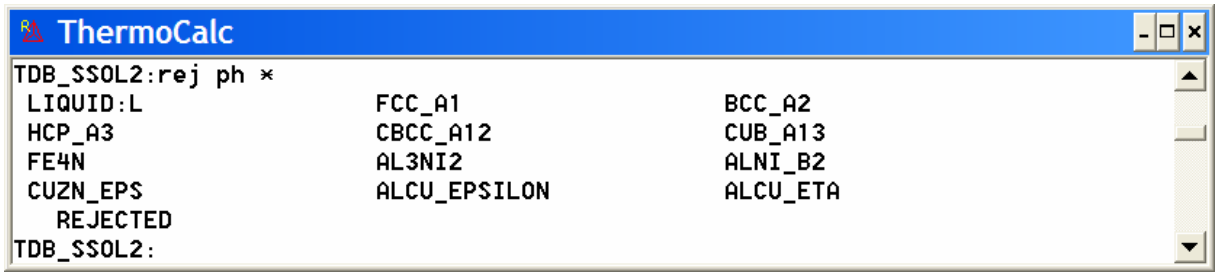
TDB-SSOL2: l-sys (↵)
…This command in full is LIST_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/ : (↵)



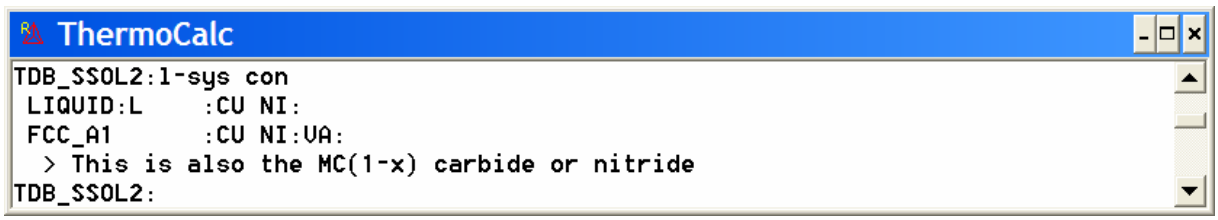
…Selection of the suitable phases of the studied system: LiQUID and FCC_A1 phases
…Reject all the phases and restore the two necessary phases, liquid and fcc

TDB-SSOL2: rej ph *
…This command in full is REJECT PHASES /ALL

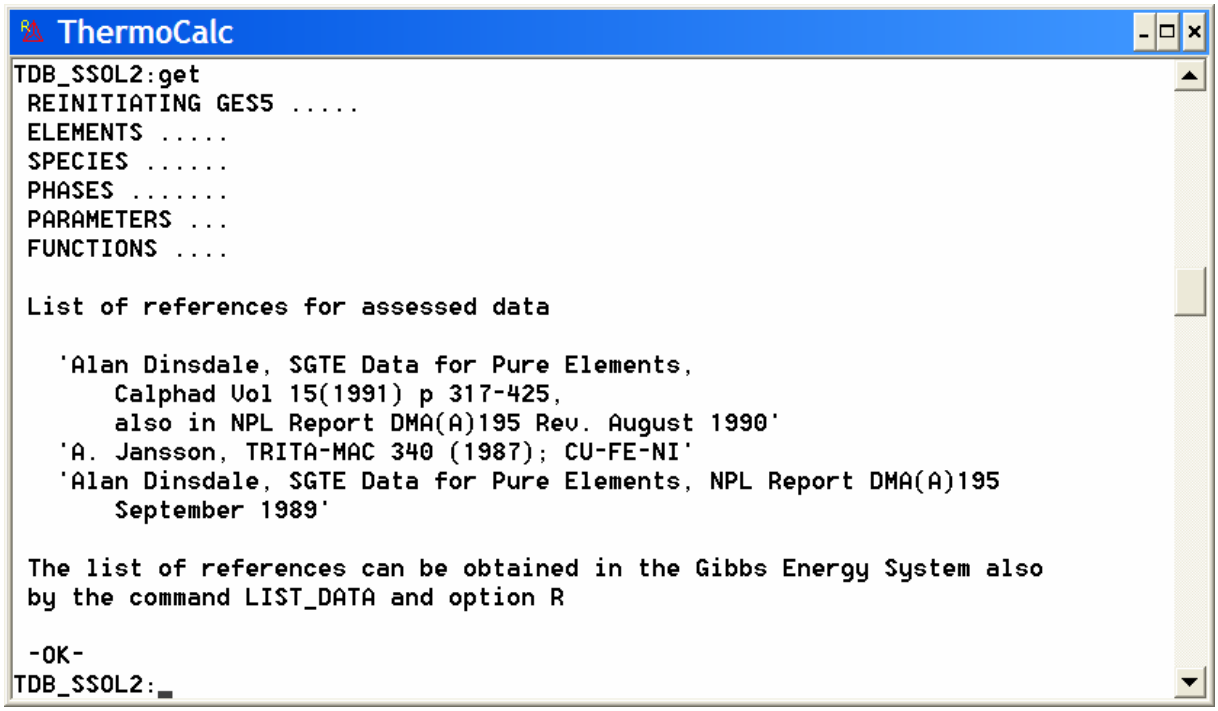


TDB-SSOL2: rest ph liquid fcc
…This command in full is RESTORE PHASES liquid fcc

TDB-SSOL2: l-sys con
…This command in full is LIST_SYSTEM CONSTITUENTS



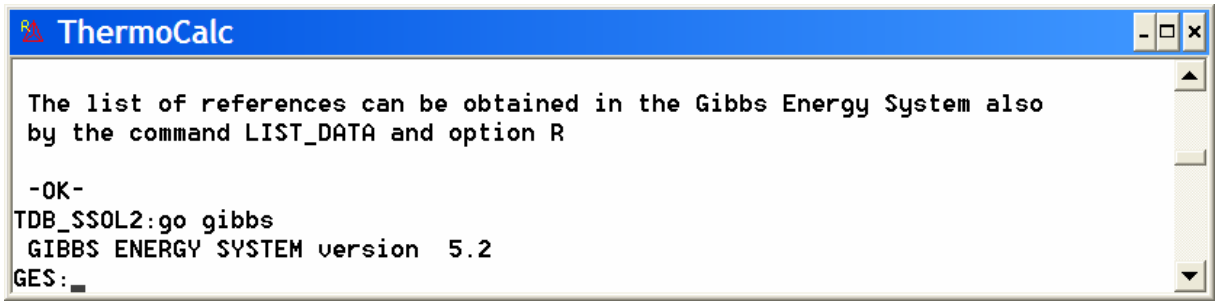
TDB-SSOL2: get
…This command in full is GET_DATA
…Retrieval of all information from the thermodynamic databank



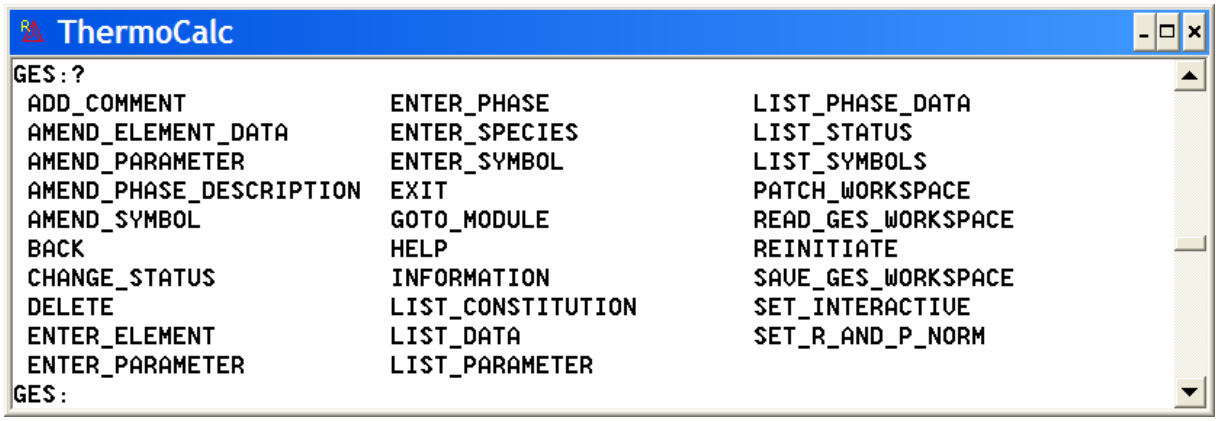
…Option 1: Reading the selected thermodynamic information of the system and finishing the exercise 1
…Option 2: Calculating the phase diagram and going directly to the exercise 2
…Option 3: Plotting the thermodynamic functions and going directly to the exercise 3

TDB-SSOL2: go gibbs

…This command in full is GOTO_MODULE GIBBS_ENERGY_SYSTEM
…Access to the **G**ibbs **E**nergy **S**ystem module (**GES**)



GES: ?

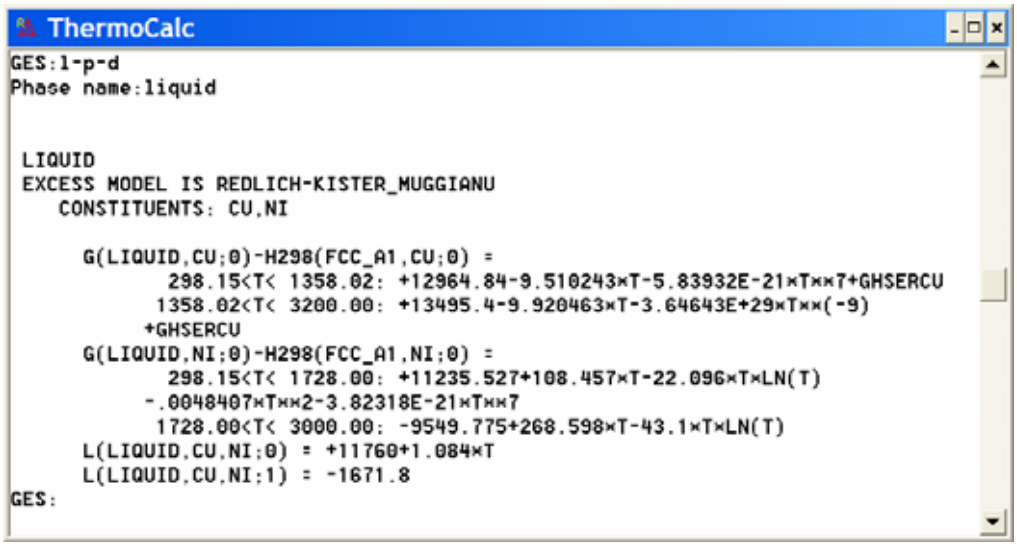


…Reading the polynomial description of the molar energy of the liquid and the fcc phases successively

GES: l-p-d

…This command in full is LIST_PHASE_DATA

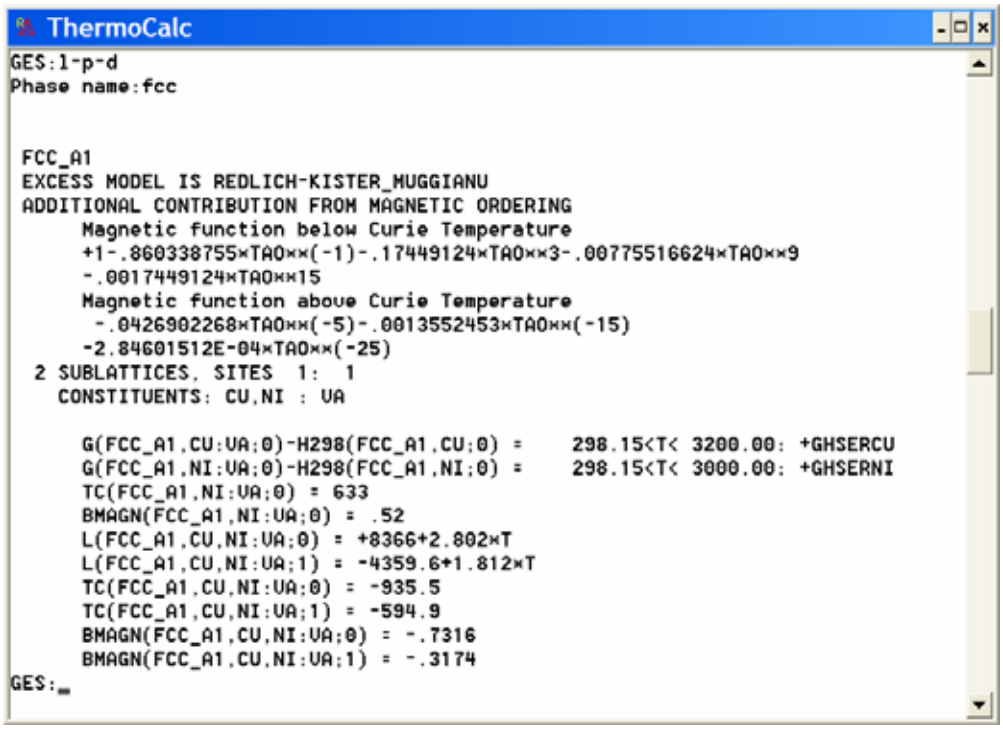
Phase name: liquid



GES: l-p-d

…This command in full is LIST_PHASE_DATA

Phase name: fcc

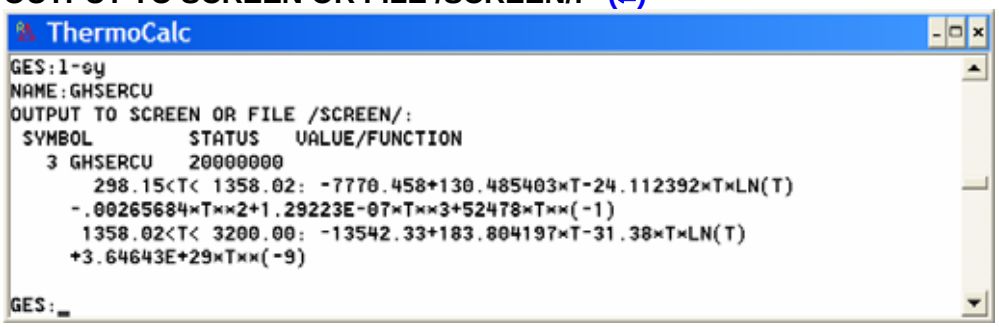


GES: l-sy

…This command in full is LIST_SYMBOL

NAME: GHSERCU

OUTPUT TO SCREEN OR FILE /SCREEN/: (↵)

