

Equilibrium Phase Diagrams

-Training Course-

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Part 3

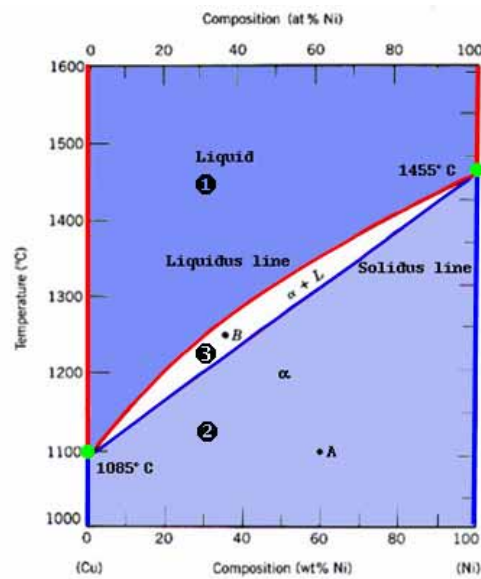
 **Thermo-Calc software. Examples**

Example 1: Cu-Ni system.....2

Example 2: Fe-Cr system.....27

EXAMPLE 1

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



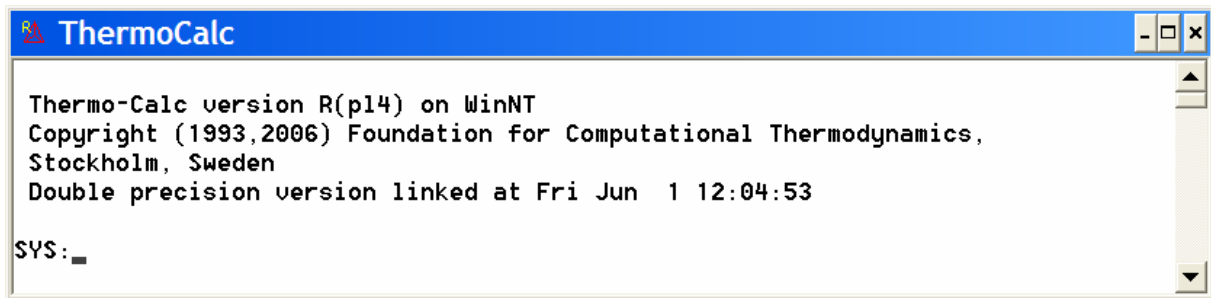
Exercise 1: Selecting the thermodynamic functions (TDB and GES modules).....2

Exercise 2: Calculating and plotting the phase diagram (POLY and POST modules).....11

Exercise 3: Plotting the molar Gibbs energy curves $G=f(X)$ (POLY and POST modules).....22

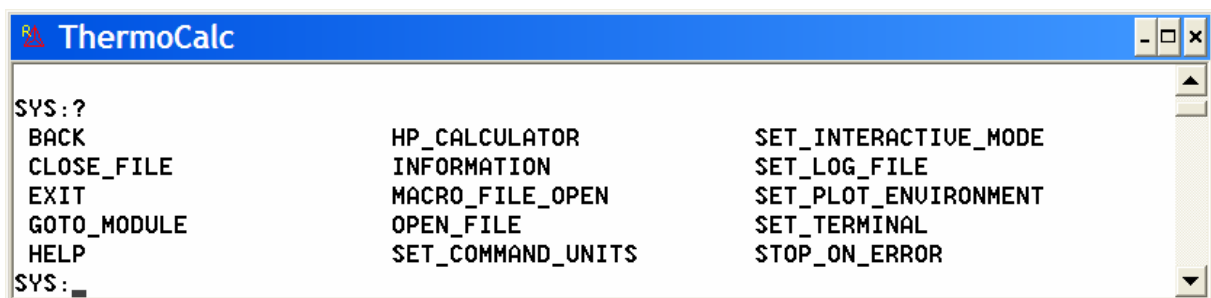
1. SELECTING THE THERMODYNAMIC FUNCTIONS OF THE SYSTEM

Running Thermo-Calc application: Execute "TCCR.exe"



SYS: ? (↵)

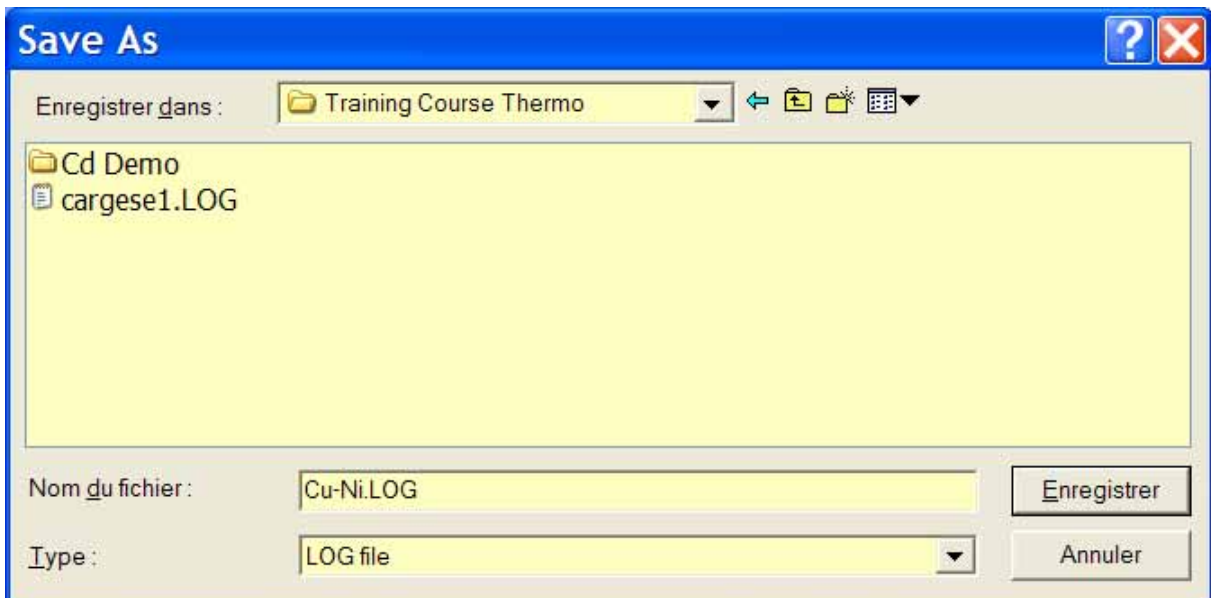
...This command lists the available commands



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

```

ThermoCalc

Thermo-Calc version R(p14) on WinNT
Copyright (1993,2006) Foundation for Computational Thermodynamics,
Stockholm, Sweden
Double precision version linked at Fri Jun  1 12:04:53

SYS:s-l-f
Heading:Cu-Ni phase diagram
SYS:

```

...Selection of the suitable database SSOL2:

SYS: go da

...This command in full is GOTO_MODULE DATABASE_RETRIEVAL
 ...Access to the Thermodynamic DataBase module (TDB)

```

ThermoCalc

SYS:go da
THERMODYNAMIC DATABASE module running on PC/WINDOWS NT
Current database: Database CECM-CTG 2007

UA                /-  DEFINED
TDB_USER:

```

TDB-USER: ?

```

ThermoCalc

TDB_USER: ?
AMEND_SELECTION      EXIT                  NEW_DIRECTORY_FILE
APPEND_DATABASE      GET_DATA             REJECT
BACK                 GOTO_MODULE          RESTORE
DATABASE_INFORMATION HELP                 SET_AUTO_APPEND_DATABASE
DEFINE_ELEMENTS      INFORMATION          SWITCH_DATABASE
DEFINE_SPECIES       LIST_DATABASE
DEFINE_SYSTEM        LIST_SYSTEM
TDB_USER:

```

TDB-USER: sw da

...This command in full is SWITCH_DATABASE
 ...All the available databases are listed

```

ThermoCalc
TDB_USER:sw da
Use one of these databases

USER      = Database CECM-CTG 2007
SBIN2     = SGTE Binary Alloys Database v.2
SSOL2     = SGTE Solution database v.2
TCMP2     = TCS Materials processing database
TTAL4     = Thermo-Tech Al-alloy database
TTNI7     = Thermo-Tech Ni-alloy database v.7
COST2     = COST507 Light Alloys Database v.2
PKP       = Kaufman Binary Alloys Database
PAQ2      = TCS Public Aqueous database
PBIN      = TCS public binary database
PCHAT     = Chatenay-Malabry binary database
PFRIB     = Fridberg dilute Fe-Alloy diffusion db
PG35      = III-U Binary Semi-Conductors Database
PGE0      = Saxena Geochemical Database
PION      = TCS public ionic database
PSUB      = TCS public ionic database
PURE4     = SGTE pure element database v.4
PTERN     = TCS public ternary database
ZRBASE    = base Zr publique, PhD C.Toffolon
COST      = COST507 Light Alloys Database v.1
USER      = User defined Database

DATABASE NAME /USER/:

```

TDB-USER: **SSOL2**

```

ThermoCalc
DATABASE NAME /USER/: SSOL2
Current database: SGTE Solution database v.2

UA  DEFINED
B2_BCC          L12_FCC          AL5FE4:
GAS:G REJECTED
TDB_SSOL2:

```

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

TDB-SSOL2: **def-el**

...This command in full is DEFINE_ELEMENTS

```

ThermoCalc
TDB_SSOL2: def-el
ELEMENTS:

```

ELEMENTS: **Cu Ni**

```

ThermoCalc
TDB_SSOL2: def-el
ELEMENTS: Cu Ni
CU          NI  DEFINED
TDB_SSOL2:

```

TDB-SSOL2: **l-sys (-)**

...This command in full is LIST_SYSTEM

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

```
ThermoCalc
TDB_SSOL2:l-sys
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
LIQUID:L      :CU NI:
FCC_A1       :CU NI:UA:
  > This is also the MC(1-x) carbide or nitride
BCC_A2       :CU NI:UA:
HCP_A3       :CU NI:UA:
  > This is also the M2C carbide and M2N nitride
CBCC_A12     :NI:UA:
  > The alpha-Mn phase
CUB_A13      :NI:UA:
  > The betha-Mn phase
FE4N        :NI:UA:
AL3NI2       :NI:NI:
  >This is the ordered HCP in A1-Ni
ALNI_B2      :NI UA:NI:
  >This is the B2 phase in A1-Ni
CUZN_EPS     :CU:
ALCU_EPSILON :CU:CU:
ALCU_ETA     :CU:CU:
TDB_SSOL2:
```

...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

```
ThermoCalc
TDB_SSOL2:rej ph *
LIQUID:L      FCC_A1      BCC_A2
HCP_A3        CBCC_A12    CUB_A13
FE4N          AL3NI2      ALNI_B2
CUZN_EPS      ALCU_EPSILON ALCU_ETA
REJECTED
TDB_SSOL2:
```

