

Chapter 9. Molar phase diagrams

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9.1. Molar axes

Compute and plot the phase diagram for Fe-C at 1 atm and between 1650 and 1850 K and 0 and 0.03 mol% C. Then, try to use enthalpy and C content as axes in the diagram.

Hint

You should realize that you may have to declare that you are not interested in the values for two-phase mixtures but for the individual phases present in the mixtures.

Instructions for T-C

POLY may have difficulties of identifying which one of the phases taking part in an equilibrium that is required when a certain feature is to be plotted. It may help to give a more specific command.

Prompts, commands and responses

```
SYS: go da
THERMODYNAMIC DATABASE module running on PC/WINDOWS NT
Current database: TCS Demo Al-Mg-Si Alloys TDB v1

VA DEFINED
TDB_DALMGSI: sw DFeCrC
Current database: TCS Demo Fe-Cr-C Alloys TDB v1

VA DEFINED
TDB_DFECRC: def-el Fe C
FE C DEFINED
TDB_DFECRC: rej p *
LIQUID:L FCC_A1 BCC_A2
HCP_A3 CEMENTITE M7C3
M23C6 GRAPHITE REJECTED
TDB_DFECRC: rest p fcc bcc liq
FCC_A1 BCC_A2 LIQUID:L
GRAPHITE RESTORED
TDB_DFECRC: get
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
```

PARAMETERS ...
 Rewind to read functions 58
 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'
 'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267 TRITA 0237 (1984);
 C-Fe'
 'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database, v1.2;
 Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters at high temperatures.'

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

-OK-

TDB_DFEERC: **go pol**

POLY version 3.32, Aug 2001
 POLY_3: **s-c T=1700 P=101325 x(C)=.01 N=1**
 POLY_3: **c-e**
 Using global minimization procedure
 Calculated 412 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: **s-a-v 1 x(C)**
 Min value /0/:
 Max value /1/: **.03**
 Increment /7.5E-04/:
 POLY_3: **s-a-v 2 T**
 Min value /0/: **1650**
 Max value /1/: **1850**
 Increment /5/:
 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: 1.000E-02 1.759E+03
 ** LIQUID
 FCC_A1
 Calculated 15 equilibria

Phase region boundary 2 at: 2.407E-02 1.768E+03
 LIQUID
 BCC_A2
 ** FCC_A1

Phase region boundary 3 at: 7.935E-03 1.768E+03
 ** BCC_A2
 FCC_A1
 Mapping terminated 2
 Calculated 49 equilibria

Phase region boundary 4 at: 2.407E-02 1.768E+03

```

LIQUID
** BCC_A2
Calculated      50 equilibria

```

```

Phase region boundary 5 at: 1.000E-02 1.759E+03

```

```

** LIQUID
FCC_A1

```

```

Mapping terminated 1

```

```

*** Last buffer saved on file: USERPROFILE\RESULT.POLY3

```

```

POLY_3: post

```

```

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

```

```

Setting automatic diagram axis

```

```

POST:

```

*) You like to include tie-lines but it may be sufficient to show every fifth one. Then, start with the ordinary T-x phase diagram. You may obtain it automatically but may use option **e** for “setting labels”, i.e., setting digits for identifying univariant phase fields.

```

POST: s-t-s 5

```

```

POST: set-lab e

```

```

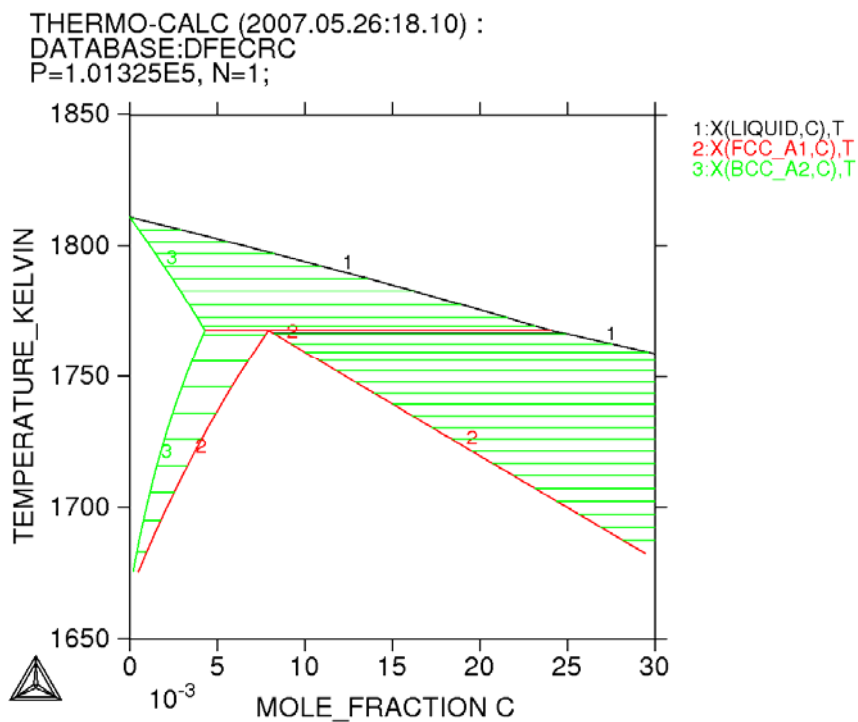
POST: plot

```

```

OUTPUT TO SCREEN OR FILE /SCREEN/:

```



```

POST: s-d-a x x(C)

```

```

Warning: maybe you should use MOLE_FRACTION C instead of X(C)