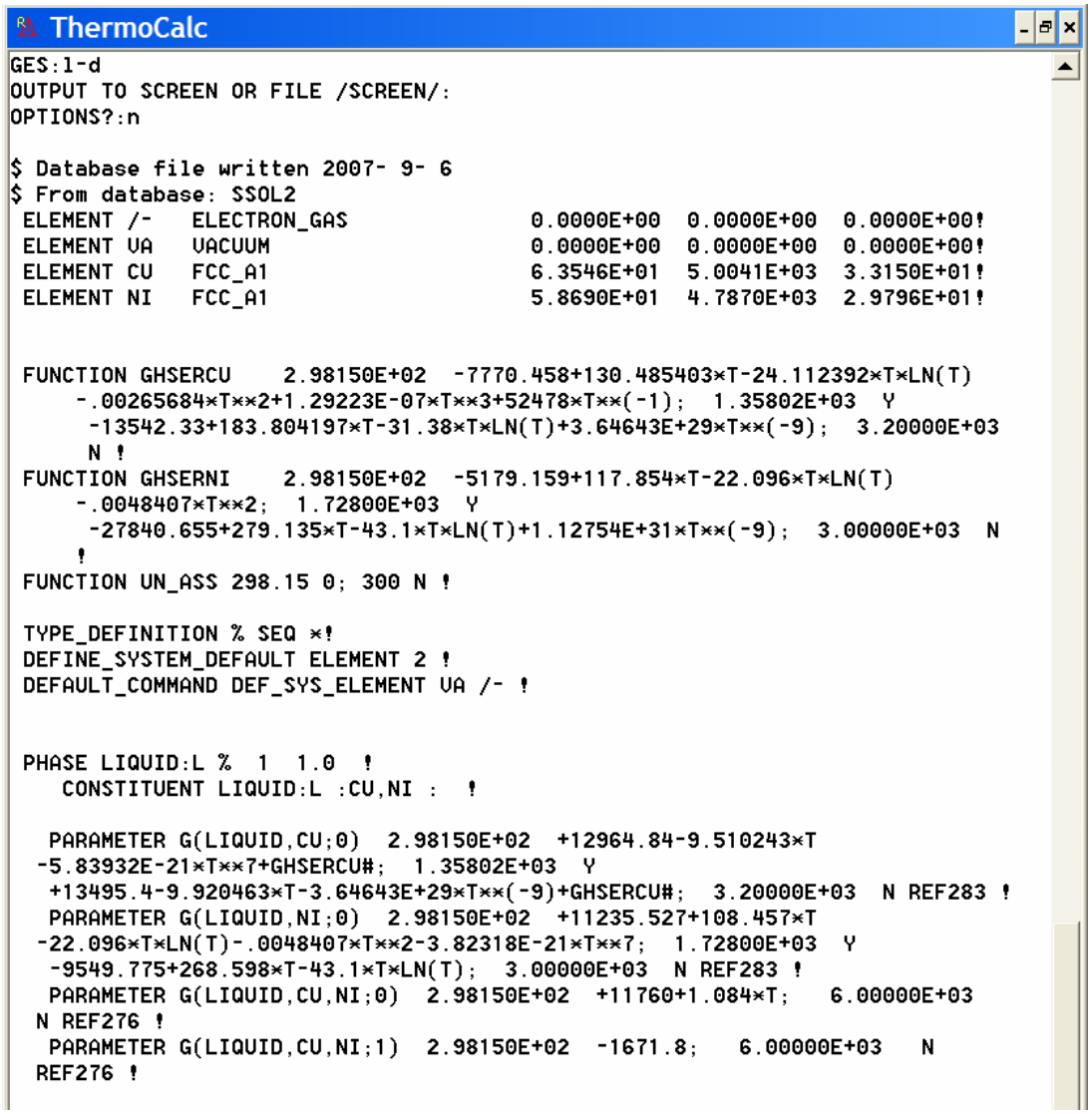


…Listing the using functions GHSERCU and GHSERNI

GES: l-sy
…This command in full is LIST_SYMBOL
NAME: GHSERNI
OUTPUT TO SCREEN OR FILE /SCREEN/: (↵)

…Listing the Cu-Ni present database of the system written in the database format of Thermo-Calc

GES: l-d
OUTPUT TO SCREEN OR FILE /SCREEN/: (↵)
OPTION?: n (↵)



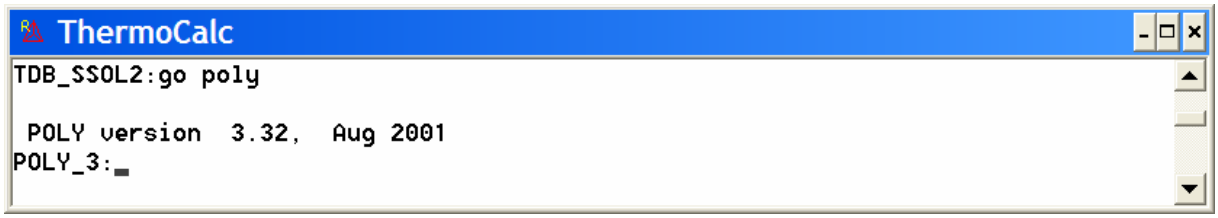
```
TYPE_DEFINITION & GES A_P_D FCC_A1 MAGNETIC  -3.0    2.80000E-01 !
PHASE FCC_A1  %&  2 1   1 !
   CONSTITUENT FCC_A1  :CU%,NI% : VA% :  !

  PARAMETER G(FCC_A1,CU:VA;0)  2.98150E+02  +GHSERCU#;  3.20000E+03  N
 REF283 !
  PARAMETER G(FCC_A1,NI:VA;0)  2.98150E+02  +GHSERNI#;  3.00000E+03  N
 REF283 !
  PARAMETER TC(FCC_A1,NI:VA;0)  2.98150E+02  633;   6.00000E+03   N REF281 !
  PARAMETER BMAGN(FCC_A1,NI:VA;0)  2.98150E+02  .52;   6.00000E+03   N
 REF281 !
  PARAMETER G(FCC_A1,CU,NI:VA;0)  2.98150E+02  +8366+2.802*T;   6.00000E+03
   N REF276 !
  PARAMETER G(FCC_A1,CU,NI:VA;1)  2.98150E+02  -4359.6+1.812*T;
 6.00000E+03   N REF276 !
  PARAMETER TC(FCC_A1,CU,NI:VA;0)  2.98150E+02  -935.5;   6.00000E+03   N
 REF276 !
  PARAMETER TC(FCC_A1,CU,NI:VA;1)  2.98150E+02  -594.9;   6.00000E+03   N
 REF276 !
  PARAMETER BMAGN(FCC_A1,CU,NI:VA;0)  2.98150E+02  -.7316;   6.00000E+03
 N REF276 !
  PARAMETER BMAGN(FCC_A1,CU,NI:VA;1)  2.98150E+02  -.3174;   6.00000E+03
 N REF276 !

LIST_OF_REFERENCES
NUMBER  SOURCE
  REF283   'Alan Dinsdale, SGTE Data for Pure Elements,
         Calphad Vol 15(1991) p 317-425,
         also in NPL Report DMA(A)195 Rev. August 1990'
  REF276   'A. Jansson, TRITA-MAC 340 (1987); CU-FE-NI'
  REF281   'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report
        DMA(A)195
         September 1989'
 !

GES:
```

2. CALCULATING AND PLOTTING THE PHASE DIAGRAM

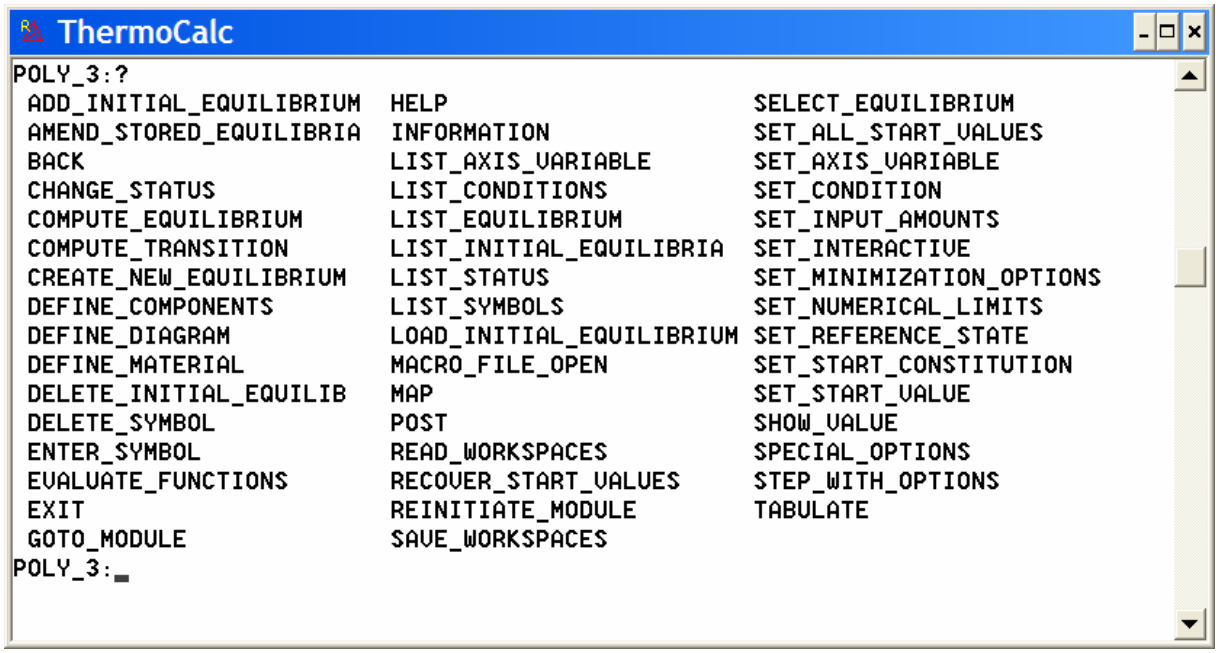
You must have preliminary retrieved the thermodynamic data in the TDB module, which implying to have done all the steps of the exercise 1, from the beginning to the "GET" command page 7 (cf. Option 2).

…Setting conditions

TDB-SSOL2: go poly
…This command in full is GOTO_MODULE POLY-3
…Access to the Equilibrium Calculation Module (POLY)

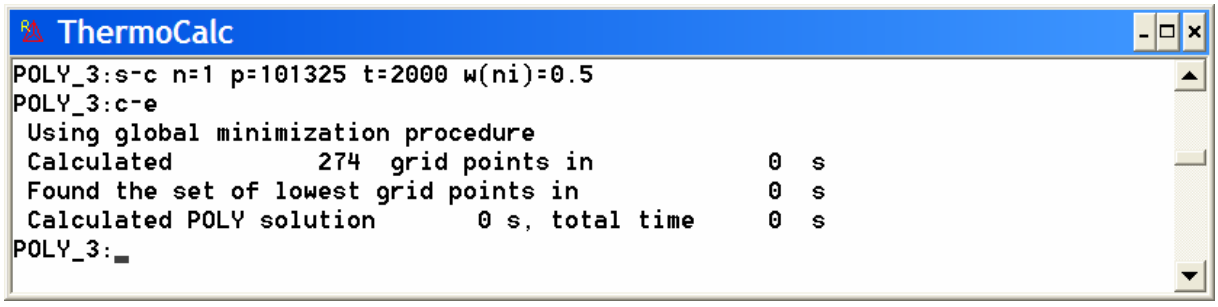


POLY_3: ?
…This command lists the available commands

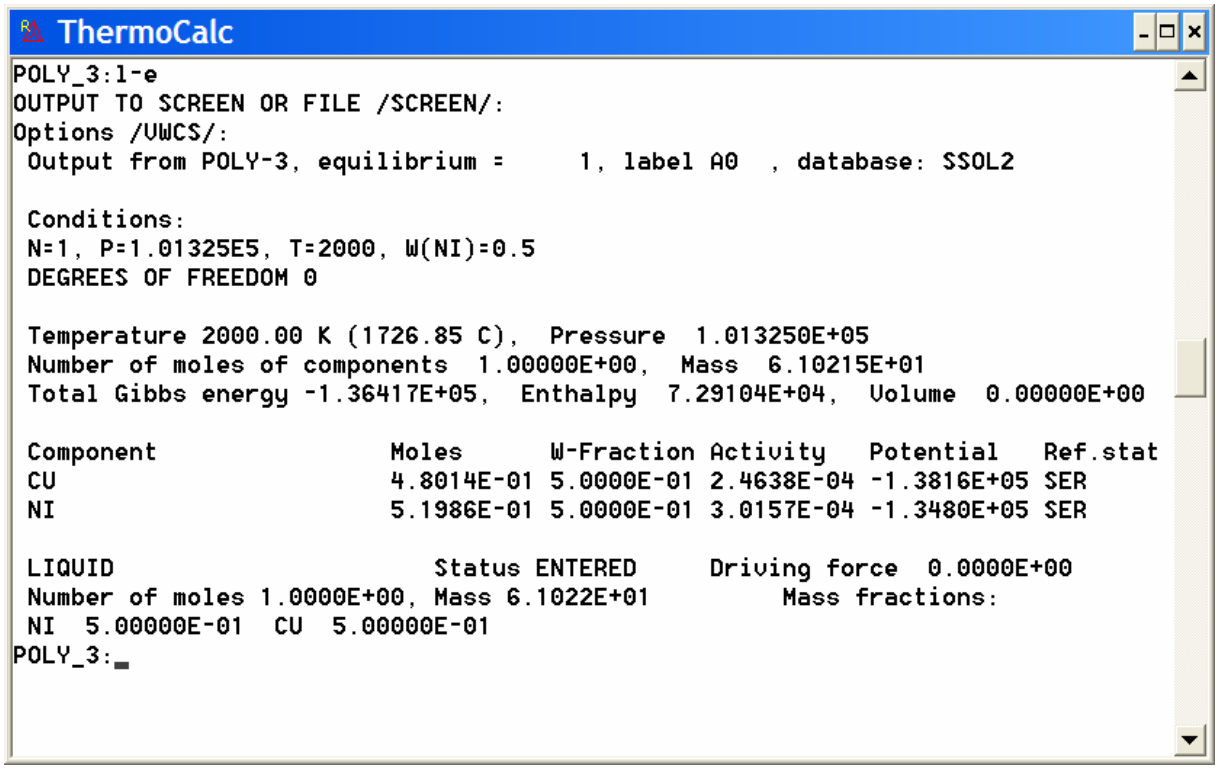


POLY_3: s-c n=1 p=101325 t=2000 w(ni)=0.5
…This command in full is SET_CONDITION
…Calculating the equilibrium for the given set of conditions
…Default units: p(Pa) and T(K); w(ni) for mass fraction or x(ni) for mole fraction