TDB-SSOL2: rest ph liquid fcc

...This command in full is RESTORE PHASES liquid fcc

```
ThermoCalc
TDB_SSOL2:rest ph liquid fcc
LIQUID:L      FCC_A1  RESTORED
TDB_SSOL2: _
```

TDB-SSOL2: l-sys con

...This command in full is LIST_SYSTEM CONSTITUENTS

```
ThermoCalc
TDB_SSOL2:l-sys con
LIQUID:L      :CU NI:
FCC_A1       :CU NI:UA:
  > This is also the MC(1-x) carbide or nitride
TDB_SSOL2:
```

TDB-SSOL2: get

...This command in full is GET_DATA

...Retrieval of all information from the thermodynamic databank

```

ThermoCalc
TDB_SSOL2:get
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

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

The list of references can be obtained in the Gibbs Energy System also
by the command LIST_DATA and option R

-OK-
TDB_SSOL2:

```

...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 Gibbs Energy System module (GES)

```

ThermoCalc

The list of references can be obtained in the Gibbs Energy System also
by the command LIST_DATA and option R

-OK-
TDB_SSOL2:go gibbs
GIBBS ENERGY SYSTEM version 5.2
GES:

```

GES: ?

```

ThermoCalc

GES: ?
ADD_COMMENT          ENTER_PHASE          LIST_PHASE_DATA
AMEND_ELEMENT_DATA   ENTER_SPECIES        LIST_STATUS
AMEND_PARAMETER      ENTER_SYMBOL         LIST_SYMBOLS
AMEND_PHASE_DESCRIPTION EXIT                 PATCH_WORKSPACE
AMEND_SYMBOL         GOTO_MODULE          READ_GES_WORKSPACE
BACK                 HELP                 REINITIATE
CHANGE_STATUS        INFORMATION          SAVE_GES_WORKSPACE
DELETE              LIST_CONSTITUTION   SET_INTERACTIVE
ENTER_ELEMENT        LIST_DATA            SET_R_AND_P_NORM
ENTER_PARAMETER      LIST_PARAMETER

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**

```
ThermoCalc
GES: l-p-d
Phase name: liquid

LIQUID
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: CU,NI

G(LIQUID, CU; 0) - H298(FCC_A1, CU; 0) =
  298.15 < T < 1358.02: +12964.84 - 9.510243 * T - 5.83932E-21 * T ** 7 + GHSERCU
  1358.02 < T < 3200.00: +13495.4 - 9.920463 * T - 3.64643E+29 * T ** (-9)
  + GHSERCU
G(LIQUID, NI; 0) - H298(FCC_A1, NI; 0) =
  298.15 < T < 1728.00: +11235.527 + 108.457 * T - 22.096 * T * LN(T)
  - .0048407 * T ** 2 - 3.82318E-21 * T ** 7
  1728.00 < T < 3000.00: -9549.775 + 268.598 * T - 43.1 * T * LN(T)
L(LIQUID, CU, NI; 0) = +11760 + 1.084 * T
L(LIQUID, CU, NI; 1) = -1671.8

GES:
```

GES: **l-p-d**

... This command in full is LIST_PHASE_DATA

Phase name: **fcc**

```
ThermoCalc
GES: l-p-d
Phase name: fcc

FCC_A1
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
ADDITIONAL CONTRIBUTION FROM MAGNETIC ORDERING
Magnetic function below Curie Temperature
+1-.860338755 * TAO ** (-1) - .17449124 * TAO ** 3 - .00775516624 * TAO ** 9
-.0017449124 * TAO ** 15
Magnetic function above Curie Temperature
-.0426902268 * TAO ** (-5) - .0013552453 * TAO ** (-15)
-2.84601512E-04 * TAO ** (-25)
2 SUBLATTICES, SITES 1: 1
CONSTITUENTS: CU, NI : UA

G(FCC_A1, CU; UA; 0) - H298(FCC_A1, CU; 0) = 298.15 < T < 3200.00: + GHSERCU
G(FCC_A1, NI; UA; 0) - H298(FCC_A1, NI; 0) = 298.15 < T < 3000.00: + GHSERNI
TC(FCC_A1, NI; UA; 0) = 633
BMAGN(FCC_A1, NI; UA; 0) = .52
L(FCC_A1, CU, NI; UA; 0) = +8366 + 2.802 * T
L(FCC_A1, CU, NI; UA; 1) = -4359.6 + 1.812 * T
TC(FCC_A1, CU, NI; UA; 0) = -935.5
TC(FCC_A1, CU, NI; UA; 1) = -594.9
BMAGN(FCC_A1, CU, NI; UA; 0) = -.7316
BMAGN(FCC_A1, CU, NI; UA; 1) = -.3174

GES: _
```

GES: **l-sy**

... This command in full is LIST_SYMBOL

NAME: **GHSERCU**

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

```
ThermoCalc
GES: l-sy
NAME: GHSERCU
OUTPUT TO SCREEN OR FILE /SCREEN/:
SYMBOL      STATUS  VALUE/FUNCTION
  3 GHSERCU  20000000
  298.15 < T < 1358.02: -7770.458 + 130.485403 * T - 24.112392 * T * LN(T)
  -.00265684 * T ** 2 + 1.29223E-07 * T ** 3 + 52478 * T ** (-1)
  1358.02 < T < 3200.00: -13542.33 + 183.804197 * T - 31.38 * T * LN(T)
  + 3.64643E+29 * T ** (-9)

GES: _
```

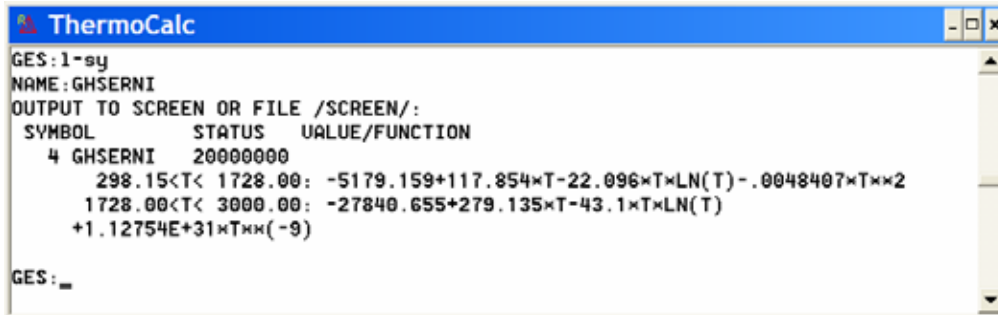

...Listing the using functions GHSERCU and GHSERNI

GES: l-sy

...This command in full is LIST_SYMBOL

NAME: GHSERNI

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



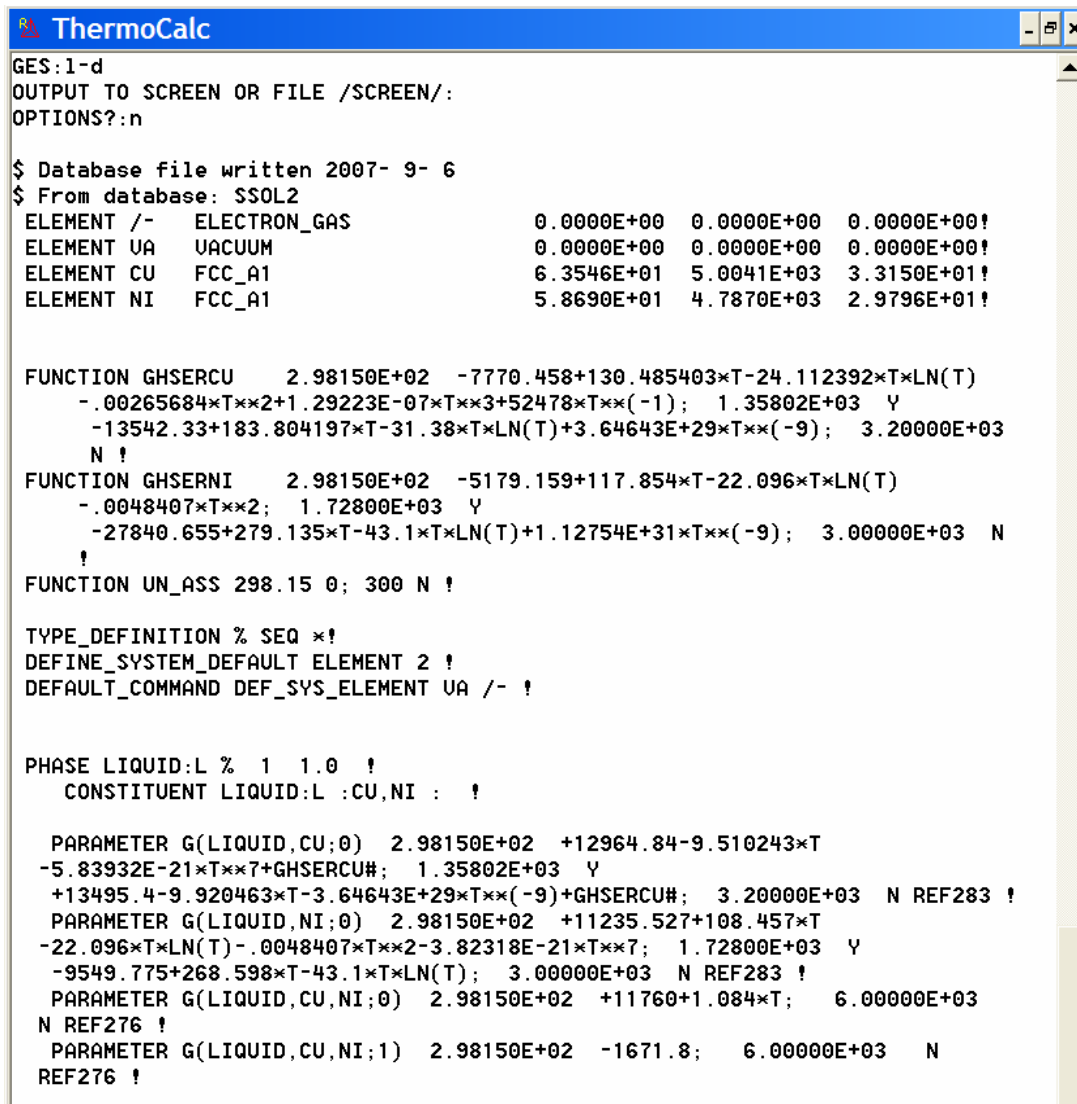
```
ThermoCalc
GES:l-sy
NAME:GHSERNI
OUTPUT TO SCREEN OR FILE /SCREEN/:
SYMBOL      STATUS      VALUE/FUNCTION
  4 GHSERNI  20000000
    298.15<T< 1728.00: -5179.159+117.854*T-22.096*T*LN(T)-.0048407*T**2
    1728.00<T< 3000.00: -27840.655+279.135*T-43.1*T*LN(T)
    +1.12754E+31*T**(-9)
GES: _
```

...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 (↵)



```
ThermoCalc
GES:l-d
OUTPUT TO SCREEN OR FILE /SCREEN/:
OPTIONS?:n

$ Database file written 2007- 9- 6
$ From database: $$SOL2
ELEMENT /-   ELECTRON_GAS      0.0000E+00  0.0000E+00  0.0000E+00!
ELEMENT UA   UACUUM            0.0000E+00  0.0000E+00  0.0000E+00!
ELEMENT CU   FCC_A1            6.3546E+01  5.0041E+03  3.3150E+01!
ELEMENT NI   FCC_A1            5.8690E+01  4.7870E+03  2.9796E+01!