```

```

POST: s-d-a y Hm

```

```

POST: plot

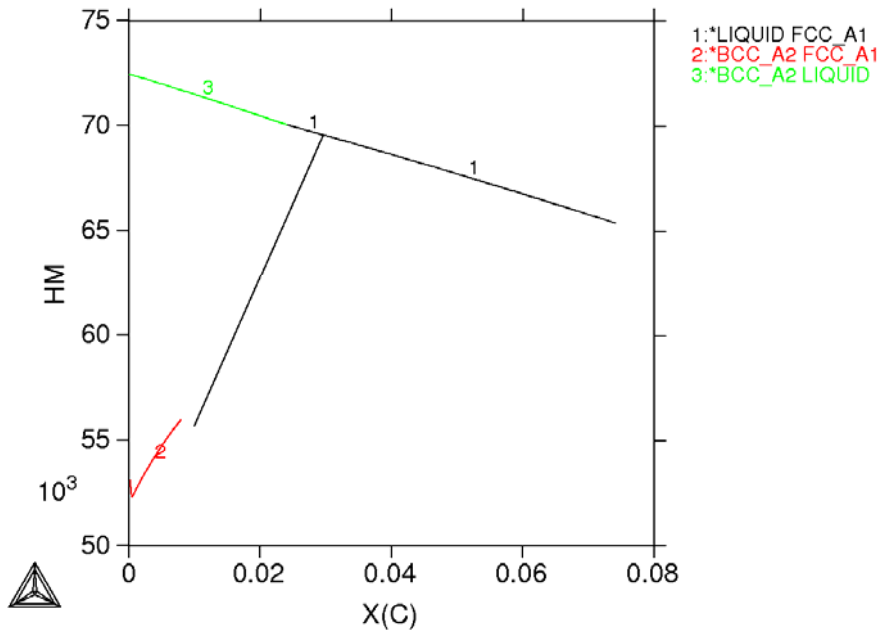
```

```

OUTPUT TO SCREEN OR FILE /SCREEN/:

```

THERMO-CALC (2007.05.26:18.11) :
 DATABASE:DFECRC
 P=1.01325E5, N=1;



POST:

) This diagram looks strange because lines are missing. You better be more specific and require that information from all () the individual phase should be used for Hm.

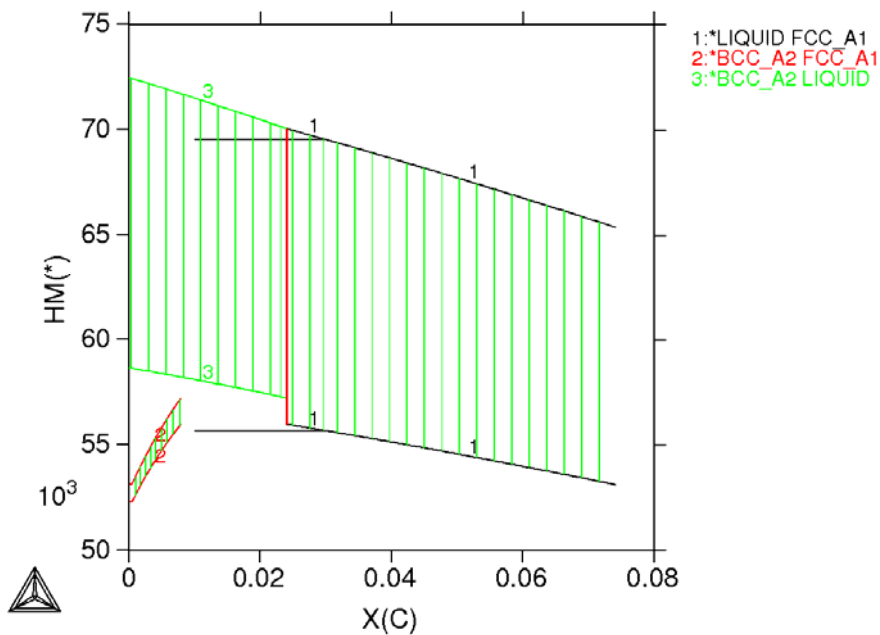
POST: **s-d-a y Hm(*)**

COLUMN NUMBER /*/:

POST: **plot**

OUTPUT TO SCREEN OR FILE /SCREEN/:

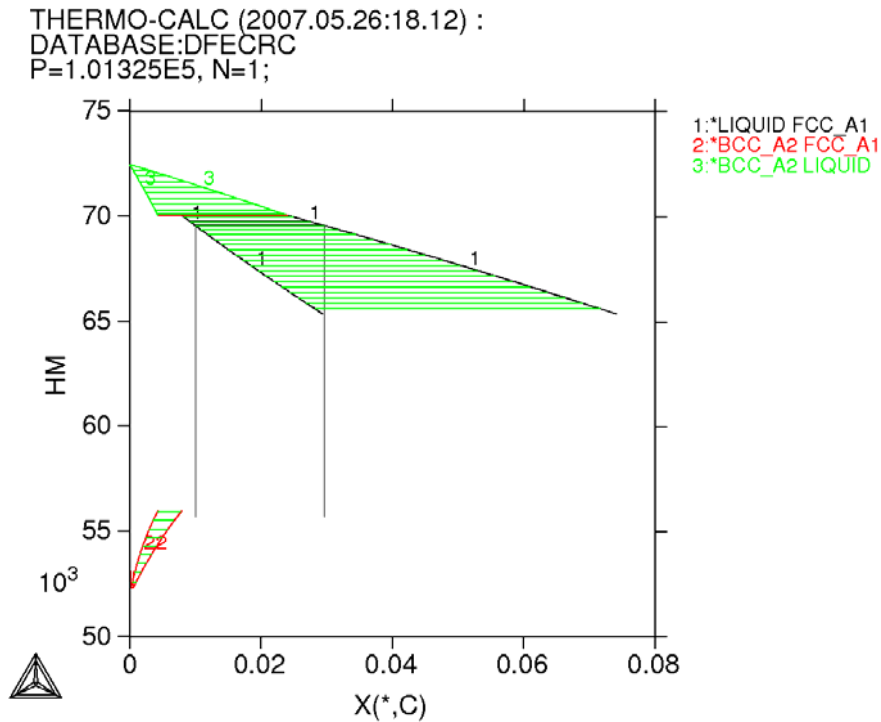
THERMO-CALC (2007.05.26:18.11) :
 DATABASE:DFECRC
 P=1.01325E5, N=1;