POLY_3: c-e
…This command in full is COMPUTE_EQUILIBRIUM



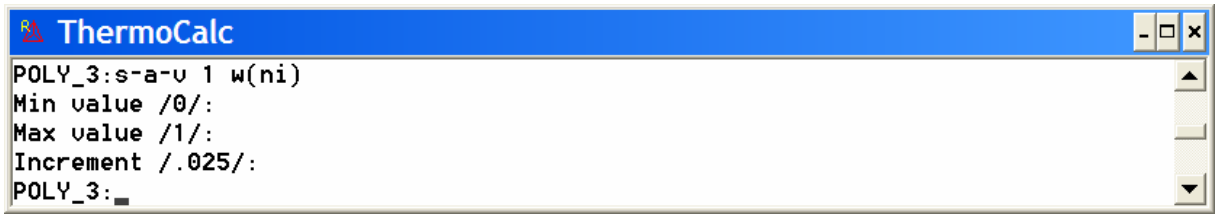
POLY_3: l-e
…This command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/ : (↵)
Options /VWCS/ : (↵)



…Generating the diagram: defining the two axis variables (1 and 2) and mapping the phase diagram

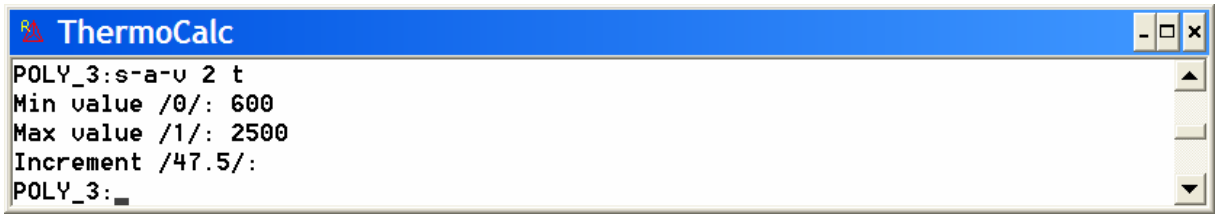
POLY_3: s-a-v 1 w(ni)
…This command in full is SET_AXIS_VARIABLE
…This means that the axis number 1 is taken to be the mass fraction of Ni

Min value /0/: 0 (↵)
Max value /0/: 1 (↵)
Increment /0.025/: (↵)

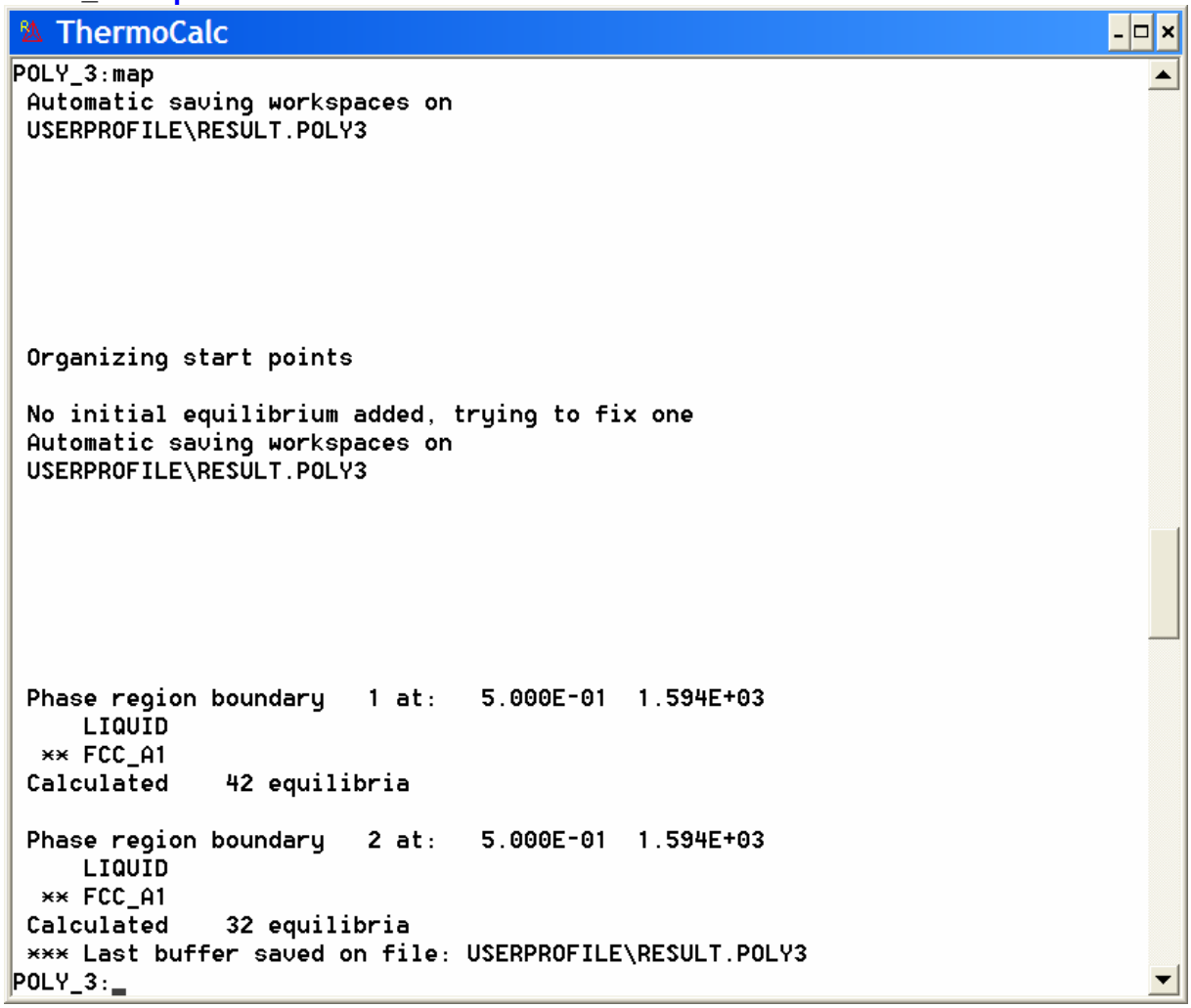


POLY_3: s-a-v 2 t
…This command in full is SET_AXIS_VARIABLE
…This means that the axis number 2 is taken to be the temperature

Min value /0/: 600 (↵)
Max value /1/: 2500 (↵)
Increment /47.5/: (↵)

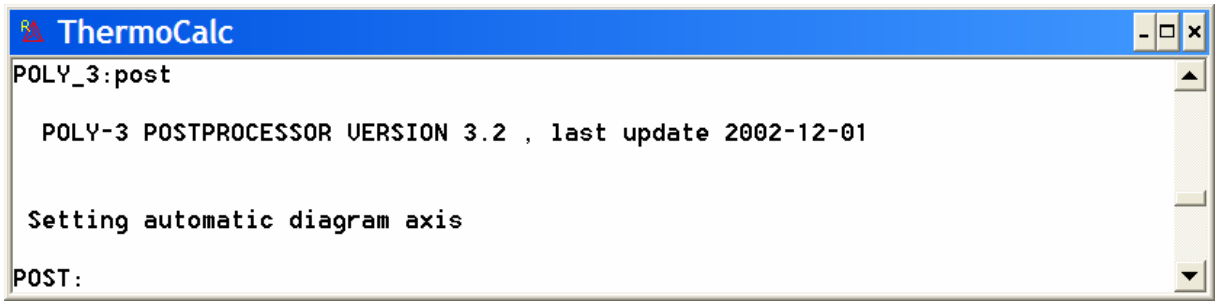


POLY_3: map



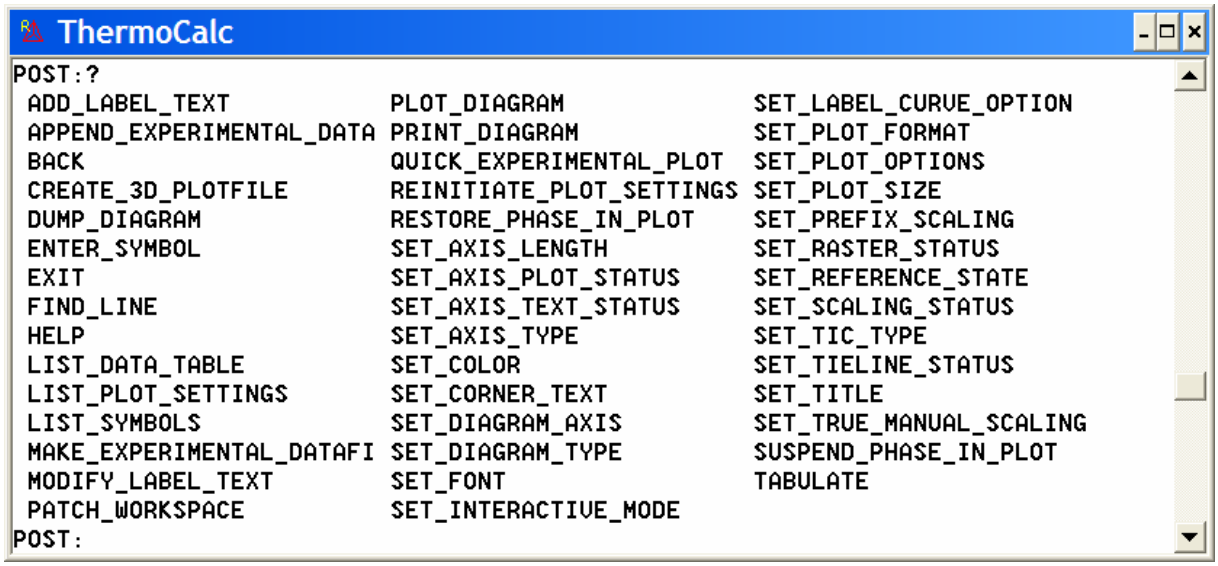
…Plotting the diagram

POLY_3: post



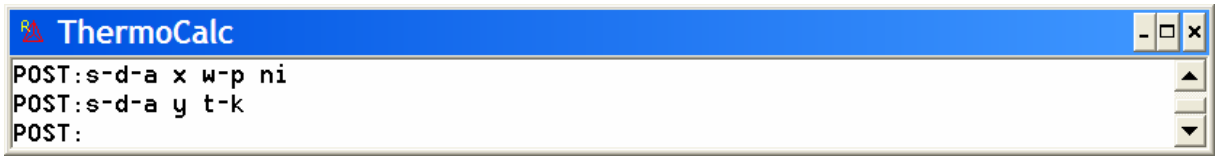
…Defining the two axis variables for plotting

POST: ?



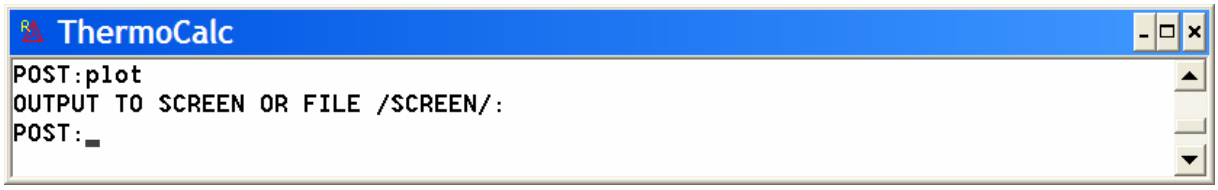
POST: s-d-a x w-p ni
…This command in full is SET_DIAGRAM_AXIS
…This means that the X axis variable is taken to be the weight-percent (w-p) of ni
…Other possible choices: weight-fraction (w-f), mole-fraction (m-f), mole-percent (m-p)

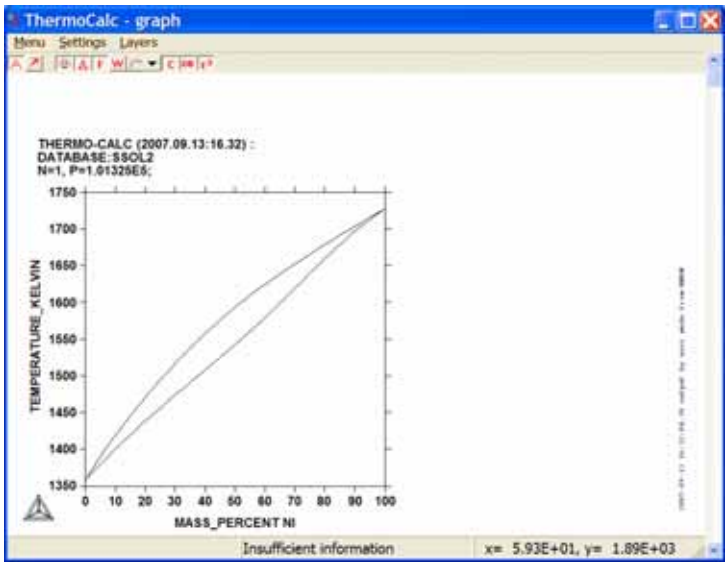
POST: s-d-a y t-k
…This means that the Y axis variable is taken to be the temperature in K (t-k)
…Other possible choice: temperature-Celsius (t-c)