FUNCTION GHSERCU  2.98150E+02 -7770.458+130.485403*T-24.112392*T*LN(T)
-.00265684*T**2+1.29223E-07*T**3+52478*T**(-1); 1.35802E+03 Y
-13542.33+183.804197*T-31.38*T*LN(T)+3.64643E+29*T**(-9); 3.20000E+03
N !
FUNCTION GHSERNI  2.98150E+02 -5179.159+117.854*T-22.096*T*LN(T)
-.0048407*T**2; 1.72800E+03 Y
-27840.655+279.135*T-43.1*T*LN(T)+1.12754E+31*T**(-9); 3.00000E+03 N
!
FUNCTION UN_ASS 298.15 0; 300 N !

TYPE_DEFINITION % SEQ *!
DEFINE_SYSTEM_DEFAULT ELEMENT 2 !
DEFAULT_COMMAND DEF_SYS_ELEMENT UA /- !

PHASE LIQUID:L % 1 1.0 !
  CONSTITUENT LIQUID:L :CU,NI : !

PARAMETER G(LIQUID,CU;0) 2.98150E+02 +12964.84-9.510243*T
-5.83932E-21*T**7+GHSERCU#; 1.35802E+03 Y
+13495.4-9.920463*T-3.64643E+29*T**(-9)+GHSERCU#; 3.20000E+03 N REF283 !
PARAMETER G(LIQUID,NI;0) 2.98150E+02 +11235.527+108.457*T
-22.096*T*LN(T)-.0048407*T**2-3.82318E-21*T**7; 1.72800E+03 Y
-9549.775+268.598*T-43.1*T*LN(T); 3.00000E+03 N REF283 !
PARAMETER G(LIQUID,CU,NI;0) 2.98150E+02 +11760+1.084*T; 6.00000E+03
N REF276 !
PARAMETER G(LIQUID,CU,NI;1) 2.98150E+02 -1671.8; 6.00000E+03 N
REF276 !
```

```

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% : UA% : !

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

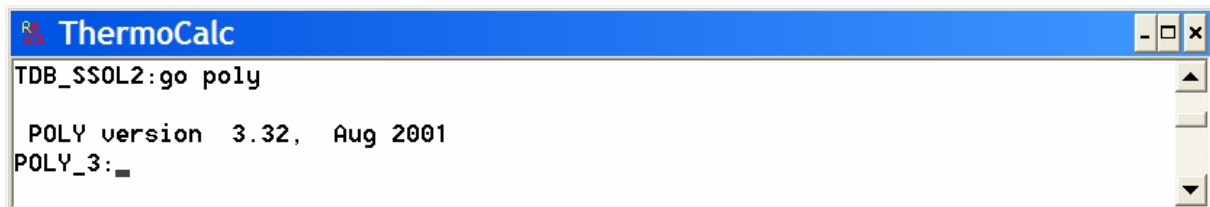
You must have preliminary retrieved the thermodynamic data in the TDB module, which implying to have done all the steps of the exercise 1, from the beginning to the “GET” command page 7 (cf. Option 2).

...Setting conditions

TDB-SSOL2: go poly

...This command in full is GOTO_MODULE POLY-3

...Access to the Equilibrium Calculation Module (POLY)

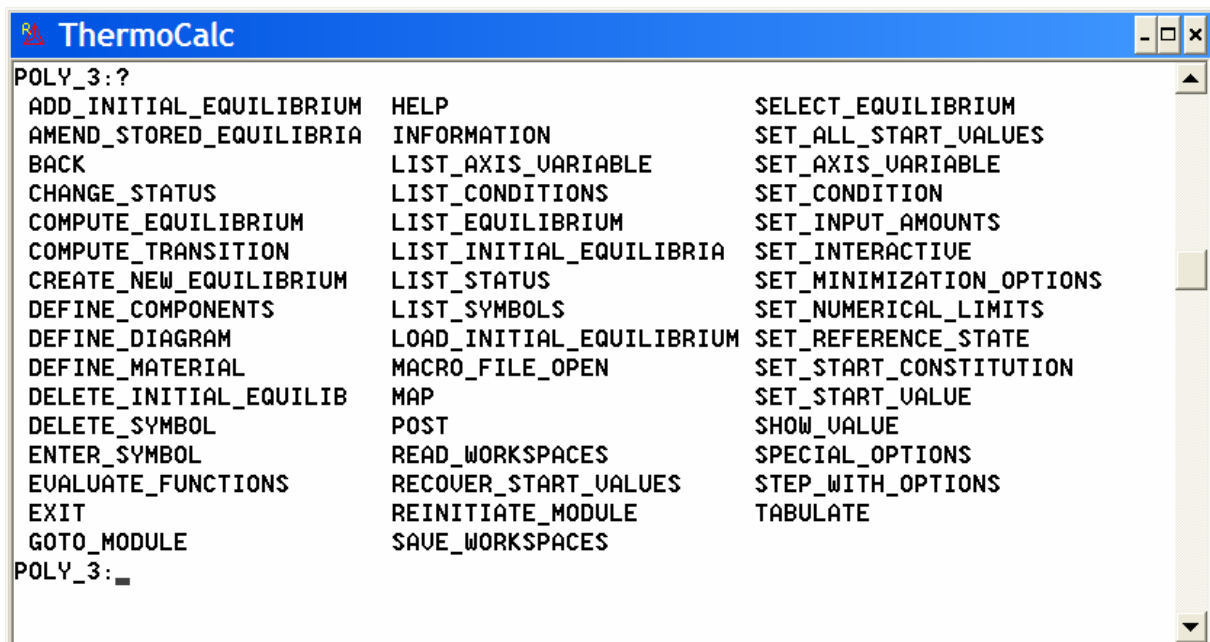


```
ThermoCalc
TDB_SSOL2:go poly

POLY version 3.32, Aug 2001
POLY_3: _
```

POLY_3: ?

...This command lists the available commands



```
ThermoCalc
POLY_3:?
ADD_INITIAL_EQUILIBRIUM  HELP
AMEND_STORED_EQUILIBRIA  INFORMATION
BACK                     LIST_AXIS_VARIABLE
CHANGE_STATUS            LIST_CONDITIONS
COMPUTE_EQUILIBRIUM      LIST_EQUILIBRIUM
COMPUTE_TRANSITION        LIST_INITIAL_EQUILIBRIA
CREATE_NEW_EQUILIBRIUM    LIST_STATUS
DEFINE_COMPONENTS         LIST_SYMBOLS
DEFINE_DIAGRAM            LOAD_INITIAL_EQUILIBRIUM
DEFINE_MATERIAL           MACRO_FILE_OPEN
DELETE_INITIAL_EQUILIB    MAP
DELETE_SYMBOL            POST
ENTER_SYMBOL              READ_WORKSPACES
EVALUATE_FUNCTIONS        RECOVER_START_VALUES
EXIT                      REINITIATE_MODULE
GOTO_MODULE               SAVE_WORKSPACES
POLY_3: _
SELECT_EQUILIBRIUM
SET_ALL_START_VALUES
SET_AXIS_VARIABLE
SET_CONDITION
SET_INPUT_AMOUNTS
SET_INTERACTIVE
SET_MINIMIZATION_OPTIONS
SET_NUMERICAL_LIMITS
SET_REFERENCE_STATE
SET_START_CONSTITUTION
SET_START_VALUE
SHOW_VALUE
SPECIAL_OPTIONS
STEP_WITH_OPTIONS
TABULATE
```

POLY_3: s-c n=1 p=101325 t=2000 w(ni)=0.5

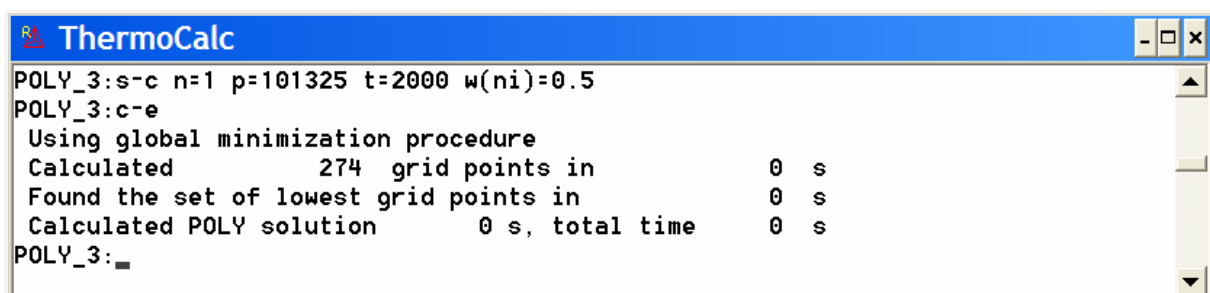
...This command in full is SET_CONDITION