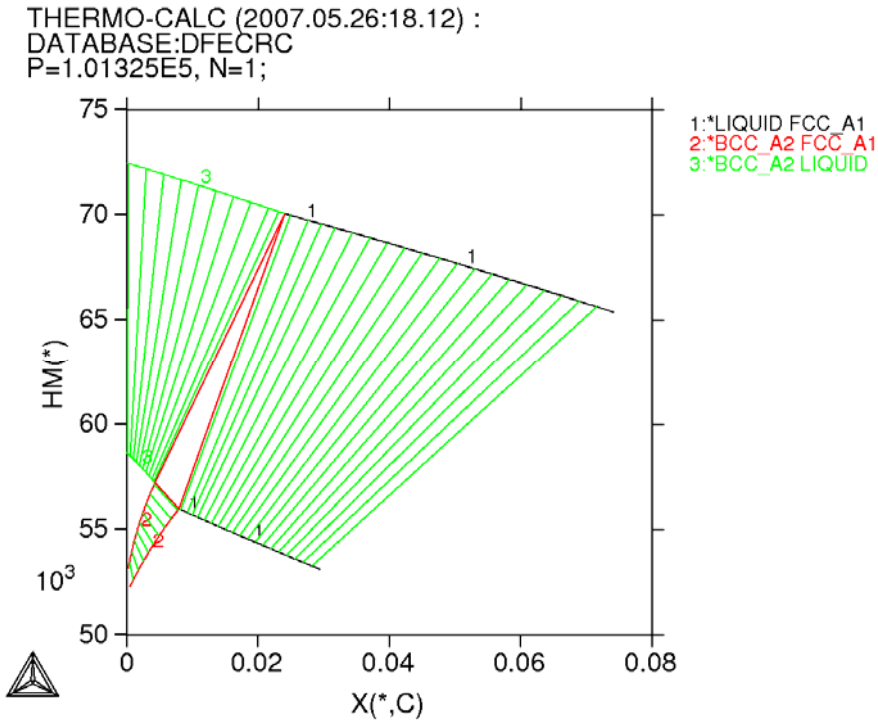
POST:

*) It did not help completely. Test if it was x(C) that needs this same help.

```
POST: s-d-a x x(*,C)
COLUMN NUMBER /*/:
POST: s-d-a y Hm
POST: plot
OUTPUT TO SCREEN OR FILE /SCREEN/:
```



```
POST:
*) Before giving up, try to "help" both variables.
POST: s-d-a y Hm(*)
COLUMN NUMBER /*/:
POST: plot
OUTPUT TO SCREEN OR FILE /SCREEN/:
```



POST:

*) Success! This looks like a true phase diagram.

OUTPUT TO SCREEN OR FILE /SCREEN/:

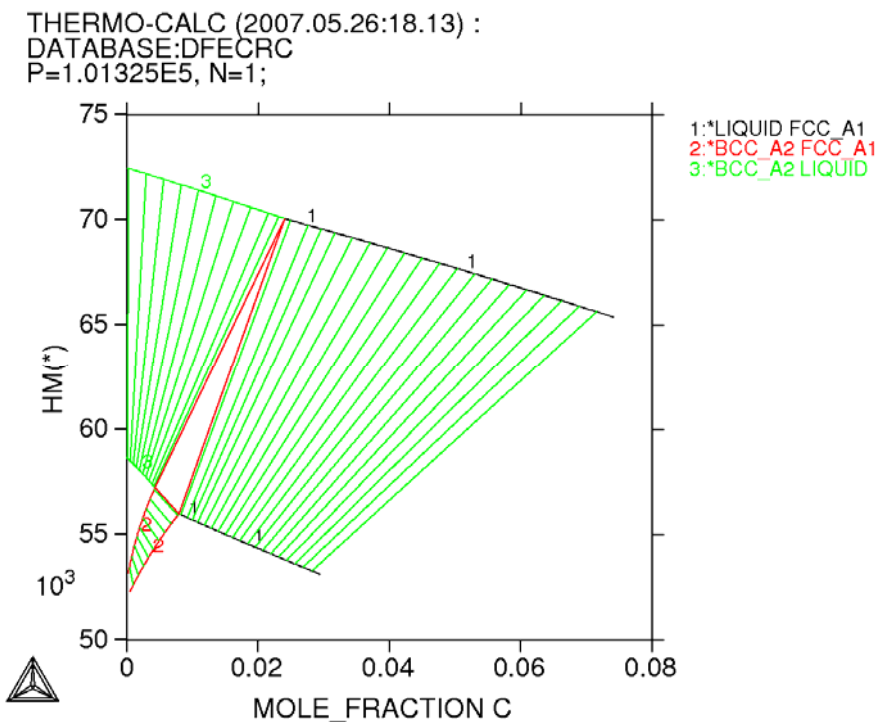
POST:

*) Finally, try to use the advice to use “m-f C” given in the warning you got from the post-processor when you first gave the command x(C).

POST: **s-d-a x m-f C**

POST: **plot**

OUTPUT TO SCREEN OR FILE /SCREEN/:



POST:

) Evidently, it works as $x(,C)$ and may thus be convenient to use more generally.

```
POST: b
POST: exit
CPU time          2 seconds
```

Comments

When plotting molar diagrams it is important that the plotting procedure identifies the values for the individual phases correctly. H_m and $x(C)$ actually represent the values for the whole system and could give the value of a phase if the plotting procedure is able to pick the composition of the correct phase. This does not always happen. It is much safer to plot the values of a given phase, $H_m(\text{phase})$ or $x(\text{phase},C)$, or of all phases as they appear, $H(*)$ or $x(*,C)$. The command "mole-fraction C" (**m-f C**) has the same meaning as $x(*,C)$ and is thus convenient to use.