…Plotting with automatic scaling (opening a “Thermo-Calc graph” window)

POST: plot
OUTPUT TO SCREEN OR FILE /SCREEN/ : (↵)

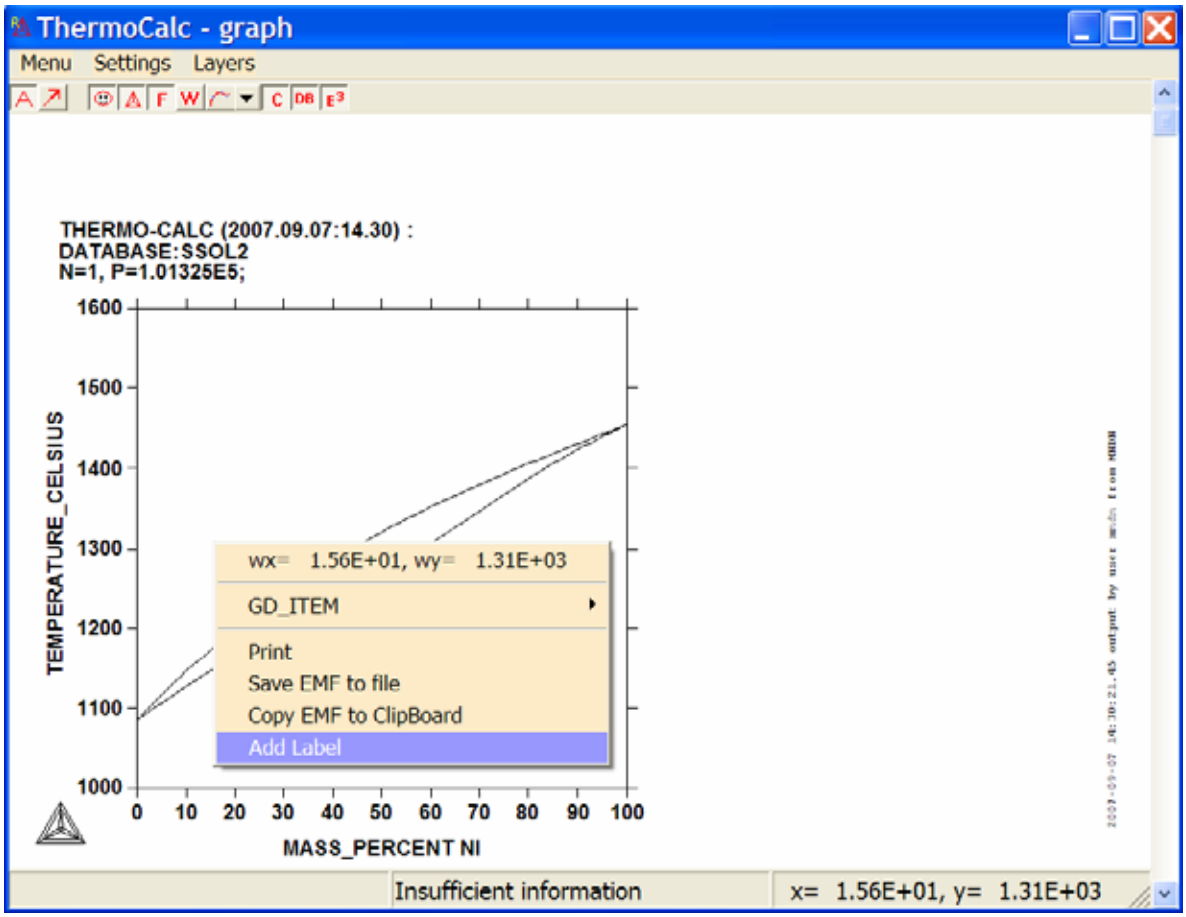




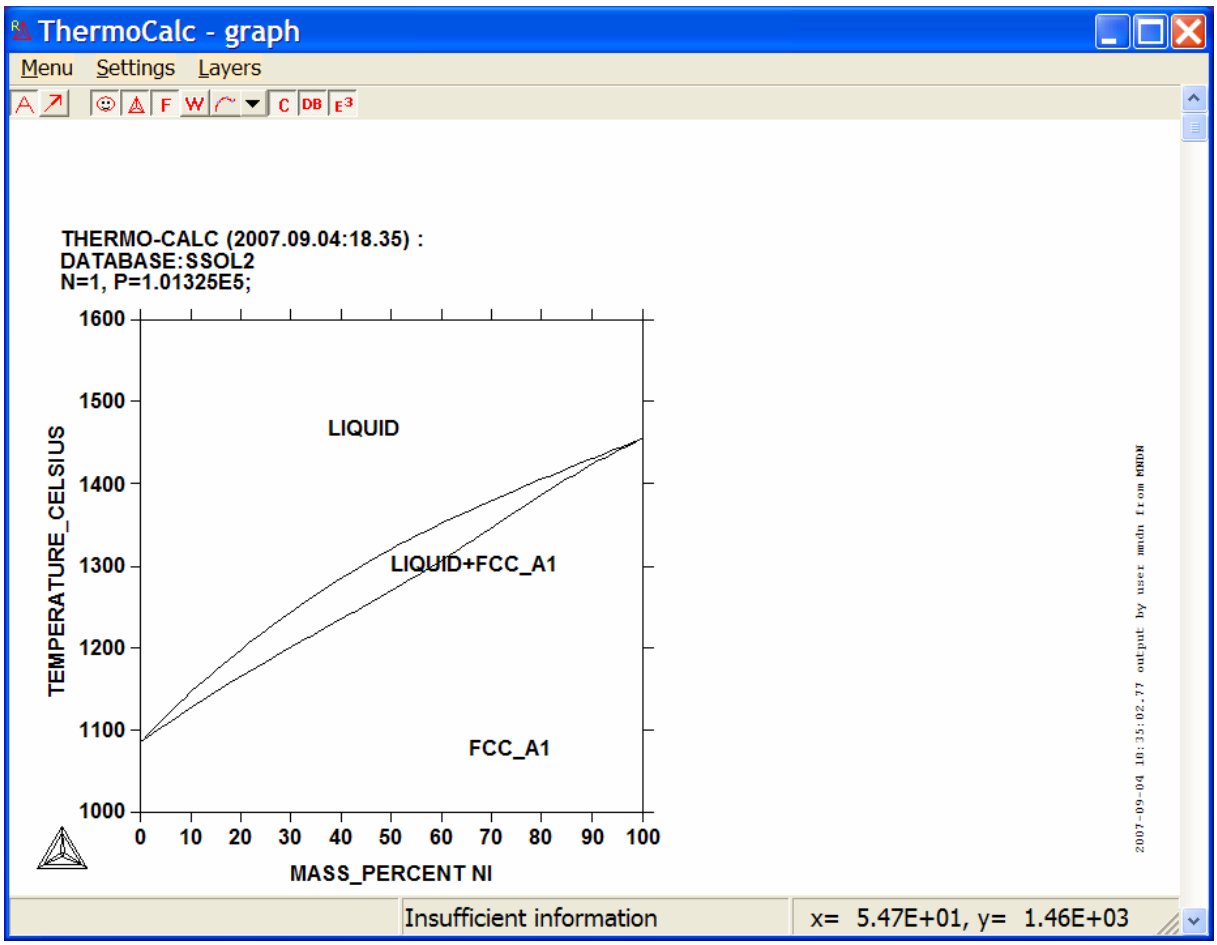
…Plotting with manual scaling

POST: s-d-a y t-c
…This command in full is SET_DIAGRAM_AXIS
POST: s-s-s
…This command in full is SET_SCALING_STATUS
AXIS (X,Y OR Z) : y
AUTOMATIC SCALING (Y or N) /N/ : n
MIN VALUE : 1000
MAX VALUE : 1600

POST: plot
OUTPUT TO SCREEN OR FILE /SCREEN/ : (↵)



Clicking the mouse-right-button on a selected point and then choosing the “Add label” option



…Plotting the tie-lines

POST: s-t-s

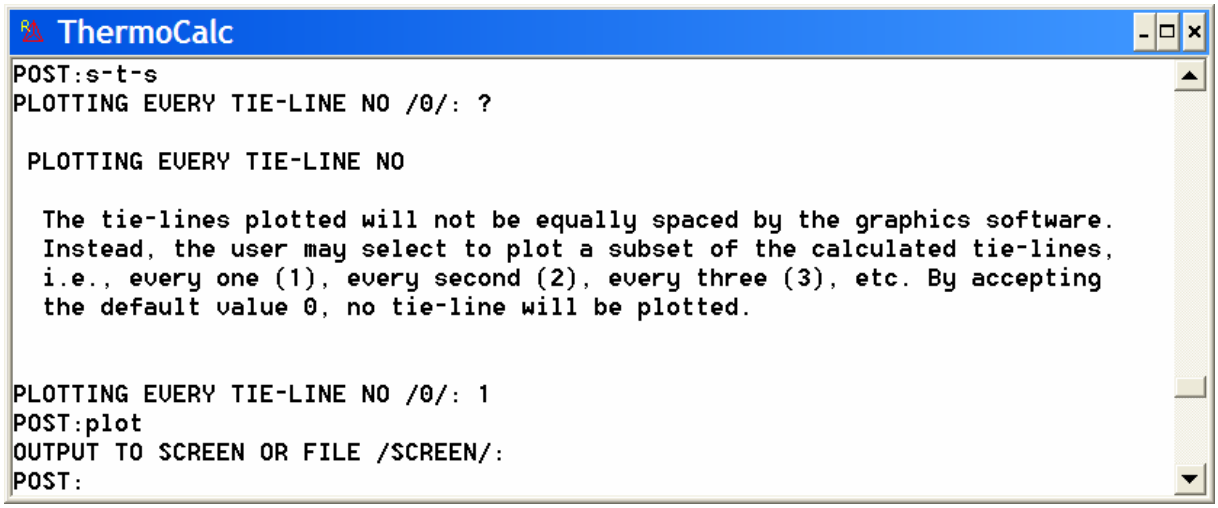
…This command in full is SET_TIELINE_STATUS

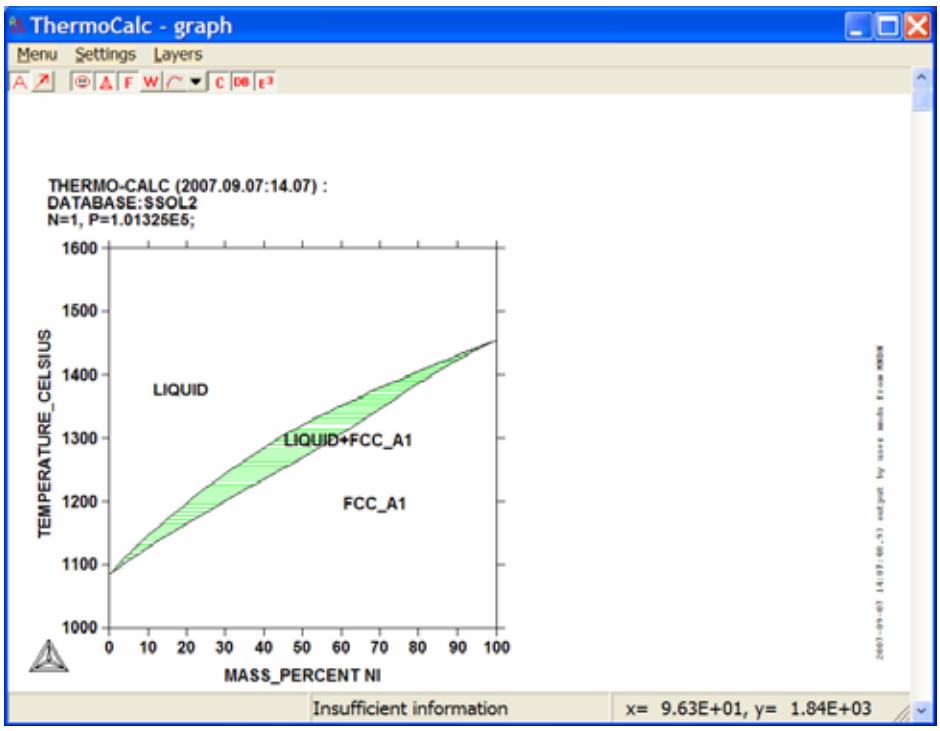
PLOTTING EVERY TIE-LINE N0 /0/: ? **(↵)**

PLOTTING EVERY TIE-LINE N0 /0/: 1 **(↵)**

POST: PLOT

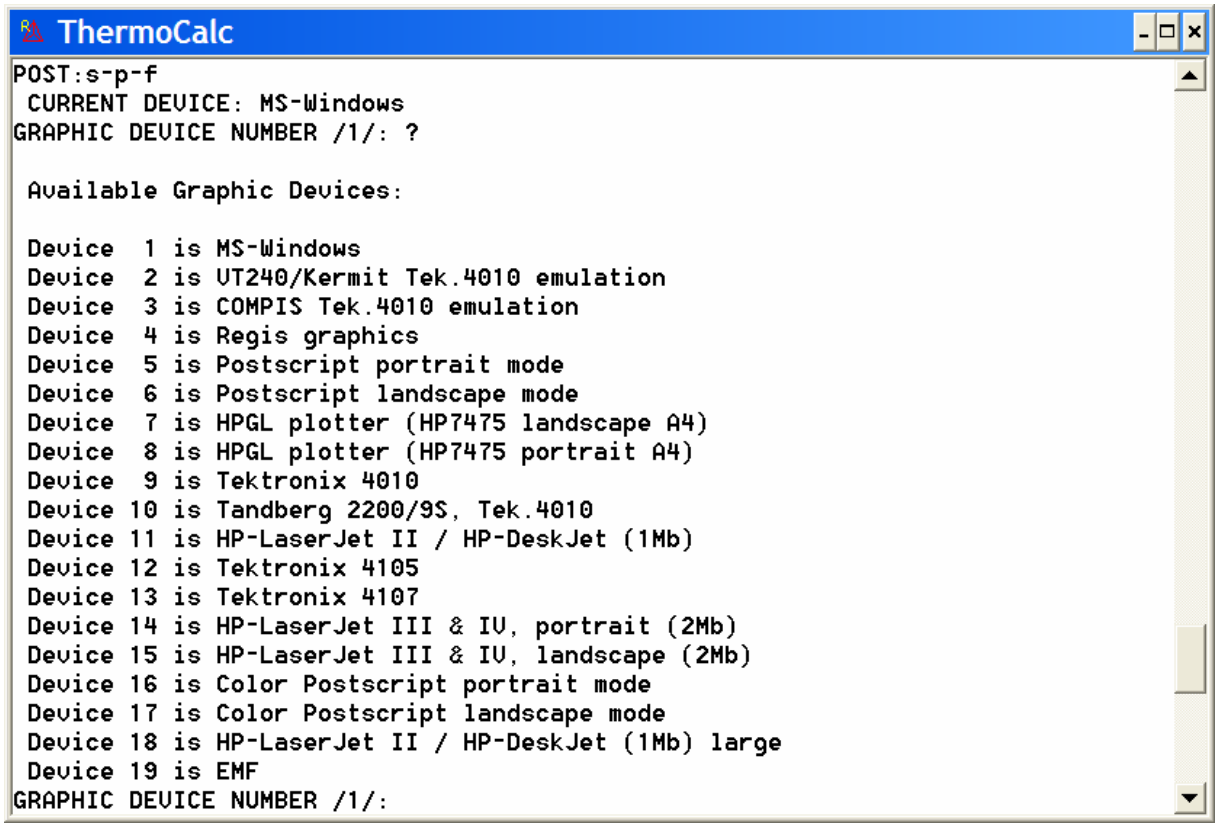
OUTPUT TO SCREEN OR FILE /SCREEN/ : **(↵)**