...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



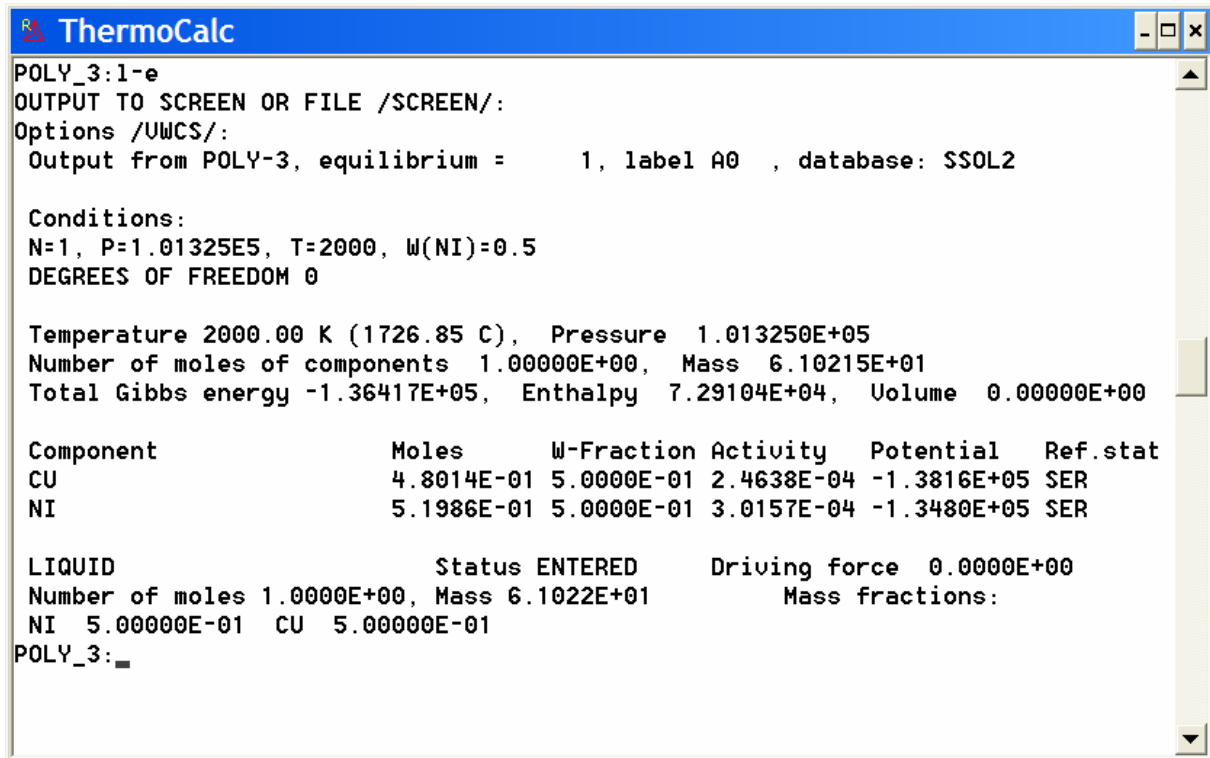
```
ThermoCalc
POLY_3:s-c n=1 p=101325 t=2000 w(ni)=0.5
POLY_3:c-e
Using global minimization procedure
Calculated      274 grid points in          0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time 0 s
POLY_3: _
```

POLY_3: l-e

...This command in full is LIST_EQUILIBRIUM

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

Options /VWCS/ : (↵)



```
POLY_3:l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium =      1, label A0  , database: SSOL2

Conditions:
N=1, P=1.01325E5, T=2000, W(NI)=0.5
DEGREES OF FREEDOM 0

Temperature 2000.00 K (1726.85 C), Pressure 1.01325E+05
Number of moles of components 1.00000E+00, Mass 6.10215E+01
Total Gibbs energy -1.36417E+05, Enthalpy 7.29104E+04, Volume 0.00000E+00

Component           Moles      W-Fraction Activity   Potential   Ref.stat
CU                   4.8014E-01 5.0000E-01 2.4638E-04 -1.3816E+05 SER
NI                   5.1986E-01 5.0000E-01 3.0157E-04 -1.3480E+05 SER

LIQUID                Status ENTERED      Driving force 0.0000E+00
Number of moles 1.0000E+00, Mass 6.1022E+01      Mass fractions:
NI 5.0000E-01  CU 5.0000E-01
POLY_3: _
```

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

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

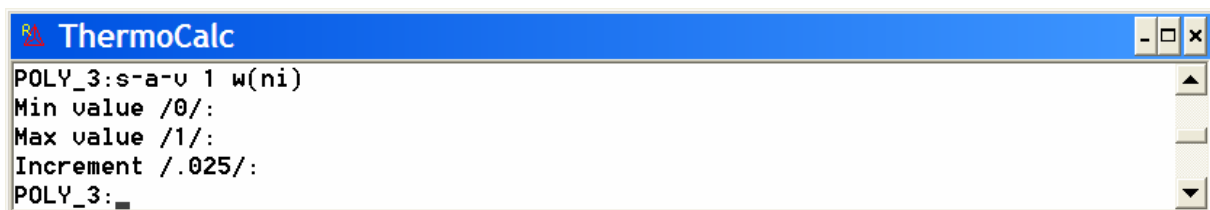
...This command in full is SET_AXIS_VARIABLE

...This means that the axis number 1 is taken to be the mass fraction of Ni

Min value /0/: 0 (↵)

Max value /1/: 1 (↵)

Increment /0.025/: (↵)



```
POLY_3:s-a-v 1 w(ni)
Min value /0/:
Max value /1/:
Increment /0.025/:
POLY_3: _
```

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/: (↵)

```
ThermoCalc
POLY_3:s-a-u 2 t
Min value /0/: 600
Max value /1/: 2500
Increment /47.5/:
POLY_3: _
```

POLY_3: map

```
ThermoCalc
POLY_3:map
Automatic saving workspaces on
USERPROFILE\RESULT.POLY3

Organizing start points

No initial equilibrium added, trying to fix one
Automatic saving workspaces on
USERPROFILE\RESULT.POLY3

Phase region boundary 1 at: 5.000E-01 1.594E+03
LIQUID
** FCC_A1
Calculated 42 equilibria

Phase region boundary 2 at: 5.000E-01 1.594E+03
LIQUID
** FCC_A1
Calculated 32 equilibria
*** Last buffer saved on file: USERPROFILE\RESULT.POLY3
POLY_3: _
```

...Plotting the diagram

POLY_3: post

```
ThermoCalc
POLY_3:post

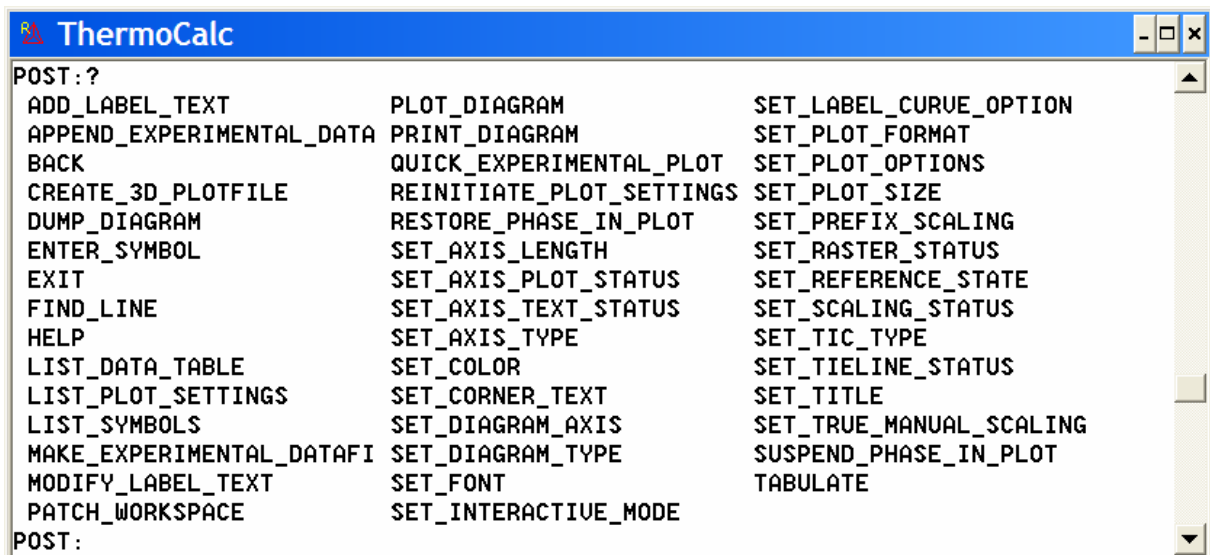
POLY-3 POSTPROCESSOR UERSION 3.2 , last update 2002-12-01

Setting automatic diagram axis

POST:
```

...Defining the two axis variables for plotting

POST: ?

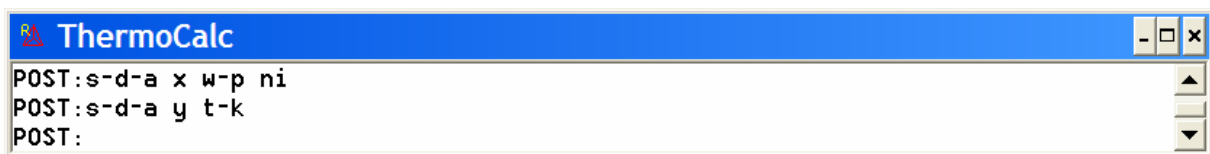


POST: s-d-a x w-p ni

...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

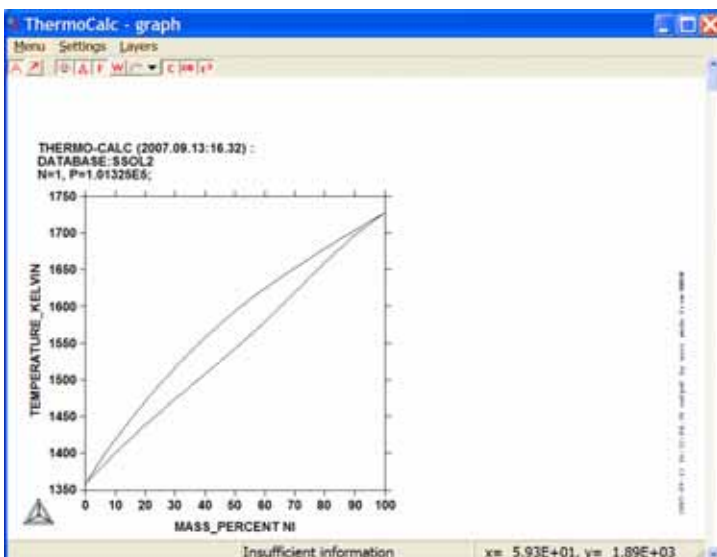
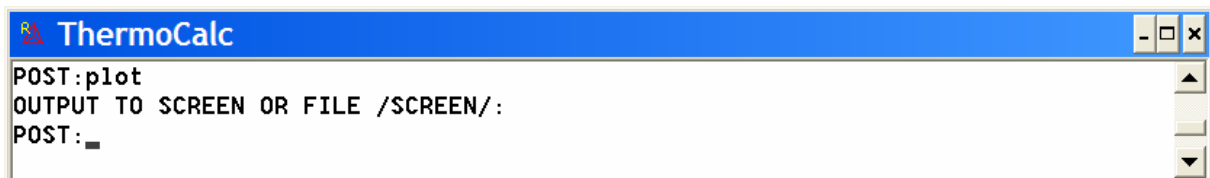
...This means that the Y axis variable is taken to be the temperature in K (t-k)
 ...Other possible choice: temperature-Celsius (t-c)