9.2. Sets of conjugate variables containing molar variables

Compute the phase equilibria for pure Fe between 500 and 1000 K and between 8E9 to 14E9 bar. Plot the results as phase diagrams with various pairs of axes. In particular combine H_m with other quantities.

Hint

As shown in Table 9.1, all combinations of axes don't give true phase diagrams.

Instructions for using T-C

In order to use a function as an axis variable, when the function is not one of those defined basically, it is necessary to enter a symbol for the function. When this function must be evaluated for more than one phase, it should be defined for each phase.

Prompts, commands and responses

```
SYS: go da
THERMODYNAMIC DATABASE module running on PC/WINDOWS NT
Current database: TCS Demo Al-Mg-Si Alloys TDB v1

VA DEFINED
TDB_DALMGSI: sw DFeCrC
Current database: TCS Demo Fe-Cr-C Alloys TDB v1

VA DEFINED
TDB_DFECRC: def-el Fe
FE DEFINED
TDB_DFECRC: rej p *
LIQUID:L          FCC_A1          BCC_A2
HCP_A3 REJECTED
TDB_DFECRC: rest p fcc bcc hcp
FCC_A1           BCC_A2          HCP_A3
RESTORED
TDB_DFECRC: get
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
```

PARAMETERS ...
 Rewind to read functions 32
 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'

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

-OK-

TDB_DFECRC: **go pol**

POLY version 3.32, Aug 2001

POLY_3:

*) Before starting the mapping you must begin with an initial equilibrium but you should then
 use as conditions those variables you like to use as variables on the axes.

POLY_3: **s-c P=9E9 T=700 N=1**

POLY_3: **c-e**

Using global minimization procedure

Calculated 3 grid points in 0 s

POLY_3: **s-a-v 1 T 500 1000**

Increment /12.5/:

POLY_3: **s-a-v 2 P 8E9 14E9**

Increment /150000000/:

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: 8.036E+02 9.000E+09
 BCC_A2

** FCC_A1

Calculated 15 equilibria

Phase region boundary 2 at: 8.036E+02 9.000E+09
 BCC_A2

** FCC_A1

Calculated 20 equilibria

Phase region boundary 3 at: 7.566E+02 1.046E+10
 BCC_A2

** FCC_A1

HCP_A3

Phase region boundary 4 at: 7.566E+02 1.046E+10
 ** FCC_A1

HCP_A3

Calculated 37 equilibria

Phase region boundary 5 at: 7.566E+02 1.046E+10
 BCC_A2

** HCP_A3

Calculated 36 equilibria

*** Last buffer saved on file: USERPROFILE\RESULT.POLY3
POLY_3: **post**

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

Setting automatic diagram axis

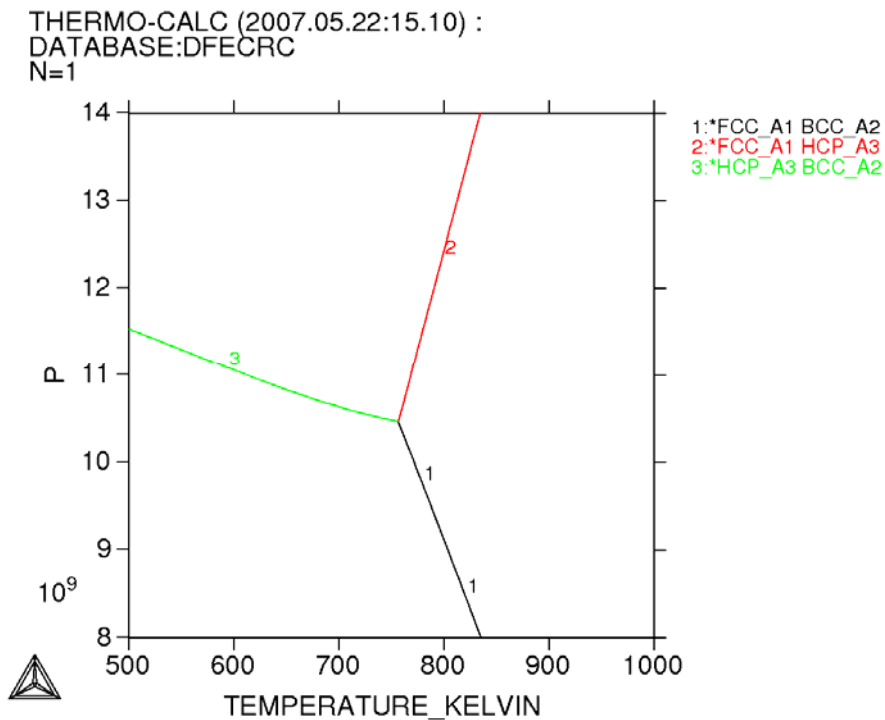
POST:

*) The automatic plotting procedure will produce a T,P phase diagram because those axes were used in the mapping. Use **set-lab e** in order to identify the phase fields.

POST: **set-lab e**

POST: **plot**

OUTPUT TO SCREEN OR FILE /SCREEN/:



POST:

) Introduce Hm instead of T on the x axis. Include tie-lines and accept every third one from the computed equilibria. In order for POST to plot Hm for all the phases you better write Hm()).