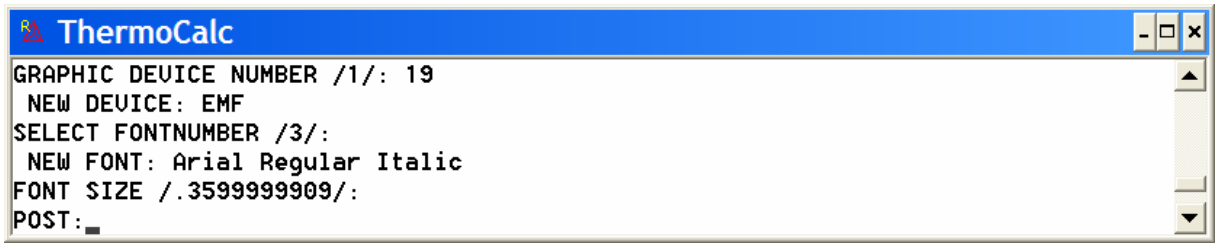


…Save the plot in a graphical format for windows (.EMF = Enhanced Windows Metafile)

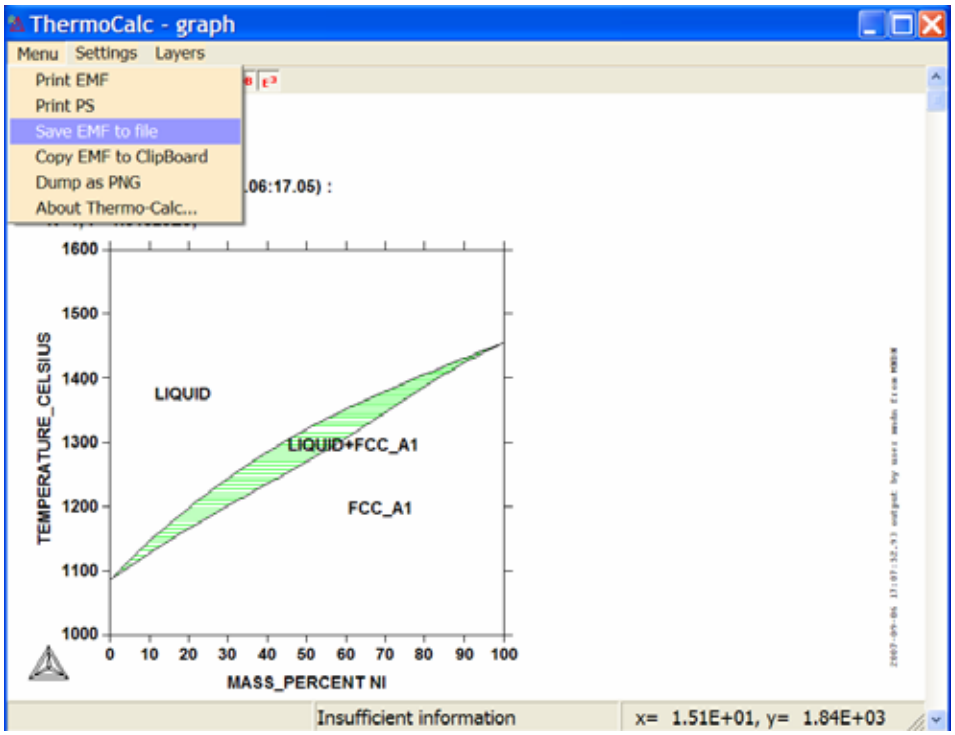
POST: s-p-f
…This command in full is SET_PLOT_FORMAT
GRAPHIC DEVICE NUMBER /1/ : ?
…This command lists the available graphic formats

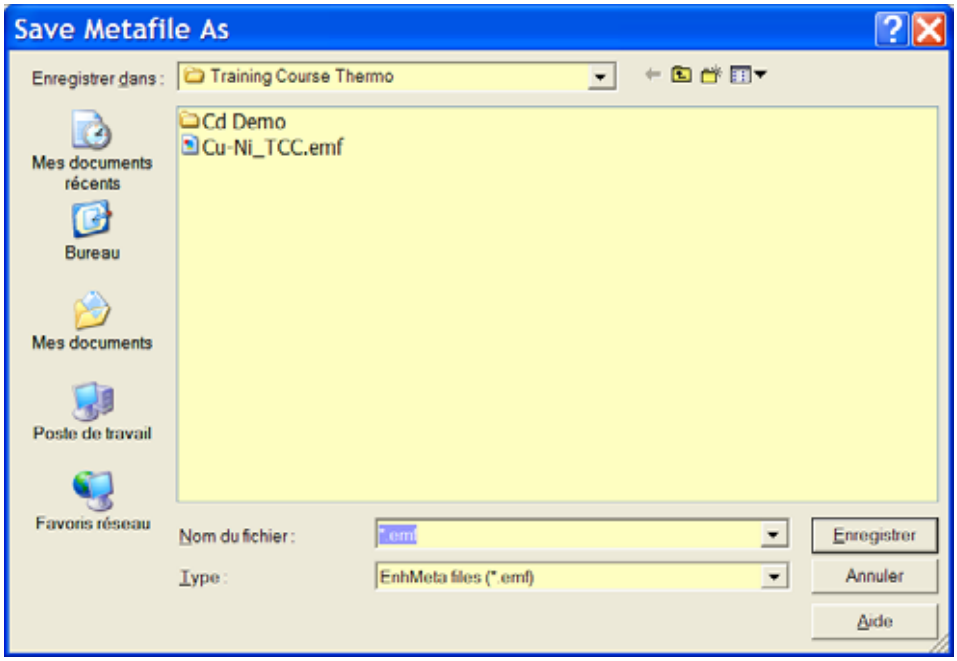


GRAPHIC DEVICE NUMBER /1/ : 19
SELECT FONTNUMBER /3/ : (↵)
FONT SIZE /0.35/ : (↵)



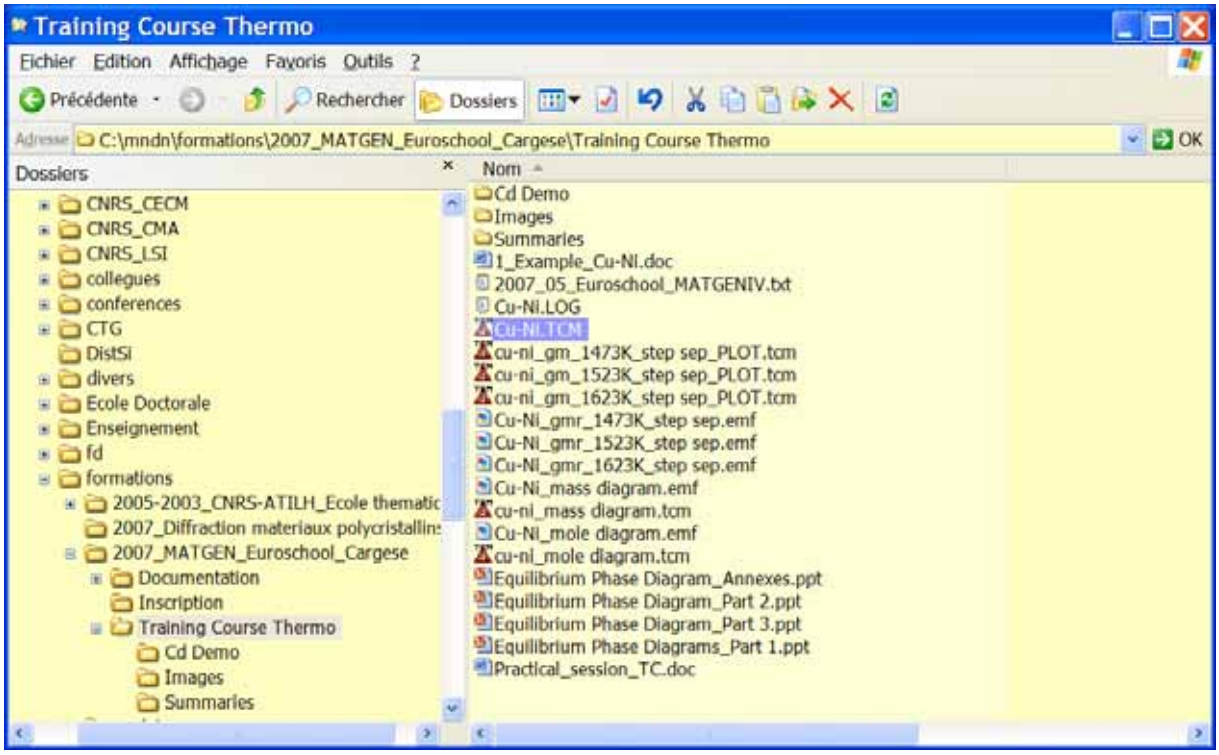
POST: PLOT
OUTPUT TO SCREEN OR FILE /SCREEN/ : (↵)





POST: exit

…All the typed commands can be read in the LOG File, “Cu-Ni.LOG”.
…If you replace the .LOG extension by the .TCM one, the file becomes a macrofile.
…Example: LOG file generated after “Exercice 1 → Option 2” and “Exercice 2”



...The TCM file can be opened by any text editor.

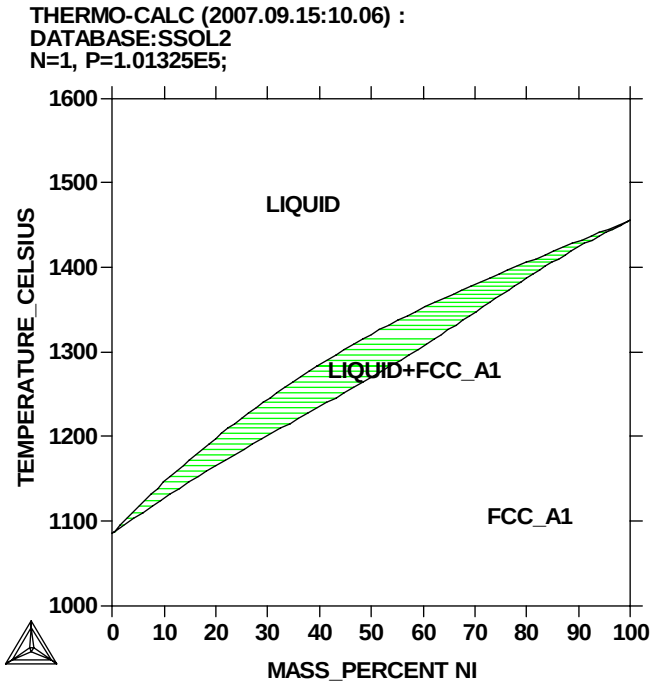
LOGFILE GENERATED ON PC/WINDOWS NT DATE 2007- 9- 7
Cu-Ni phase diagram

go da
?
sw da
SSOL2
def-el
Cu Ni
l-sys
CONSTITUENT
rej ph *
rest ph liquid fcc
l-sys con
get
go poly
?
s-con n=1 p=101325 t=2000 w(ni)=0.5
c-e
l-e
SCREEN
VWCS
s-a-v 1 w(ni)
0
1

```
.025
s-a-v 2 t
600
2500
47.5
map
post
?
s-d-a x w-p ni
s-d-a y t-k
plot
SCREEN
s-d-a y t-c
s-s-s
y
n
1000
1600
plot
SCREEN
ADD_LABEL    7.238283E+01    1.097146E+03 ,,,,,,,,,,,,,;!

PLOT,,;!
ADD_LABEL    1.117161E+02    1.063025E+03 ,,,,,,,,,,,,,;!

PLOT,,;!
ADD_LABEL    2.961776E+01    1.465977E+03 ,,,,,,,,,,,,,;!

PLOT,,;!
ADD_LABEL    4.176093E+01    1.269376E+03 ,,,,,,,,,,,,,;!

PLOT,,;!
s-t-s
?
1
plot
SCREEN
s-p-f
?
19


plot
SCREEN
exit

********** end of the TCM file **********************************************
```

…Replace the command of the last line “exit” by “set-inter”
…Save the file
…Your TCM file can be executed!