...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

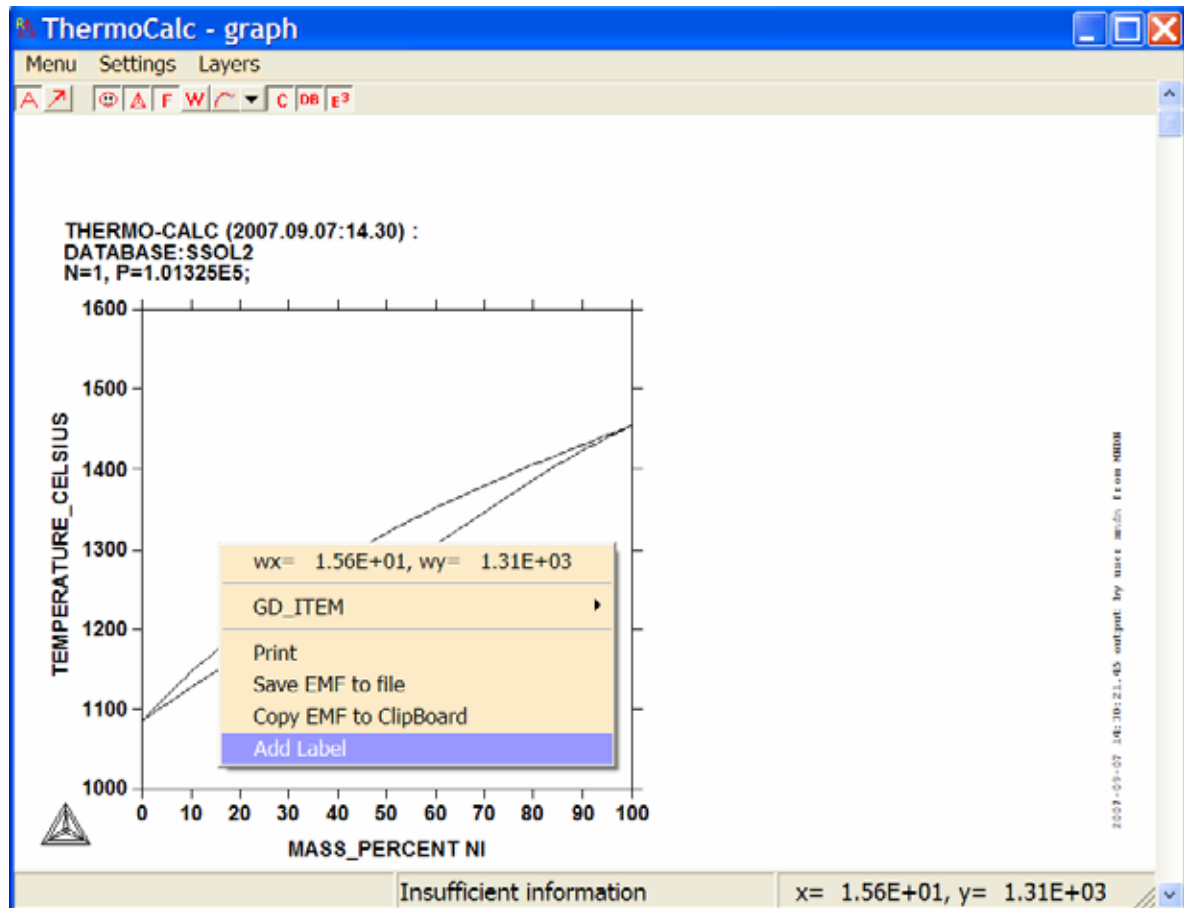
MIN VALUE : 1000

MAX VALUE : 1600

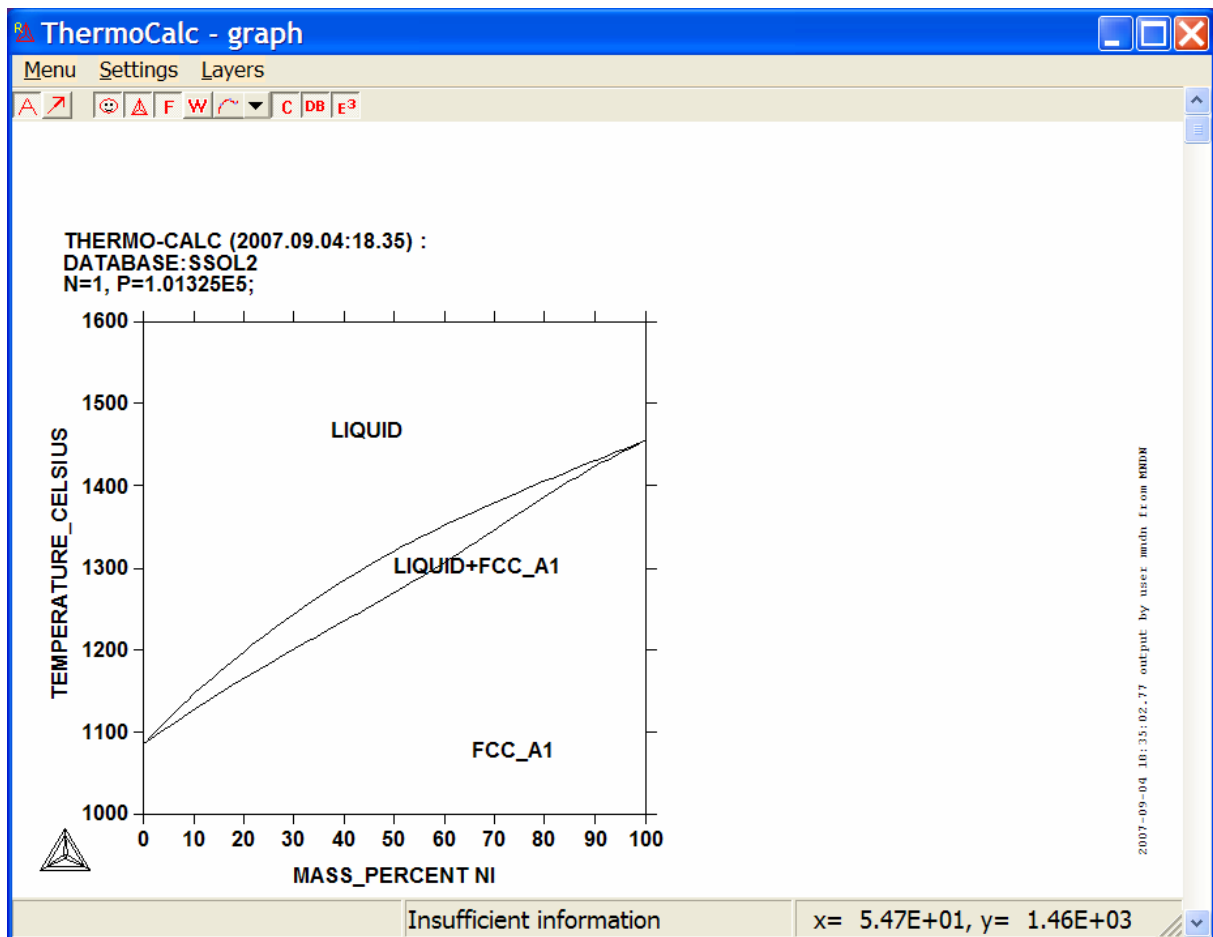
```
ThermoCalc
POST:s-d-a y t-c
POST:s-s-s
AXIS (X, Y OR Z) :y
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE :1000
MAX VALUE :1600
POST:
```

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 NO /0/: ? (↵)

PLOTTING EVERY TIE-LINE NO /0/: 1 (↵)

POST: PLOT

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

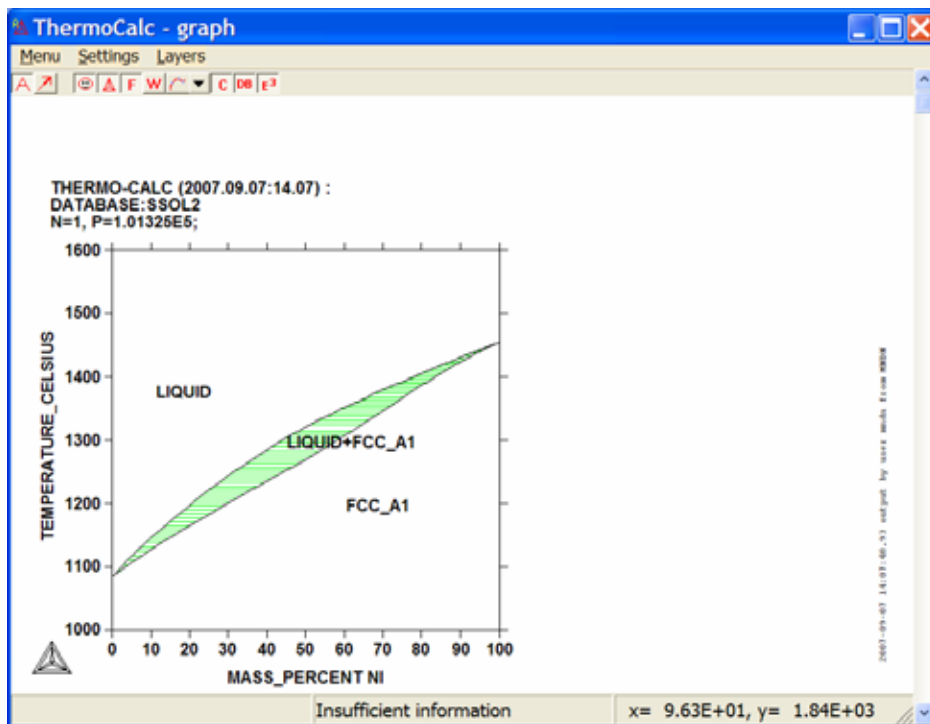
```

ThermoCalc
POST:s-t-s
PLOTTING EVERY TIE-LINE NO /0/: ?

PLOTTING EVERY TIE-LINE NO

The tie-lines plotted will not be equally spaced by the graphics software.
Instead, the user may select to plot a subset of the calculated tie-lines,
i.e., every one (1), every second (2), every three (3), etc. By accepting
the default value 0, no tie-line will be plotted.

PLOTTING EVERY TIE-LINE NO /0/: 1
POST:plot
OUTPUT TO SCREEN OR FILE /SCREEN/:
POST:
  