POST: **s-d-a x Hm(*)**

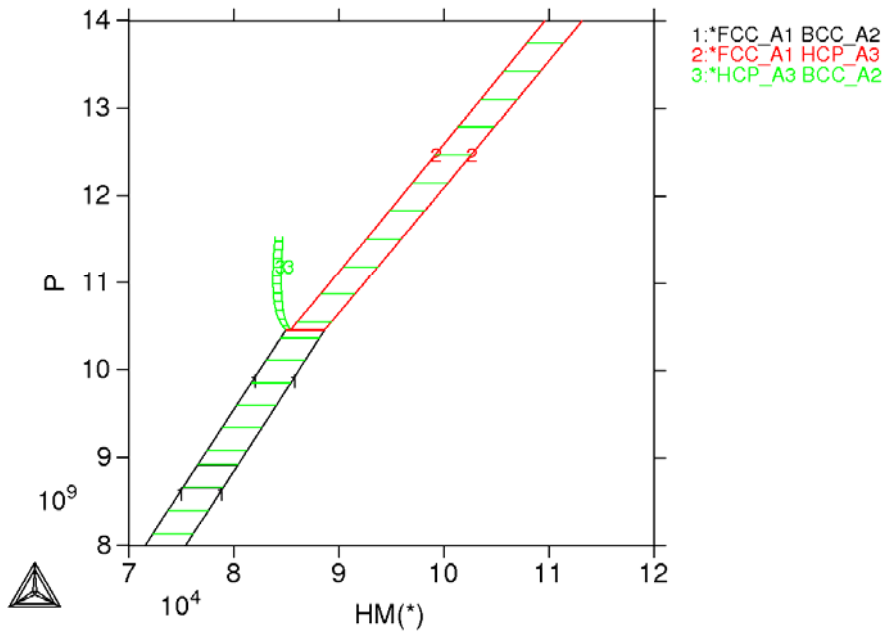
COLUMN NUMBER /*/:

POST: **s-t-s 3**

POST: **plot**

OUTPUT TO SCREEN OR FILE /SCREEN/:

THERMO-CALC (2007.06.08:14.47) :
 DATABASE:DFECRC
 N=1



POST:

*) Restore the T axis and introduce Vm instead of P on the y axis.

POST: **s-d-a x T**

COLUMN NUMBER /*/:

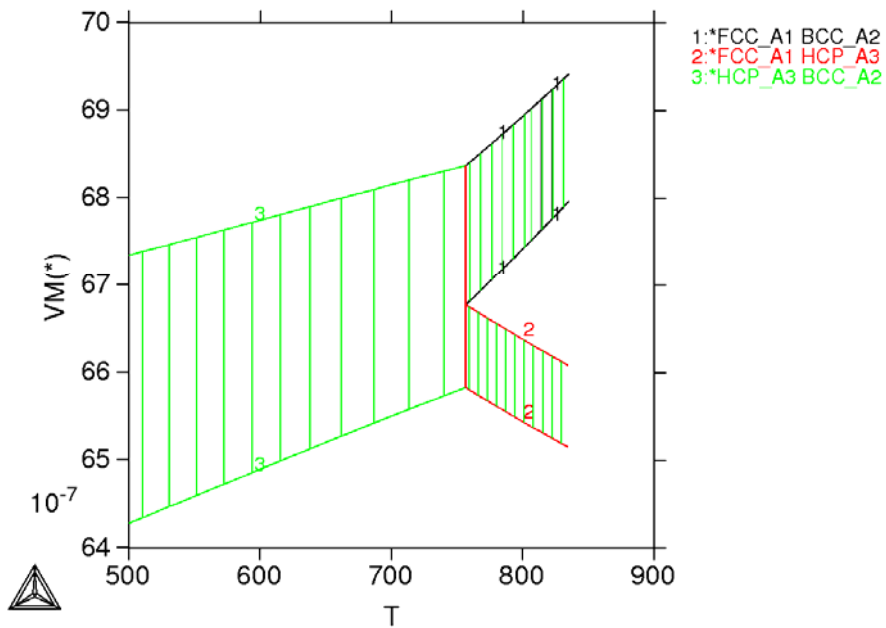
POST: **s-d-a y Vm(*)**

COLUMN NUMBER /*/:

POST: **plot**

OUTPUT TO SCREEN OR FILE /SCREEN/:

THERMO-CALC (2007.06.08:14.44) :
 DATABASE:DFECRC
 N=1



POST:

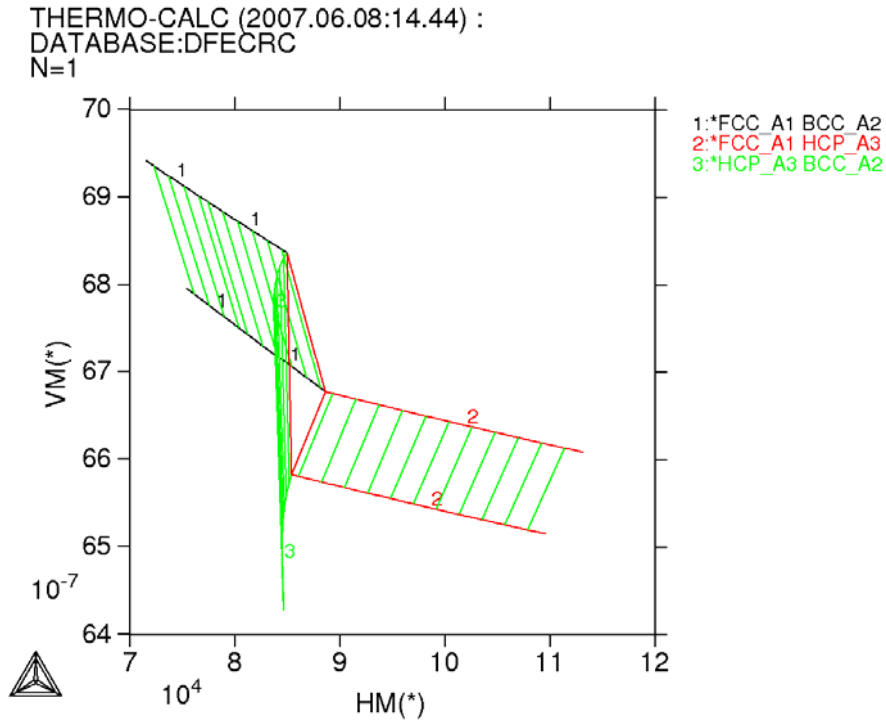
*) Use both Hm and Vm axes.