…Execute the TCM file



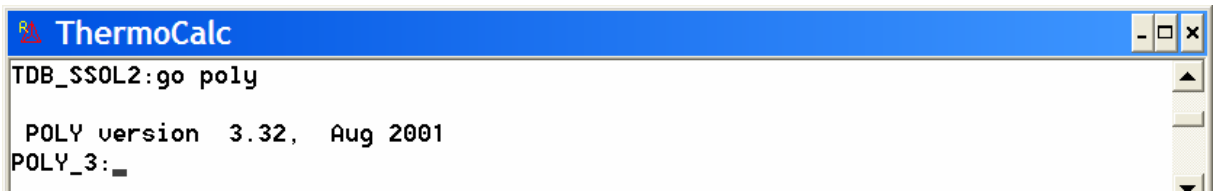
2007-09-15 10:06:04.20 output by user mndn from MNDN

3. PLOTTING THE MOLAR GIBBS ENERGY CURVES G=f(X)

You must have preliminary retrieved the thermodynamic data in the TDB module, which implying to have done all the steps of the exercise 1, from the beginning to the "GET" command page 7 (cf. Option 3).
Don't forget at the beginning to create a new set-log-file with another name

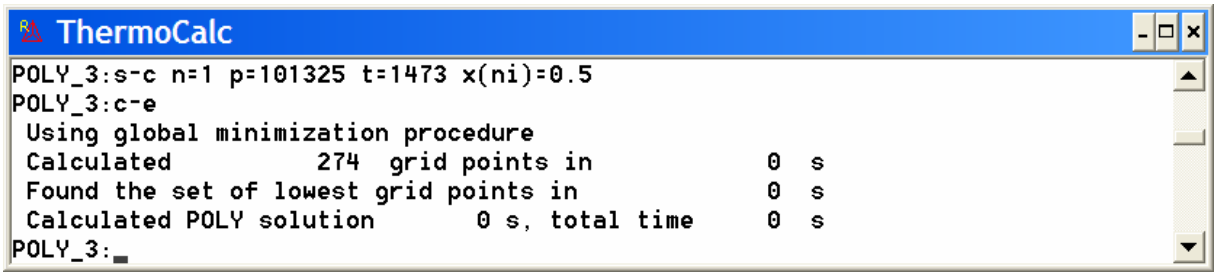
…Plotting the molar Gibbs energy functions G=f(X) for T=1200°C (1473K)

TDB-SSOL2: go poly
…This command in full is GOTO_MODULE POLY-3
…Access to the Equilibrium Calculation Module (POLY)



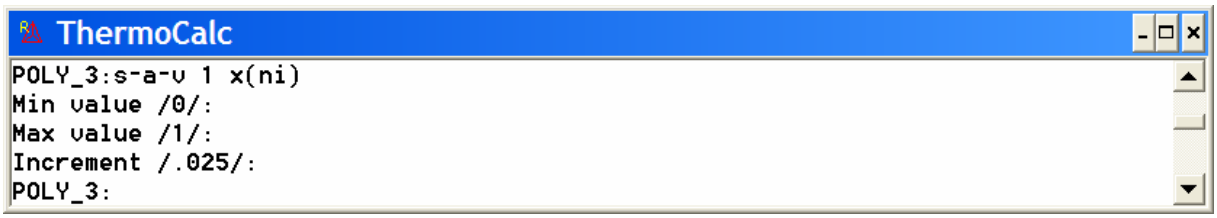
…Calculating the equilibrium for the given set of conditions (T=1473K = 1200°C)

POLY_3: s-c n=1 p=101325 t=1473 x(ni)=0.5
…This command in full is SET_CONDITION
…Calculating the equilibrium for the given set of conditions
POLY_3: c-e
…This command in full is COMPUTE_EQUILIBRIUM



…In order to plot G=f(X), only one variable X axis

POLY_3: s-a-v 1 x(ni)
…This command in full is SET_AXIS_VARIABLE
Min value /0/: 0 (↵)
Max value /0/: 1 (↵)
Increment /0.025/: (↵)



…Calculating G=f(X) for all the phases

POLY: step sep
…These commands in full are STEP_WITH_OPTIONS and SEPARATE_PHASES
…"sep" option: This is used when the user wants to plot Gm curves versus composition

ThermoCalc

```
POLY_3:step sep,
 Convergence problems, increasing smallest sitefraction from 1.00E-30
 to hardware precision 2.00E-12.  You can restore using SET-NUMERICAL-LIMITS

 Phase Region from   0.502463     for:
     LIQUID
     FCC_A1

 Phase Region from   0.502463     for:
     LIQUID
     FCC_A1
 *** Buffer saved on file *** USERPROFILE\RESULT.POLY3
POLY_3:
```

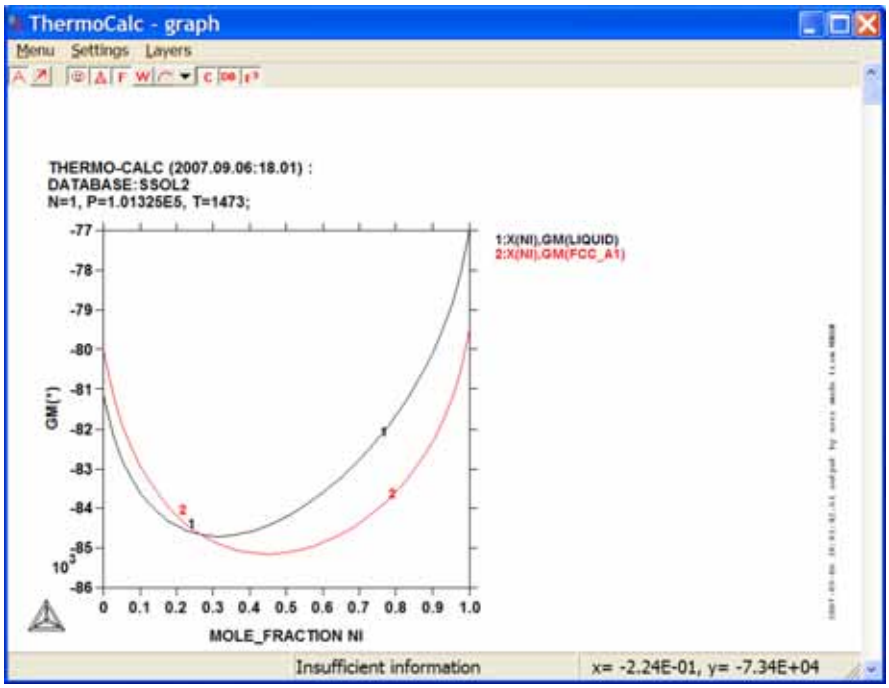
POLY: post
POST: s-d-a x m-f ni
…This command in full is SET_DIAGRAM_AXIS
POST: s-d-a y gm(*)
…This means that the Y axis variable is taken to be the molar Gibbs energies of all phases (default unit: J/mol)
COLUMN NUMBER /*/ : (↵)

ThermoCalc

```
POLY_3:post

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST:s-d-a x m-f ni
POST:s-d-a y gm(*)
COLUMN NUMBER /*/:
POST:
```

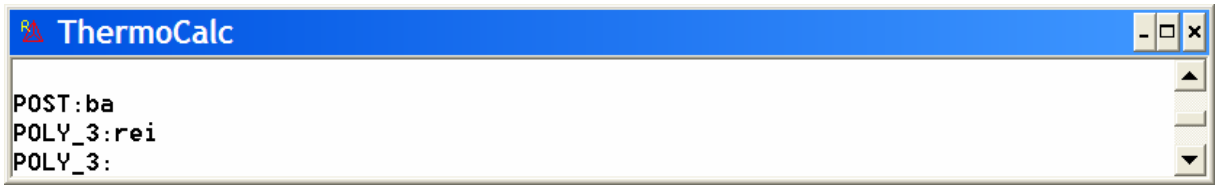
…A table g1 is created with three columns: X(Ni) Gm(liquid) Gm(fcc_a1) (it can be tabulated by the l-d-t command)

POST: s-l-c-o f
…This command in full is SET_LABEL_CURVE_OPTION
POST: plot screen

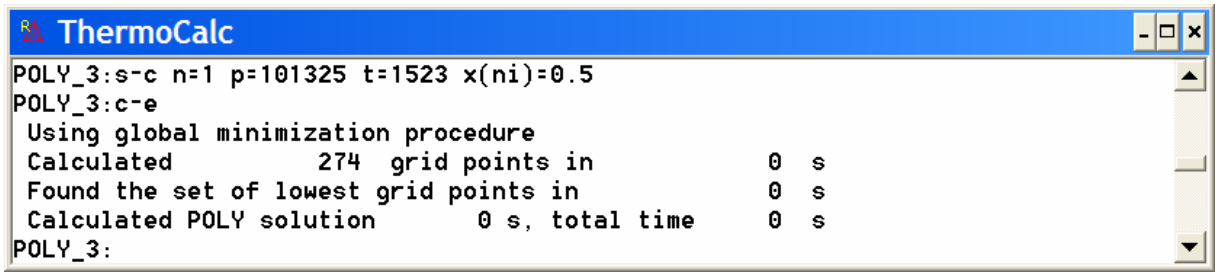


…Plotting the molar Gibbs energy functions for T=1250°C (1523K)

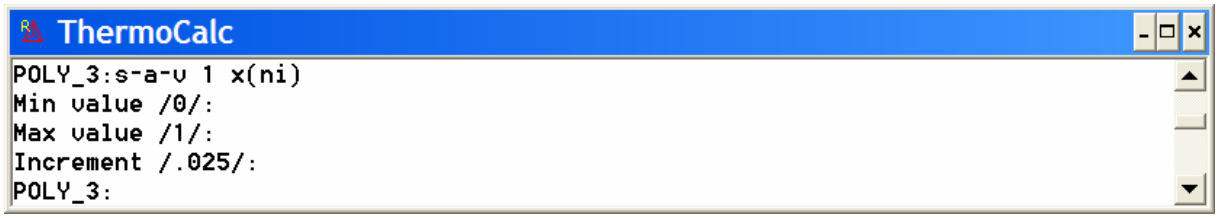
POST: ba
…This command in full is BACK
POLY: rei
…This command in full is REINITIATE_MODULE



POLY_3: s-c n=1 p=101325 t=1523 x(ni)=0.5
…Calculating the equilibrium for the given set of conditions
POLY_3: c-e

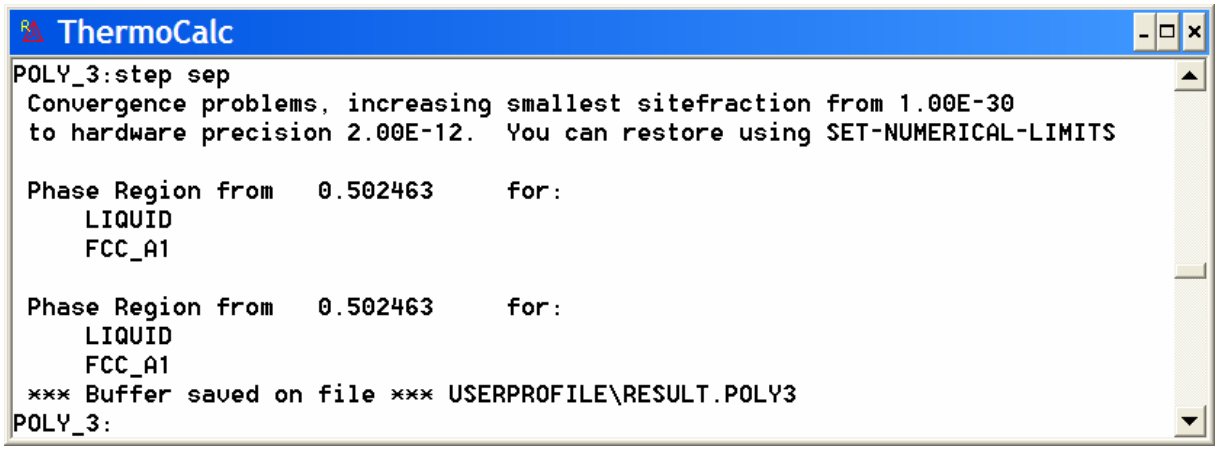


POLY_3: s-a-v 1 x(ni)