```

...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

```

ThermoCalc
POST:s-p-f
CURRENT DEVICE: MS-Windows
GRAPHIC DEVICE NUMBER /1/ : ?

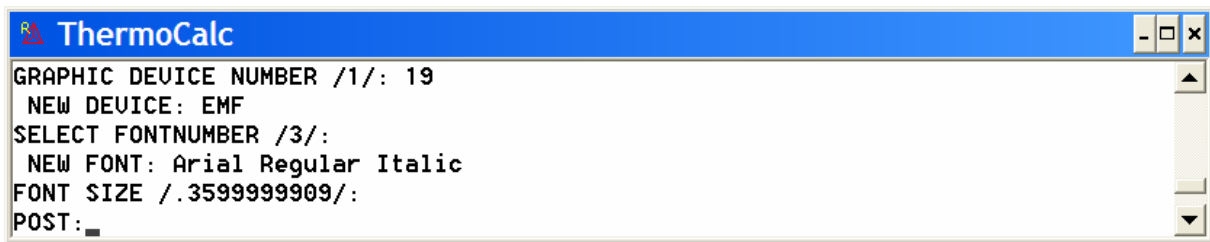
Available Graphic Devices:

Device 1 is MS-Windows
Device 2 is UT240/Kermit Tek.4010 emulation
Device 3 is COMPIS Tek.4010 emulation
Device 4 is Regis graphics
Device 5 is Postscript portrait mode
Device 6 is Postscript landscape mode
Device 7 is HPGL plotter (HP7475 landscape A4)
Device 8 is HPGL plotter (HP7475 portrait A4)
Device 9 is Tektronix 4010
Device 10 is Tandberg 2200/9S, Tek.4010
Device 11 is HP-LaserJet II / HP-DeskJet (1Mb)
Device 12 is Tektronix 4105
Device 13 is Tektronix 4107
Device 14 is HP-LaserJet III & IV, portrait (2Mb)
Device 15 is HP-LaserJet III & IV, landscape (2Mb)
Device 16 is Color Postscript portrait mode
Device 17 is Color Postscript landscape mode
Device 18 is HP-LaserJet II / HP-DeskJet (1Mb) large
Device 19 is EMF
GRAPHIC DEVICE NUMBER /1/ :
  
```

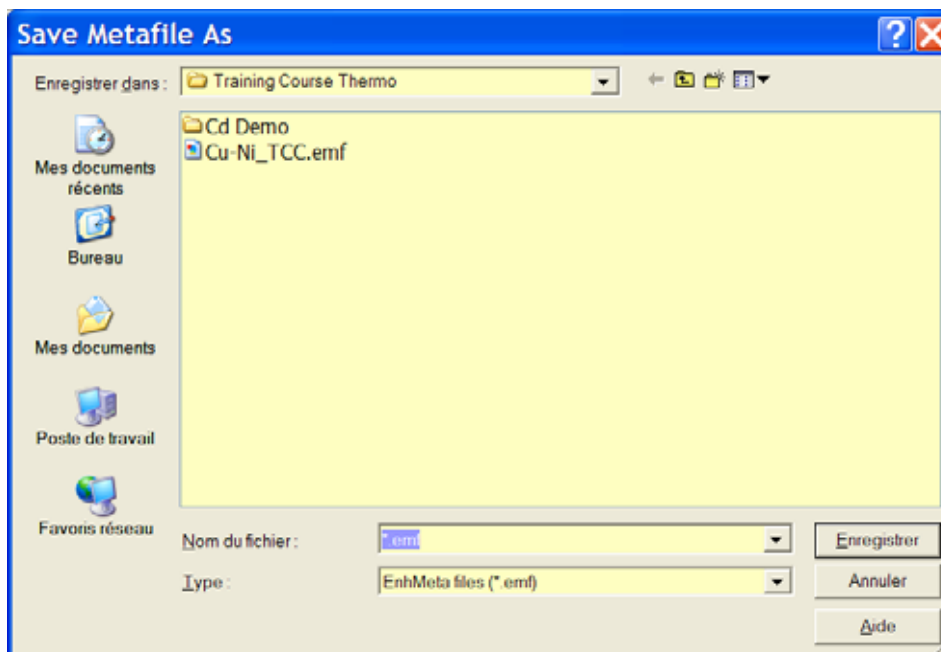
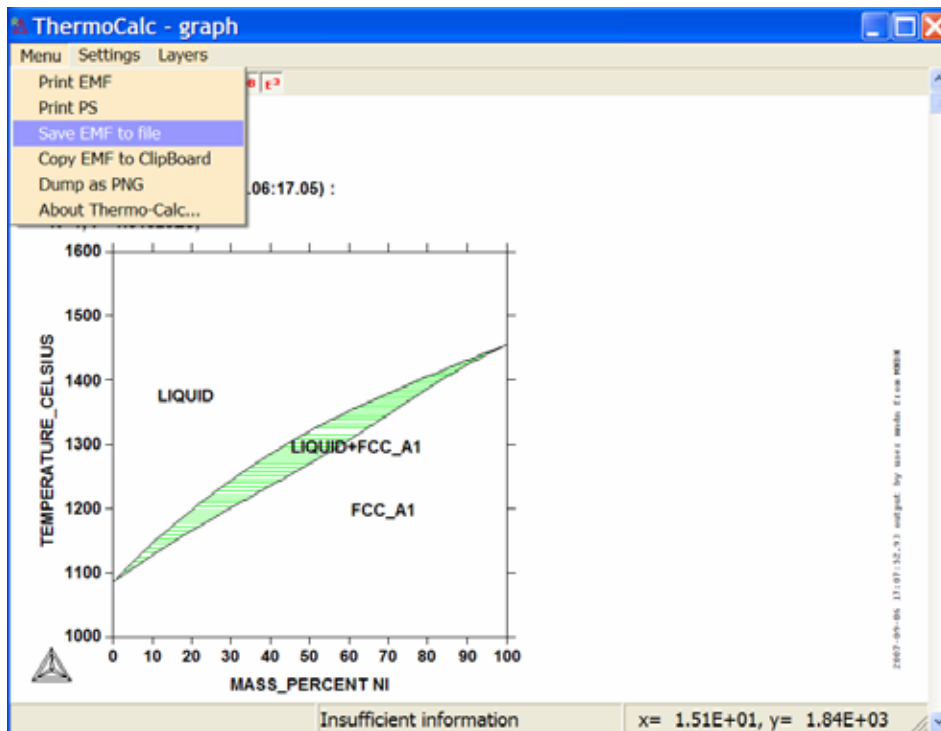
GRAPHIC DEVICE NUMBER /1/ : 19

SELECT FONTNUMBER /3/ : (↓)

FONT SIZE /0.35/ : (↓)

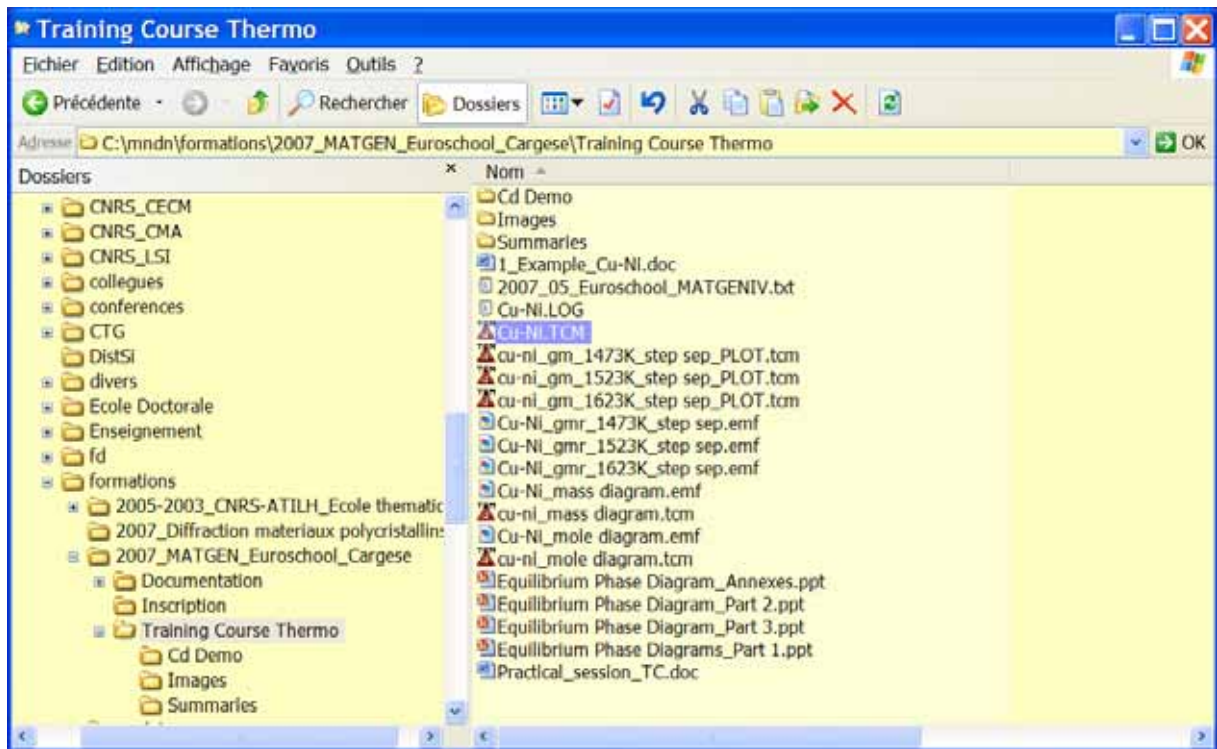


POST: PLOT
 OUTPUT TO SCREEN OR FILE /SCREEN/ : (↵)



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”



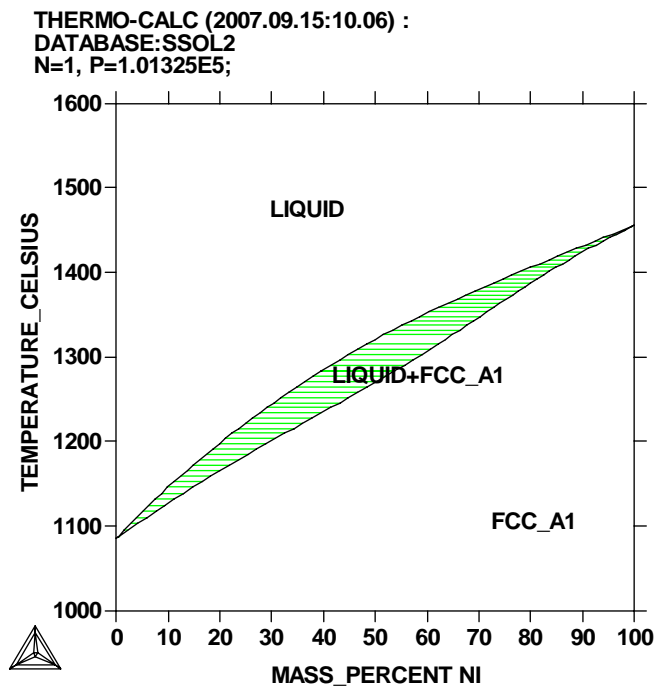
...The TCM file can be opened by any text editor.