POST: **s-d-a x Hm(*)**

COLUMN NUMBER /*/:

POST: **plot**

OUTPUT TO SCREEN OR FILE /SCREEN/:



POST:

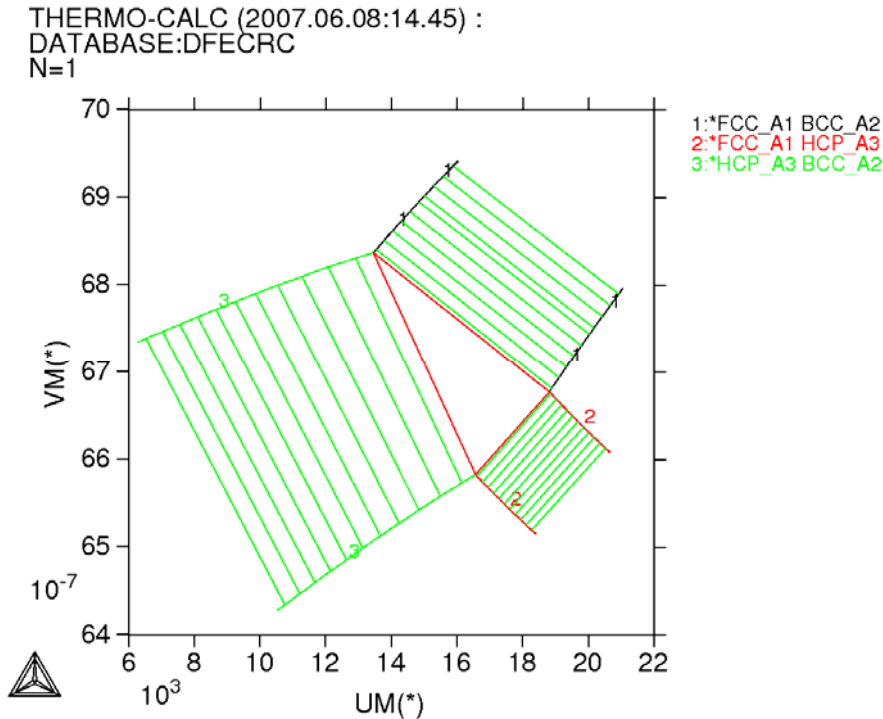
*) Two two-phase fields now overlap and the diagram is not a true phase diagram. According to the fourth row in Table 9.1 you may combine Vm with Um to get a true phase diagram.

POST: **s-d-a x Um(*)**

COLUMN NUMBER /*/:

POST: **plot**

OUTPUT TO SCREEN OR FILE /SCREEN/:



POST: b
 POLY_3: exit
 CPU time 1 seconds

Comments

Starting from the T,P phase diagram, you will obtain true phase diagrams by introducing $H_m(^*)$ instead of T and by introducing $V_m(^*)$ instead of P but not by using both $H_m(^*)$ and $V_m(^*)$. In order to obtain a true phase diagram with $V_m(^*)$ and another molar variable you may use $U_m(^*)$, as indicated by Table 9.1.

9.4. Sections of molar phase diagrams

Consider a carbon free Fe-6 mass% Cr alloy being carburised. Demonstrate with a diagram how the alloy would move from phase field to phase field as the C content is increasing. Construct the diagram for temperatures between 650 and 1550°C. Then, try to figure out the number of phases in the various phase fields. Finally, compute diagrams showing how the amounts of the phases change with the C content during carburisation and with temperature during cooling.

Hint

Evidently, you are asked to compute a so-called isopleth with a constant ratio of Fe to Cr. It will give the same result whether you define this ratio with mass fractions or mole fractions.

Instructions for using T-C

With POLY you can give the condition for an isopleth by constructing a linear expression that is zero.

Prompts, commands and responses

Evidently, you should calculate an isoplethal section by just adding C.

SYS: **go da**

THERMODYNAMIC DATABASE module running on PC/WINDOWS NT
Current database: TCS Demo Al-Mg-Si Alloys TDB v1

VA DEFINED

TDB_DALMGSI: **sw DFeCrC**

Current database: TCS Demo Fe-Cr-C Alloys TDB v1

VA DEFINED

TDB_DFECRC: **def-el Fe Cr C**

FE CR C

DEFINED

TDB_DFECRC: **get**

REINITIATING GES5

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

Rewind to read functions 100

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'
'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'
'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267 TRITA 0237 (1984);
C-FE'
'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92 TRITA 0270
(1986); CR-FE'
'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database, v1.2;
Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters at high temperatures.'
'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636 TRITA 0207 (1986);
C-CR-FE'

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

-OK-

TDB_DFECRC: **go pol**

POLY version 3.32, Aug 2001

POLY_3:

*) You don't like graphite to take part in the equilibria but could use it as reference if you
keep it suspended.

POLY_3: **ch-st p gra=sus**

POLY_3:

*) You will soon step in C content and would then like the ratio between Fe and Cr to stay
constant. Already when computing the single equilibrium you should prepare for this
condition.