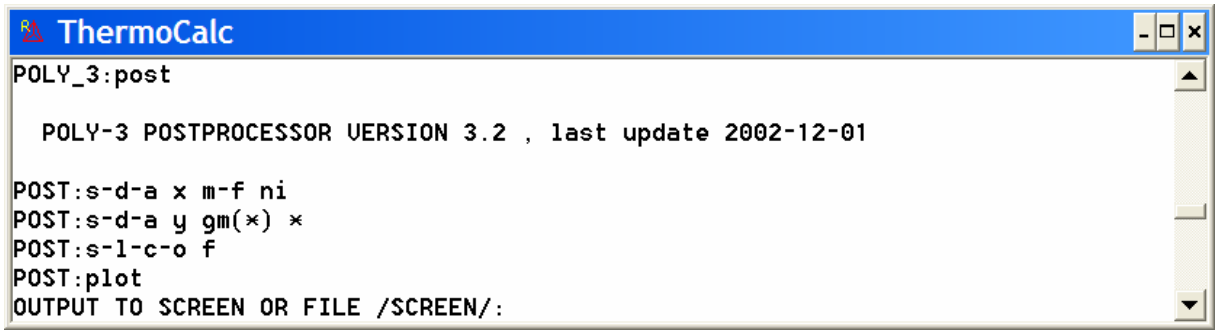


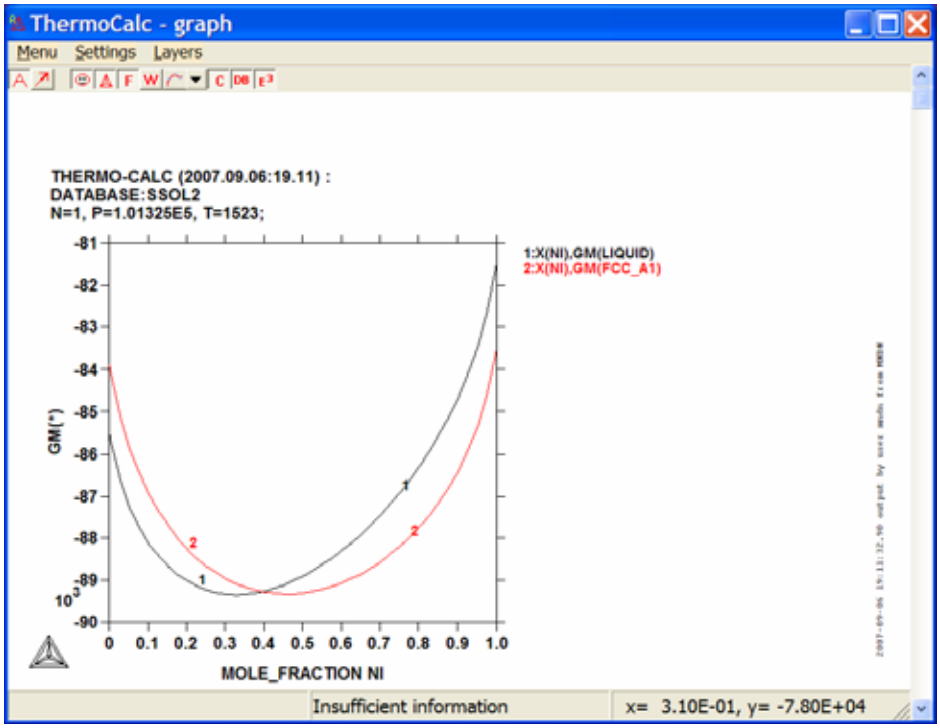
…Calculating G=f(X) for all the phases

POLY: step sep



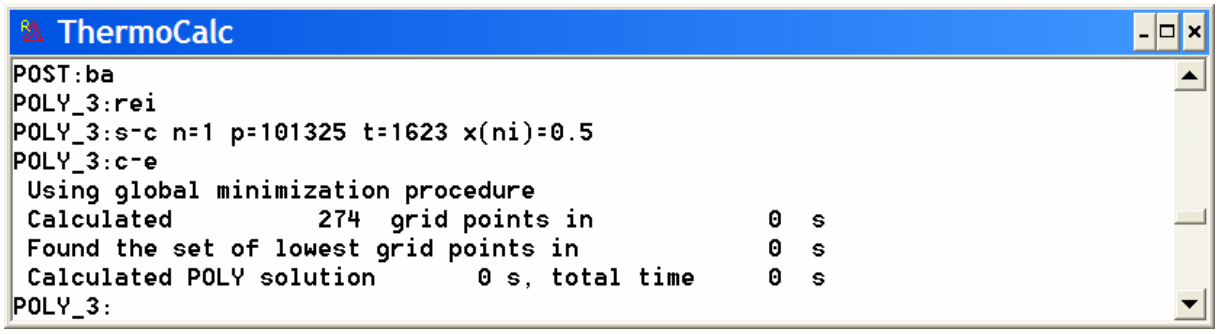
POLY: post
POST: s-d-a x m-f ni
POST: s-d-a y gm(*) *
COLUMN NUMBER /*/ : (↵)
POST: s-l-c-o f
POST: plot



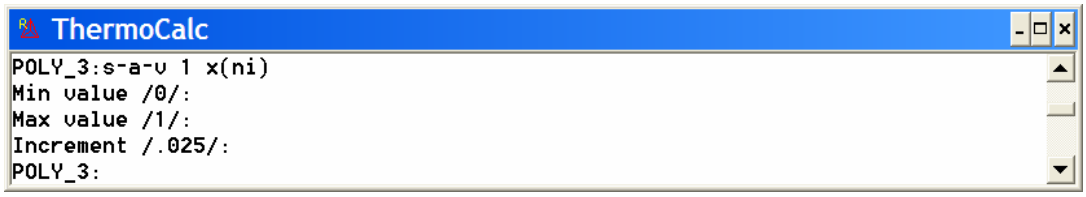


…Plotting the molar Gibbs energy functions for T=1350°C (1623K)

POST: ba
POLY: rei
POLY_3: s-c n=1 p=101325 t=1623 x(ni)=0.5
POLY_3: c-e

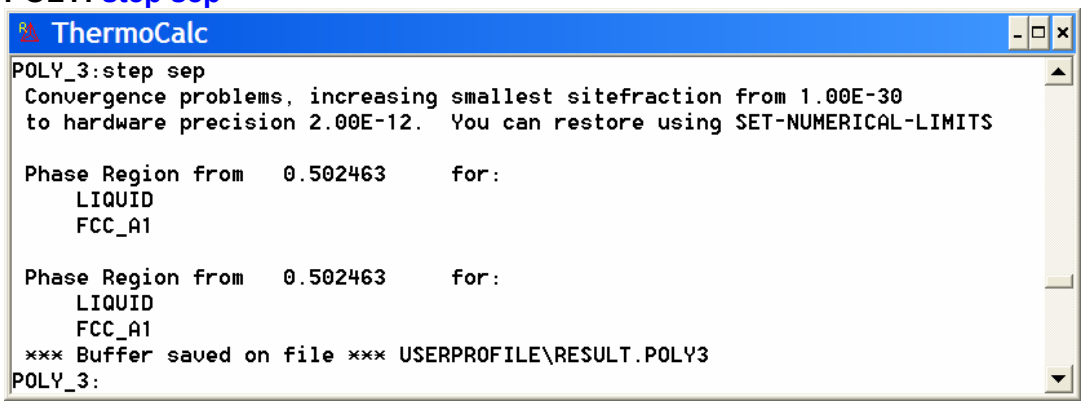


POLY_3: s-a-v 1 x(ni)

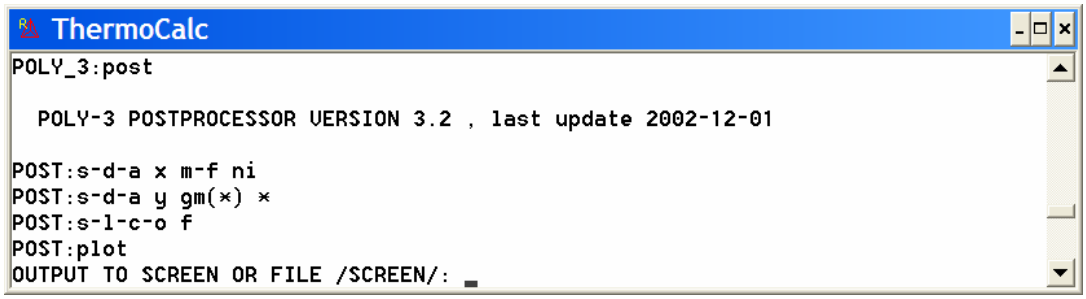


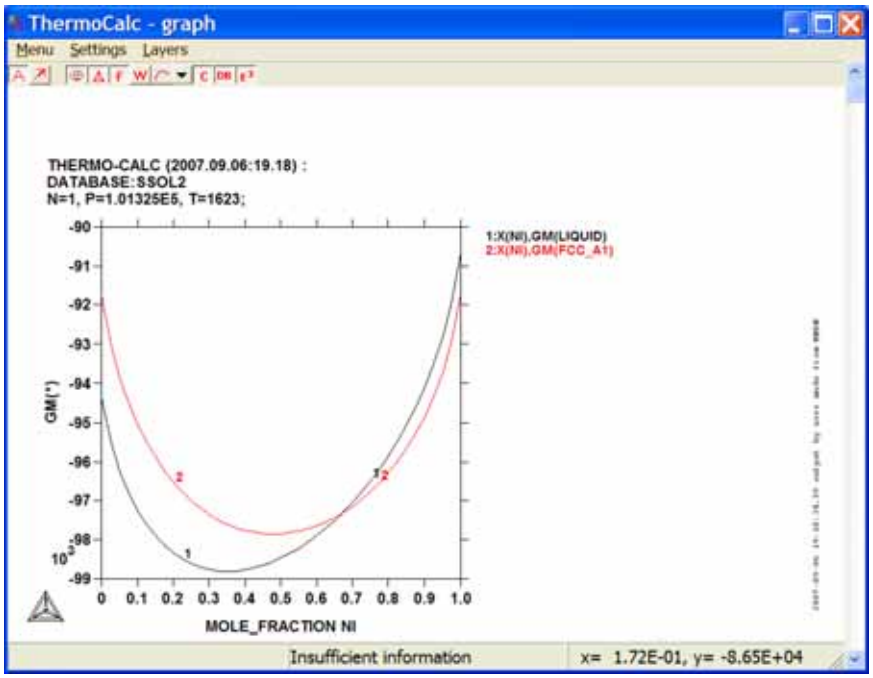
...Calculating G=f(X) for all the phases

POLY: step sep



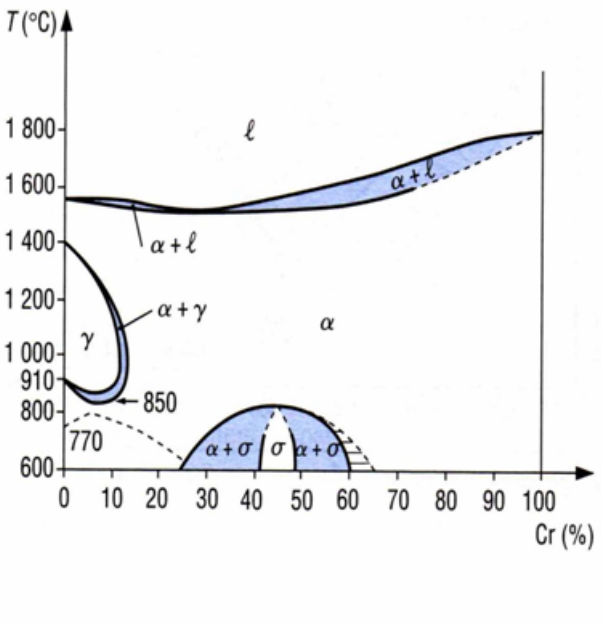
POLY: post
POST: s-d-a x m-f ni
POST: s-d-a y gm(*) *
COLUMN NUMBER /*/ : (↵)
POST: s-l-c-o f
POST: plot





EXAMPLE 2

Calculation of the Fe-Cr phase diagram between 600 and 2200°C



1. SELECTING THE THERMODYNAMIC FUNCTIONS OF THE SYSTEM

Running Thermo-Calc application: Execute “TCCR.exe”

SYS: s-l-f
…This command in full is SET_LOG_FILE
…Choose the path and the name of the file
Heading: Fe-Cr phase diagram
…The heading for the Fe-Cr.LOG file

SYS: go da
…This command in full is GOTO_MODULE DATABASE_RETRIEVAL
…Access to the **T**hermodynamic **D**ata**B**ase module (**TDB**)

TDB-USER: sw da
…This command in full is SWITCH_DATABASE
…All the available databases are listed

TDB-USER: PTERN
…Define the system in terms of elements: selection of Fe and Cr

TDB-PTERN: def-el
…This command in full is DEFINE_ELEMENTS
ELEMENTS: fe cr

TDB-PTERN: l-sys con
…This command in full is LIST_SYSTEM CONSTITUENTS

TDB-PTERN: rej ph *
…This command in full is REJECT PHASES /ALL

TDB-PTERN: rest ph liquid fcc bcc sigma
…This command in full is RESTORE PHASES liquid fcc bcc sigma

TDB-PTERN: l-sys con
…This command in full is LIST_SYSTEM CONSTITUENTS

TDB-PTERN: get
…This command in full is GET_DATA
…Retrieval of all information from the thermodynamic databank

…Option 1: Reading the selected thermodynamic information of the system and finishing the exercise 1
…Option 2: Calculating the phase diagram and going directly to the exercise 2

TDB-PTERN: go gibbs
…This command in full is GOTO_MODULE GIBBS_ENERGY_SYSTEM
…Access to the **G**ibbs **E**nergy **S**ystem module (**GES**)

…Reading the polynomial description of the molar energy of the liquid and the fcc phases successively

GES: l-p-d
…This command in full is LIST_PHASE_DATA
Phase name: liquid

GES: l-p-d
…This command in full is LIST_PHASE_DATA
Phase name: fcc

GES: l-p-d
…This command in full is LIST_PHASE_DATA
Phase name: bcc

GES: l-p-d
…This command in full is LIST_PHASE_DATA
Phase name: sigma

2. CALCULATING AND PLOTTING THE PHASE DIAGRAM

You must have preliminary retrieved the thermodynamic data in the TDB module, which implying to have done all the steps of the exercise 1, from the beginning to the "GET" command page 28 (cf. Option 2).