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
  
```


...Execute the TCM file



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

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

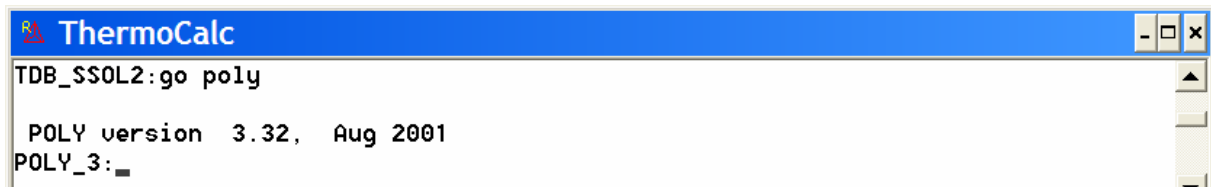
You must have preliminary retrieved the thermodynamic data in the TDB module, which implying to have done all the steps of the exercise 1, from the beginning to the “GET” command page 7 (cf. Option 3).

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 $T=1200^{\circ}\text{C}$ (1473K)

TDB-SSOL2: **go poly**

...This command in full is GOTO_MODULE POLY-3
...Access to the Equilibrium Calculation Module (POLY)



```
ThermoCalc
TDB_SSOL2:go poly

POLY version 3.32, Aug 2001
POLY_3: _
```

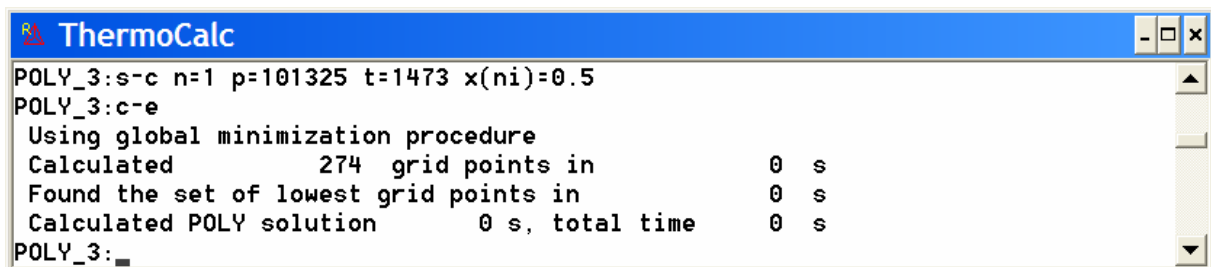
...Calculating the equilibrium for the given set of conditions ($T=1473\text{K} = 1200^{\circ}\text{C}$)

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



```
ThermoCalc
POLY_3:s-c n=1 p=101325 t=1473 x(ni)=0.5
POLY_3:c-e
Using global minimization procedure
Calculated 274 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: _
```

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

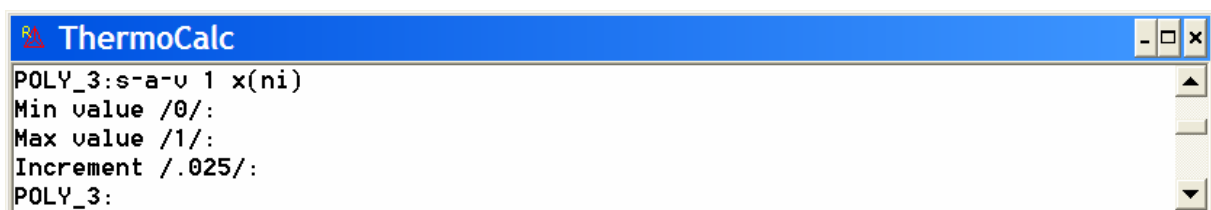
POLY_3: **s-a-v 1 x(ni)**

...This command in full is SET_AXIS_VARIABLE

Min value /0/: 0 (↵)

Max value /0/: 1 (↵)

Increment /0.025/: (↵)



```
ThermoCalc
POLY_3:s-a-v 1 x(ni)
Min value /0/:
Max value /1/:
Increment /.025/:
POLY_3: _
```

...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 G_m 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:

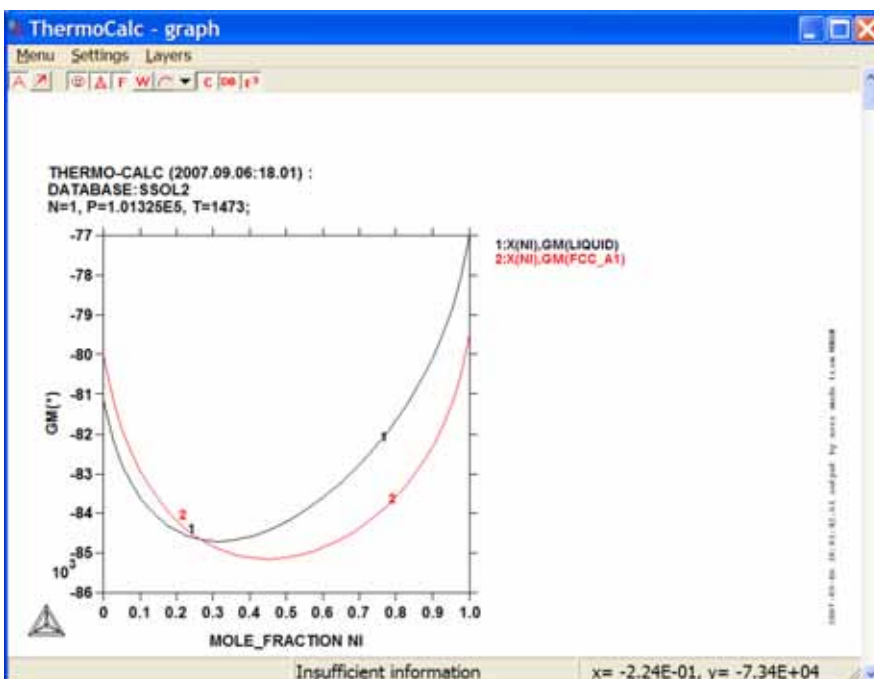
```

...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

```
ThermoCalc
POST:ba
POLY_3:rei
POLY_3:
```

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

```
ThermoCalc
POLY_3:s-c n=1 p=101325 t=1523 x(ni)=0.5
POLY_3:c-e
Using global minimization procedure
Calculated          274 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:
```

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

```
ThermoCalc
POLY_3:s-a-v 1 x(ni)
Min value /0/:
Max value /1/:
Increment /.025/:
POLY_3:
```

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

POLY: step sep

```
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

POST: s-d-a y gm(*) *

COLUMN NUMBER /*/: (↵)

POST: s-l-c-o f

POST: plot

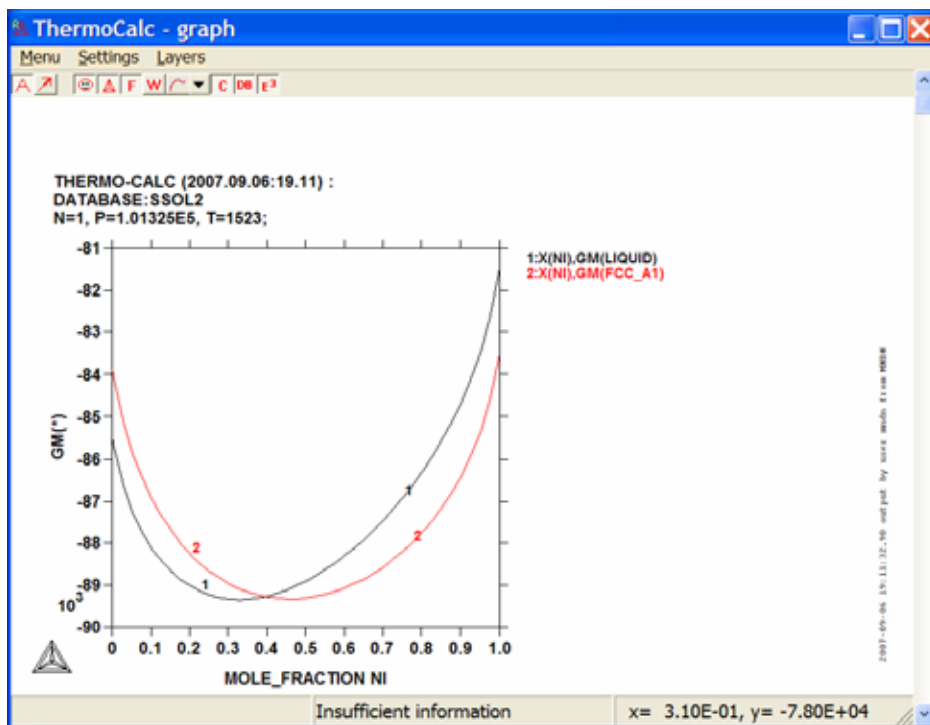

```

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(*) *
POST:s-l-c-o f
POST:plot
OUTPUT TO SCREEN OR FILE /SCREEN/:

```



...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

```

ThermoCalc
POST:ba
POLY_3:rei
POLY_3:s-c n=1 p=101325 t=1623 x(ni)=0.5
POLY_3:c-e
Using global minimization procedure
Calculated          274 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:

```

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

```

ThermoCalc
POLY_3:s-a-u 1 x(ni)
Min value /0/:
Max value /1/:
Increment /.025/:
POLY_3:

```

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

POLY: step sep

```

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

POST: s-d-a y gm(*) *

COLUMN NUMBER /*/: (,)

POST: s-l-c-o f

POST: plot

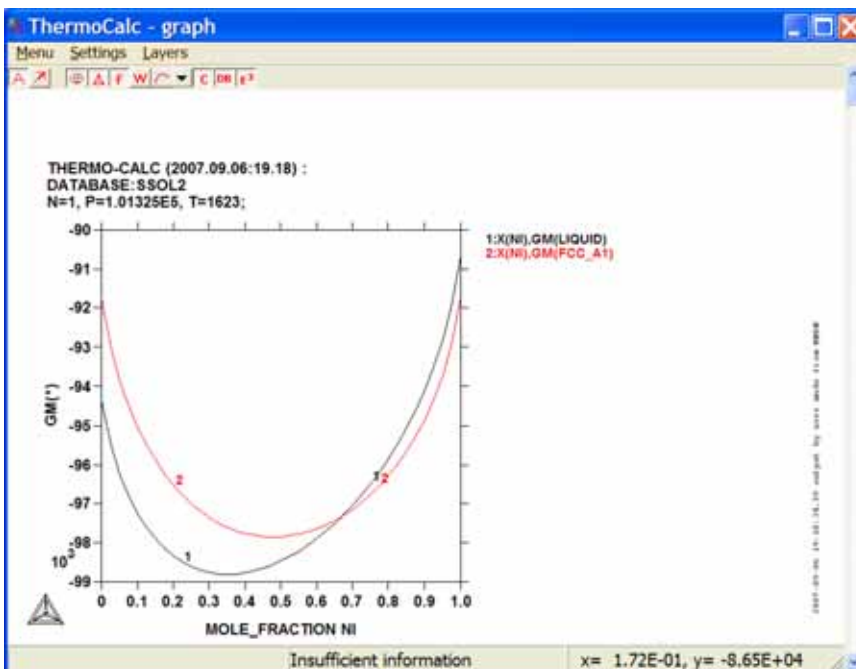
```

ThermoCalc
POLY_3:post

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

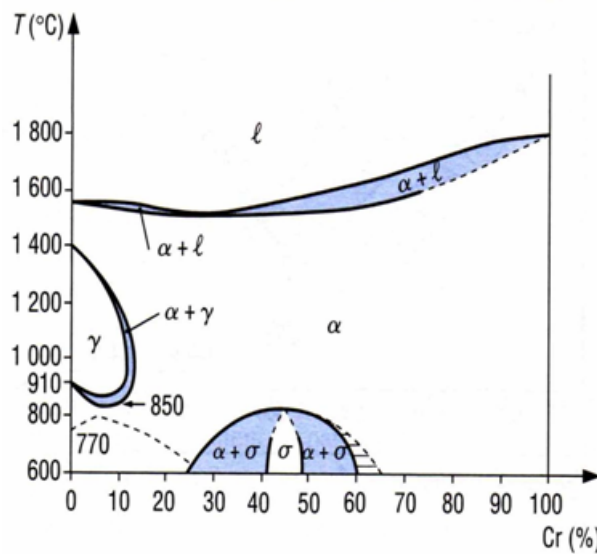
POST:s-d-a x m-f ni
POST:s-d-a y gm(*) *
POST:s-l-c-o f
POST:plot
OUTPUT TO SCREEN OR FILE /SCREEN/:

```



EXAMPLE 2

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



Exercise 1: Selecting the thermodynamic functions (TDB and GES modules).....28

Exercise 2: Calculating and plotting the phase diagram (POLY and POST modules).....29

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 Thermodynamic DataBase 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 Gibbs Energy System 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

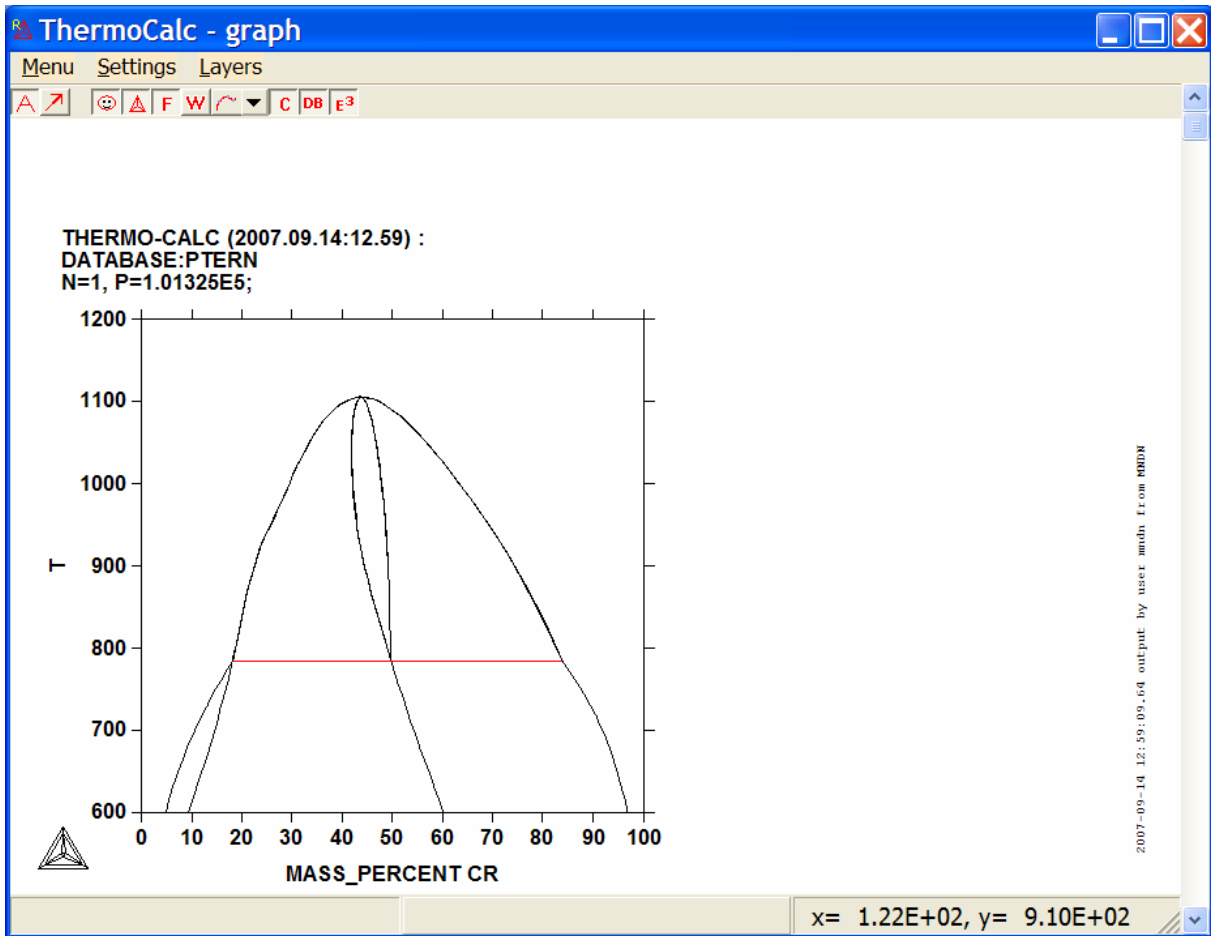
Phase region boundary 4 at: 8.468E-01 7.848E+02
  BCC_A2#1
  ** BCC_A2#2
Calculated 23 equilibria

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

```

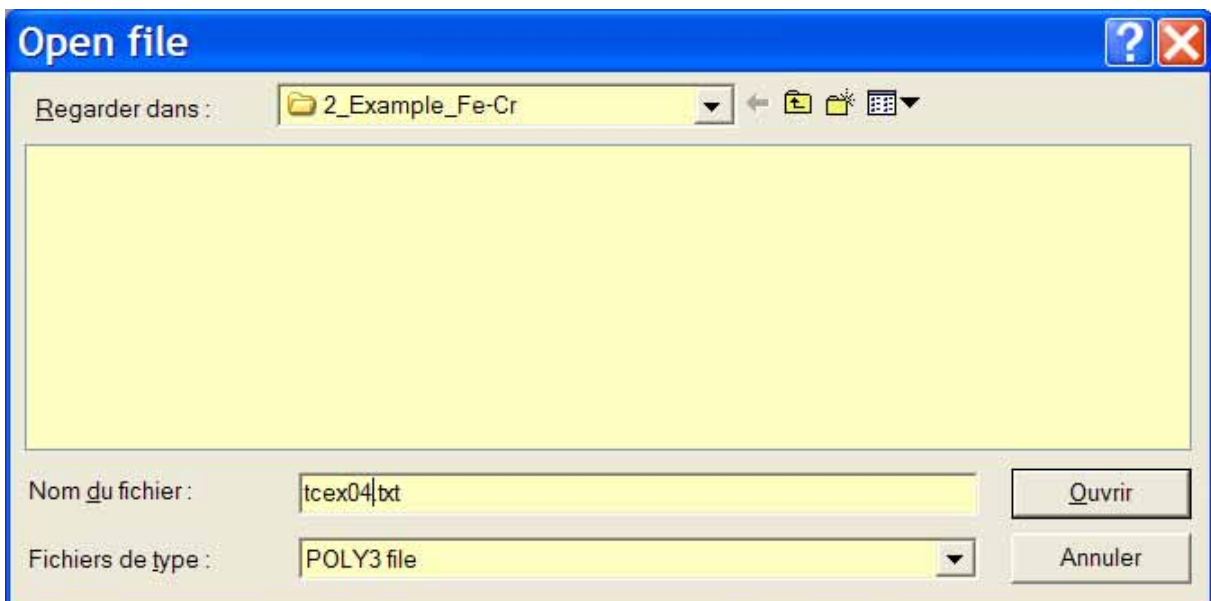
POST: s-d-a x w-p cr
POST: s-d-a y t
POST: PLOT SCREEN



```

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 isopleth (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 refers
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

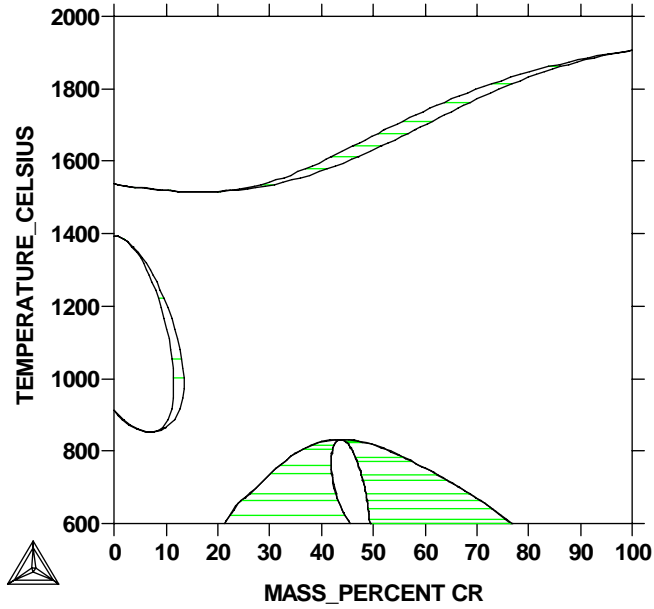
Calculated 43 equilibria

*** 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

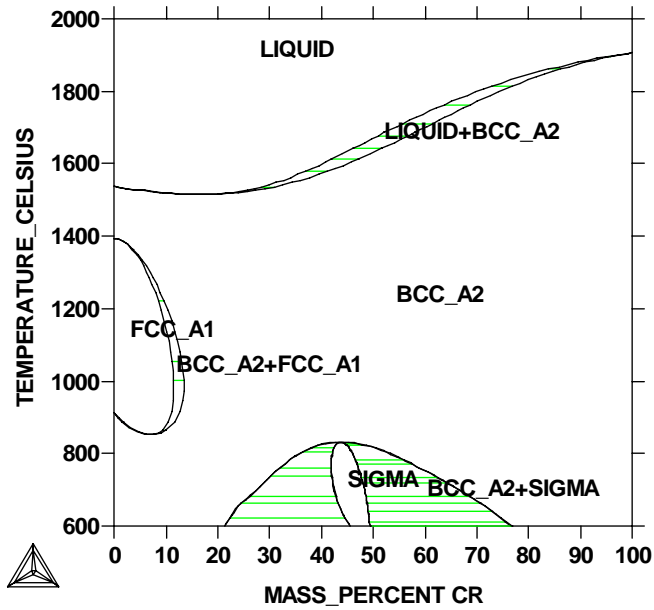
THERMO-CALC (2007.09.14:13.05) :
 DATABASE:PTERN
 N=1, P=1.01325E5;



2007-09-14 13:05:35.14 output by user mmdn from MMDN

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

THERMO-CALC (2007.09.12:20.23) :
 DATABASE:PTERN
 N=1, P=1.01325E5;



2007-09-12 20:23:33.85 output by user mmdn from MMDN