POLY_3: **s-c P=101325 T=1800 N=1 w(C)=.01**

POLY_3: **s-c 94*w(Cr)-6*w(Fe)=0**

POLY_3: **c-e**

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 87413 grid points in 1 s

20 ITS, CPU TIME USED 1 SECONDS

POLY_3: **s-a-v 1 w(C) 0 .1**

Increment /.0025/:

POLY_3: **s-a-v 2 T 923 1823**

Increment /22.5/:

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

Tie-lines not in the plane of calculation

Phase region boundary 1 at: 1.000E-02 1.724E+03

LIQUID

** FCC_A1

Calculated 5 equilibria

Phase region boundary 2 at: 5.684E-03 1.750E+03

LIQUID

BCC_A2

** FCC_A1

Calculated 7 equilibria

Phase region boundary 3 at: 9.984E-04 1.745E+03

** LIQUID

BCC_A2

FCC_A1

Calculated 3 equilibria

Phase region boundary 4 at: 2.379E-03 1.743E+03

LIQUID

** BCC_A2

FCC_A1

Terminating at known equilibrium

Calculated 4 equilibria

Phase region boundary 5 at: 2.379E-03 1.743E+03

** BCC_A2

FCC_A1

Calculated 11 equilibria

Phase region boundary 6 at: 2.379E-03 1.743E+03

** LIQUID

FCC_A1

Calculated 14 equilibria

Phase region boundary 7 at: 1.825E-02 1.483E+03

** LIQUID

FCC_A1

M7C3

Calculated 5 equilibria

Phase region boundary 8 at: 2.417E-02 1.451E+03

** LIQUID

CEMENTITE

FCC_A1

M7C3

Phase region boundary 9 at: 3.065E-02 1.451E+03

LIQUID

** CEMENTITE

FCC_A1

Calculated 8 equilibria

Phase region boundary 10 at: 4.373E-02 1.445E+03

LIQUID

CEMENTITE

** FCC_A1

Calculated 12 equilibria

Phase region boundary 11 at: 6.717E-02 1.434E+03

** LIQUID

CEMENTITE

FCC_A1

Terminating at known equilibrium

Calculated 19 equilibria

Phase region boundary 12 at: 6.717E-02 1.434E+03

** LIQUID

CEMENTITE

Calculated 6 equilibria

Phase region boundary 13 at: 6.717E-02 1.503E+03

** LIQUID

CEMENTITE

M7C3

Calculated 10 equilibria

Phase region boundary 14 at: 8.474E-02 1.489E+03

LIQUID

** CEMENTITE

M7C3

Calculated 12 equilibria

Phase region boundary 15 at: 6.181E-02 1.502E+03

LIQUID

CEMENTITE

** M7C3

Convergence problems, increasing smallest sitefraction from 1.00E-30

to hardware precision 2.00E-12. You can restore using SET-NUMERICAL-LIMITS

Terminating at known equilibrium

Calculated 5 equilibria

Phase region boundary 16 at: 6.181E-02 1.502E+03

LIQUID

** M7C3

Calculated 20 equilibria

Phase region boundary 17 at: 6.181E-02 1.502E+03

LIQUID

** CEMENTITE

Terminating at known equilibrium

Calculated 10 equilibria

Phase region boundary 18 at: 8.474E-02 1.489E+03

** CEMENTITE

M7C3

Calculated 30 equilibria

Phase region boundary 19 at: 8.474E-02 1.489E+03
 ** LIQUID
 M7C3
 *** Sorry cannot continue *** 4

Calculated 8 equilibria

Phase region boundary 20 at: 6.717E-02 1.503E+03
 LIQUID
 CEMENTITE
 ** M7C3
 Terminating at known equilibrium
 Calculated 5 equilibria

Phase region boundary 21 at: 6.717E-02 1.503E+03
 CEMENTITE
 ** M7C3
 *** Buffer saved on file: USERPROFILE\RESULT.POLY3
 Calculated 32 equilibria

Phase region boundary 22 at: 6.717E-02 1.434E+03
 CEMENTITE
 ** FCC_A1
 Calculated 22 equilibria

Phase region boundary 23 at: 6.717E-02 1.007E+03
 BCC_A2
 CEMENTITE
 ** FCC_A1
 Calculated 21 equilibria

Phase region boundary 24 at: 2.184E-02 1.022E+03
 BCC_A2
 CEMENTITE
 ** FCC_A1
 M7C3

Phase region boundary 25 at: 1.107E-02 1.022E+03
 BCC_A2
 ** CEMENTITE
 M7C3
 Calculated 9 equilibria

Phase region boundary 26 at: 1.107E-02 1.022E+03
 BCC_A2
 ** FCC_A1
 M7C3
 Calculated 8 equilibria

Phase region boundary 27 at: 5.874E-05 1.084E+03
 BCC_A2
 FCC_A1
 ** M7C3
 Calculated 3 equilibria

Phase region boundary 28 at: 1.373E-03 1.082E+03
 ** BCC_A2
 FCC_A1
 M7C3

```

Terminating at known equilibrium
Calculated      8 equilibria

Phase region boundary  29 at:   1.373E-03  1.082E+03
** BCC_A2
   FCC_A1
Calculated      7 equilibria

Phase region boundary  30 at:   1.373E-03  1.082E+03
   FCC_A1
** M7C3
Terminating at known equilibrium
Calculated     21 equilibria

Phase region boundary  31 at:   5.874E-05  1.084E+03
   BCC_A2
** M7C3
Calculated      7 equilibria

Phase region boundary  32 at:   1.020E-05  9.865E+02
   BCC_A2
   M23C6
** M7C3
Mapping terminated 2
Calculated      5 equilibria

Phase region boundary  33 at:   1.020E-05  9.865E+02
   BCC_A2
** M23C6
   M7C3
Mapping terminated 2
Calculated      5 equilibria

Phase region boundary  34 at:   1.020E-05  9.865E+02
   BCC_A2
** M23C6
Calculated      9 equilibria

Phase region boundary  35 at:   5.874E-05  1.084E+03
   BCC_A2
** FCC_A1
Calculated      6 equilibria

Phase region boundary  36 at:   2.407E-02  1.022E+03
** BCC_A2
   CEMENTITE
   FCC_A1
Terminating at known equilibrium
Calculated     20 equilibria

Phase region boundary  37 at:   2.407E-02  1.022E+03
   CEMENTITE
   FCC_A1
** M7C3
Terminating at known equilibrium
Calculated     22 equilibria

Phase region boundary  38 at:   1.500E-02  1.022E+03
** BCC_A2
   FCC_A1
   M7C3