…Setting conditions

TDB-PTERN: go poly

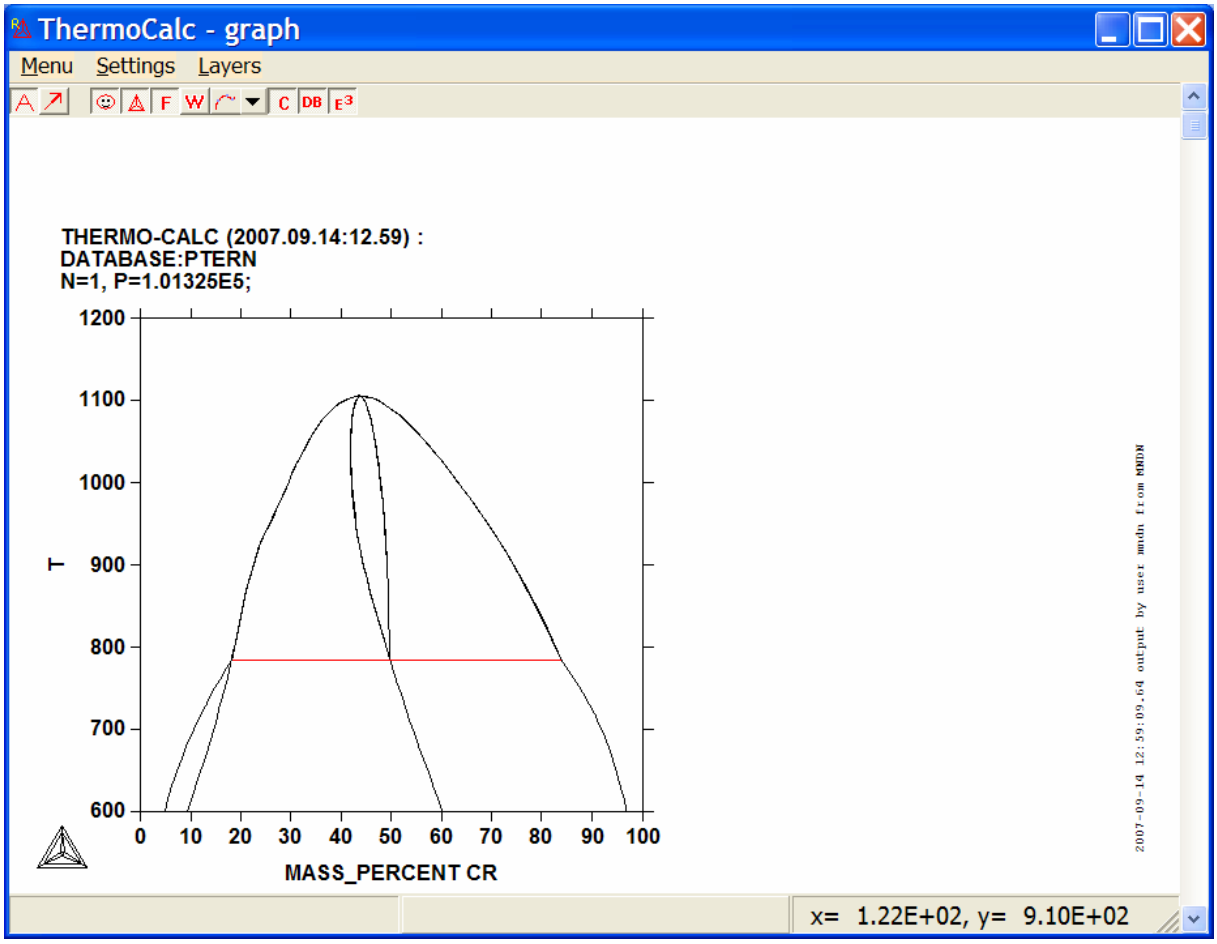
…Example 4 of the "Guide of examples" of Thermo-Calc

POLY-3:

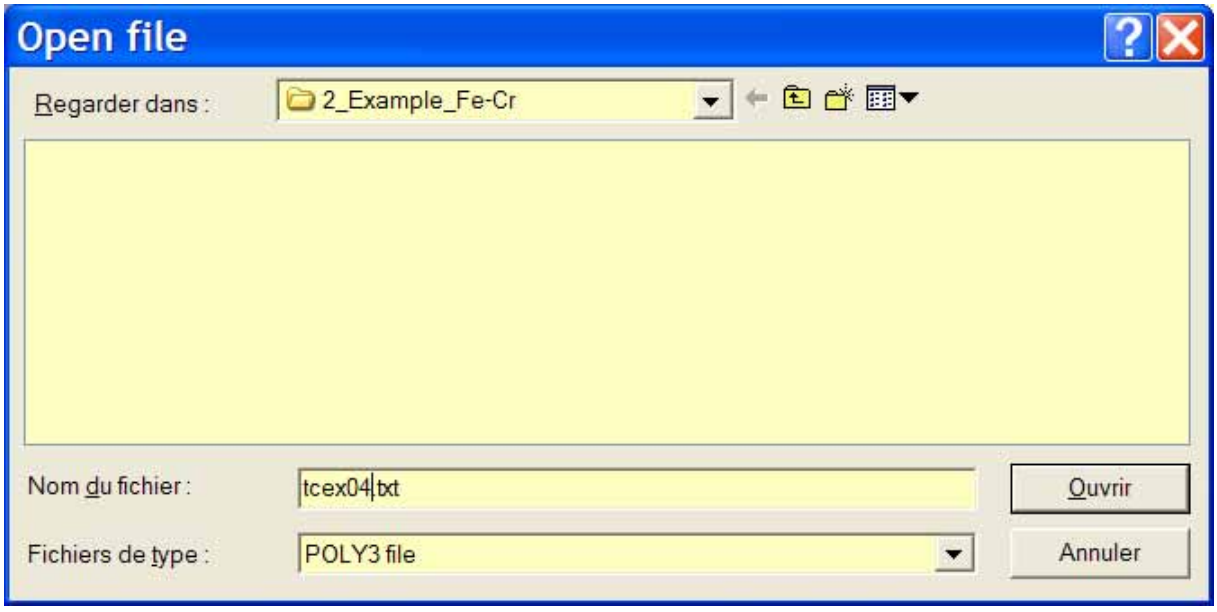
```
POLY_3: @@ There is a miscibility gap in BCC Fe-Cr. Prior to version R, we
POLY_3: @@ must tell the program by the command SPECIAL/SET_MISCIBILITY_GAP.
POLY_3: @@ From version R, the Global Minimization procedure can find the
POLY_3: @@ miscibility gap automatically.
POLY_3: @@ Let us first calculate the low temperature region.
POLY_3: s-c x(cr)=.6 t=700 p=101325 n=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated  548 grid points in  0 s
 Found the set of lowest grid points in   0 s
 Creating a new composition set BCC_A2#2
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: PTERN

 Conditions:
 X(CR)=0.6, T=700, P=1.01325E5, N=1
 DEGREES OF FREEDOM 0

 Temperature  700.00 K ( 426.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass  5.35364E+01
 Total Gibbs energy -2.30650E+04,  Enthalpy  1.31808E+04,  Volume  7.26677E-06

 Component               Moles      W-Fraction Activity   Potential   Ref.stat
 CR                      6.0000E-01 5.8274E-01 2.3706E-02 -2.1779E+04 SER
 FE                      4.0000E-01 4.1726E-01 1.3646E-02 -2.4994E+04 SER

 BCC_A2#1                   Status ENTERED     Driving force  0.0000E+00
 Number of moles 3.9881E-01, Mass 2.2098E+01         Mass fractions:
 FE  8.93536E-01  CR  1.06464E-01

 BCC_A2#2                   Status ENTERED     Driving force  0.0000E+00
 Number of moles 6.0119E-01, Mass 3.1438E+01         Mass fractions:
 CR  9.17510E-01  FE  8.24897E-02
POLY_3:@?
POLY_3: @@ Now make a calculation at a higher temperature
POLY_3: s-c t=900
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated  548 grid points in  0 s
 Found the set of lowest grid points in   0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: PTERN

 Conditions:
 X(CR)=0.6, T=900, P=1.01325E5, N=1
 DEGREES OF FREEDOM 0

 Temperature  900.00 K ( 626.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass  5.35364E+01
 Total Gibbs energy -3.49339E+04,  Enthalpy  2.36270E+04,  Volume  5.01460E-06

 Component               Moles      W-Fraction Activity   Potential   Ref.stat
```

```
 CR                      6.0000E-01 5.8274E-01 1.2780E-02 -3.2625E+04 SER
 FE                      4.0000E-01 4.1726E-01 5.9093E-03 -3.8397E+04 SER

 BCC_A2#1                    Status ENTERED     Driving force  0.0000E+00
 Number of moles 3.6758E-01, Mass 1.9458E+01        Mass fractions:
 CR  7.42505E-01  FE  2.57495E-01

 SIGMA                       Status ENTERED     Driving force  0.0000E+00
 Number of moles 6.3242E-01, Mass 3.4078E+01        Mass fractions:
 FE  5.08488E-01  CR  4.91512E-01
POLY_3: @?<Hit return to continue>
POLY_3: @@ The fe-cr phase diagram has three non-connected two-phase regions.
POLY_3: @@ This requires three initial equilibria and a special procedure to help the
POLY_3: @@ program to find these regions. But first we map the diagram once just to
POLY_3: @@ see the result of the first equilibrium calculation.
POLY_3: s-a-v 1 x(cr)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  0
Max value /1/:  1
Increment /.025/:
POLY_3: s-a-v 2
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/:  t
Min value /0/:  600
Max value /1/:  2200
Increment /40/:
POLY_3: @@ Always a SAVE command before MAP (or STEP) unless
POLY_3: @@ you want to overlay this calculation with an earlier one
POLY_3: save tcex04 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Organizing start points

 No initial equilibrium added, trying to fix one

 Phase region boundary   1 at:   7.559E-01  9.000E+02
    BCC_A2#1
  ** SIGMA
 Calculated    13 equilibria

 Phase region boundary   2 at:   8.468E-01  7.848E+02
    BCC_A2#1
    BCC_A2#2
  ** SIGMA

 Phase region boundary   3 at:   5.140E-01  7.848E+02
  ** BCC_A2#2
    SIGMA
 Terminating at known equilibrium
 Calculated    64 equilibria

 Phase region boundary   4 at:   8.468E-01  7.848E+02
    BCC_A2#1
  ** BCC_A2#2
 Calculated    23 equilibria

 Phase region boundary   5 at:   7.559E-01  9.000E+02
    BCC_A2#1
  ** SIGMA
 Terminating at known equilibrium
 *** Last buffer saved on file: tcex04.POLY3
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis
```

POST: s-d-a x w-p cr
POST: s-d-a y t
POST: PLOT SCREEN

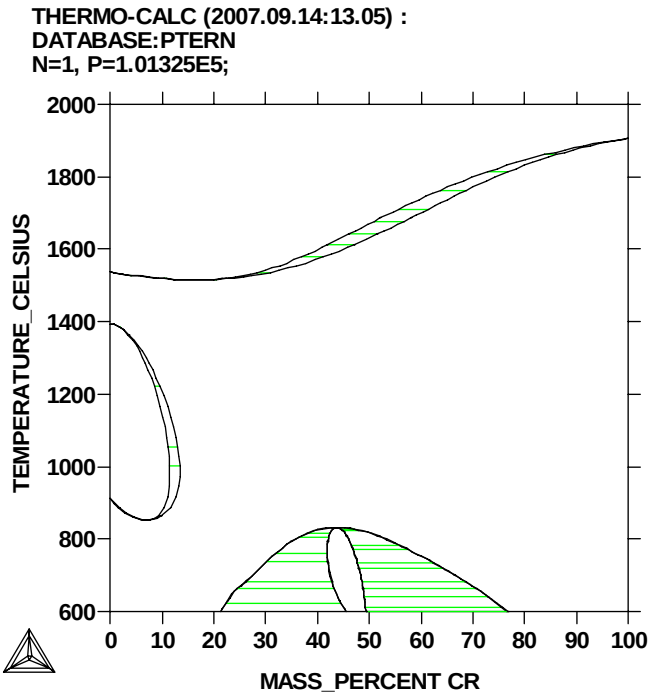



```
POST: @@ The bcc+sigma and bcc+bcc has been calculated correctly.
POST: @@ The program did not find any other two-phase regions as these are
POST: @@ not connected. Then we continue as follows...
POST: back
POLY_3: @@ Always a READ command after using the post processor
POLY_3: read tcex04
   ... the command in full is READ_WORKSPACES
POLY_3:
```



```
POLY_3:
POLY_3: @@ Chose new start point compositions and add these with a direction
POLY_3: s-c t=1300 x(cr)=.02
   ... the command in full is SET_CONDITION
POLY_3: add
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
Direction /Default/: ?
 Direction

  The direction is important when the initial equilibrium point is in a
  single-phase region or when the diagram is an isoplet (tie-lines not in
  the plane of calculation). In such cases, the program will search for a
  line in the diagram (i.e., a line where the amount of a phase is zero)
  in the given direction.

  Direction code(s):
      1 or 2   for positive direction of axis 1 or 2, respectively.
     -1 or -2  for negative direction of axis 1 or 2, respectively.
      Default  for all directions.

  From the TCC version M, the default direction is treated in a new way.
  The ADD command with the default direction will scan along the axis
  variables and generate start points each time the scan procedure crosses
  a phase boundary. In addition, it will generate 4 start points, scanning
  cross the middle of each axis, if there is any solubility line that does
  not reach the axes. At the MAP command, a search for lines in the diagram
  will be made along each direction of the axis variables in the diagram.
  In this way, it should guarantee that all possible phase boundary lines
  in a phase diagram are found. Of course, it may take a little longer time
  to execute than using the minimum number of start points, as some lines
  may be calculated more than once. But the POLY module remembers all node
  points and will subsequently stop calculations along a line when it finds
  a known node point.

  It is also possible to create a sequence of start points from one initial
  equilibria by appending a ">" after the direction at the ADD command.
  For example:

   Direction /default/: 2>

  This will generate one start point for each set of phase change in the
  positive direction of the axis 2; this will ensure successful finding
  of all phase boundary lines (not just the first one) in this direction.

  This is particularly useful when you have a phase diagram with several
  lines with no intersection. It is thus possible to calculate e.g. an
  isopleth for a much more limited composition range. It is also useful
  for calculating CVD diagrams.

Direction /Default/: 1
POLY_3: s-c t=1900 x(cr)=.5
   ... the command in full is SET_CONDITION
POLY_3: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: list-in
   ... the command in full is LIST_INITIAL_EQUILIBRIA
 No 1  +1  X(CR)=2E-2, T=1300, P=101325, N=1
 No 2  -2  X(CR)=0.5, T=1900, P=101325, N=1.
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ The command ADD gives us a new startingpoint for the mapping. 1 referes
POLY_3: @@ to positive direction on the x-axis and -2 means negative direction on the
POLY_3: @@ y-axis.

POLY_3: @@
POLY_3: @@ It is important NOT to give a SAVE command this time as that would destroy
POLY_3: @@ the results from the previous calculation.
POLY_3: map
 Organizing start points

Using ADDED start equilibria

 Calculated    57 equilibria

 Phase region boundary   1 at:   1.208E-01  1.300E+03
  ** BCC_A2#1
     FCC_A1
 Calculated    21 equilibria

 Phase region boundary   2 at:   1.208E-01  1.300E+03
  ** BCC_A2#1
     FCC_A1
 Calculated    24 equilibria

 Phase region boundary   3 at:   4.580E-01  1.900E+03
     LIQUID
  ** BCC_A2#1
 Calculated    41 equilibria

 Phase region boundary   4 at:   4.580E-01  1.900E+03
     LIQUID
  ** BCC_A2#1
 Calculated    43 equilibria
 *** Last buffer saved on file: tcex04.POLY3
POLY_3: post
```

POST: s-d-a x w-p cr
POST: s-d-a y t-c
POST: s-s-s y n 600 2000
POST: s-t-s 6
POST: PLOT SCREEN



Clicking the mouse-right-button on a selected point and then choosing the “Add label” option