```

Terminating at known equilibrium

Calculated 9 equilibria

Phase region boundary 39 at: 1.500E-02 1.022E+03

** CEMENTITE

FCC_A1

M7C3

*** Buffer saved on file: USERPROFILE\RESULT.POLY3

Terminating at known equilibrium

Calculated 22 equilibria

Phase region boundary 40 at: 2.184E-02 1.022E+03

BCC_A2

CEMENTITE

** M7C3

Calculated 9 equilibria

Phase region boundary 41 at: 6.717E-02 1.007E+03

** BCC_A2

CEMENTITE

Calculated 10 equilibria

Phase region boundary 42 at: 4.373E-02 1.445E+03

LIQUID

** FCC_A1

Terminating at known equilibrium

Calculated 18 equilibria

Phase region boundary 43 at: 4.373E-02 1.445E+03

LIQUID

** CEMENTITE

Terminating at known equilibrium

Calculated 10 equilibria

Phase region boundary 44 at: 3.065E-02 1.451E+03

LIQUID

FCC_A1

** M7C3

Terminating at known equilibrium

Calculated 8 equilibria

Phase region boundary 45 at: 2.724E-02 1.451E+03

** LIQUID

CEMENTITE

FCC_A1

Terminating at known equilibrium

Calculated 19 equilibria

Phase region boundary 46 at: 2.724E-02 1.451E+03

CEMENTITE

FCC_A1

** M7C3

Terminating at known equilibrium

Calculated 22 equilibria

Phase region boundary 47 at: 2.417E-02 1.451E+03

** CEMENTITE

FCC_A1

M7C3

Terminating at known equilibrium

Calculated 22 equilibria

```

Phase region boundary 48 at: 1.825E-02 1.483E+03
  FCC_A1
  ** M7C3
Terminating at known equilibrium
Calculated 21 equilibria

Phase region boundary 49 at: 9.984E-04 1.745E+03
  ** LIQUID
  BCC_A2
Calculated 7 equilibria

Phase region boundary 50 at: 9.984E-04 1.745E+03
  BCC_A2
  ** FCC_A1
Calculated 10 equilibria

Phase region boundary 51 at: 5.684E-03 1.750E+03
  LIQUID
  ** BCC_A2
Calculated 7 equilibria

Phase region boundary 52 at: 1.000E-02 1.724E+03
  LIQUID
  ** FCC_A1
Terminating at known equilibrium
*** Last buffer saved on file: USERPROFILE\RESULT.POLY3
POLY_3: post

```

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

Setting automatic diagram axis

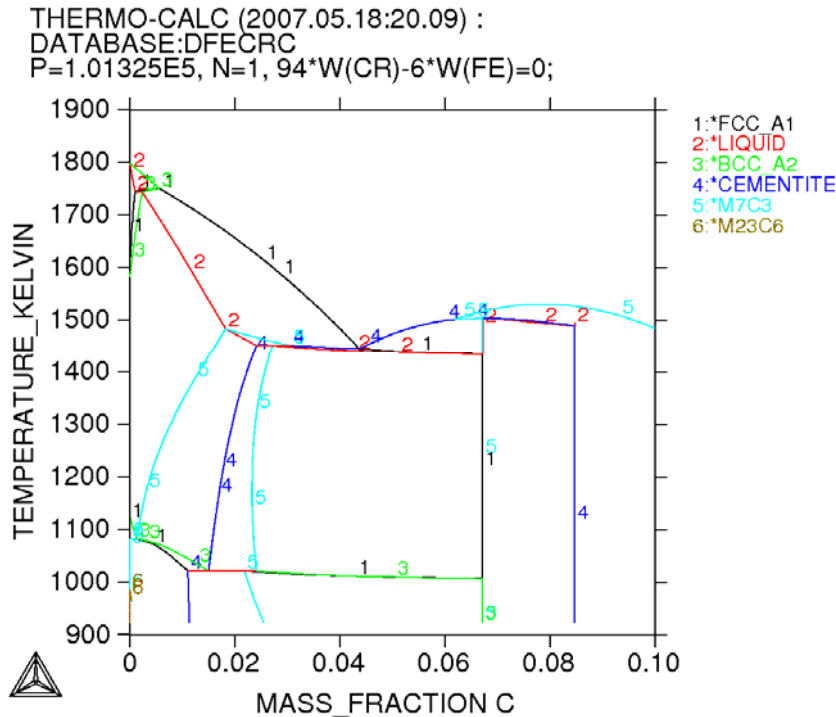
POST:

*) Instead of defining the two axes of your choice, you can accept the automatic procedure.
Identify the phase boundaries with labels.

POST: **set-lab e**

POST: **plot**

OUTPUT TO SCREEN OR FILE /SCREEN/:



POST:

*) The numbers representing the equilibria in the diagram help you to interpret the diagram. You may also consult the list of results from the mapping. It may be interesting to try to find the invariant four-phase equilibria. Of course, you could also magnify the T axis just around them.

POST: **b**

POLY_3:

*) Before producing diagrams with new kinds of axes you should empty POLY from memories of the first diagram. Use **reinitiate** and prepare for stepping in C content at a fixed temperature, e.g. 1200 K.

POLY_3: **rein**

POLY_3: **ch-st p gra=sus**

POLY_3: **s-c P=101325 T=1200 N=1 w(C)=.01**

POLY_3: **s-c 94*w(Cr)-6*w(Fe)=0**

POLY_3: **c-e**

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 87413 grid points in 1 s

33 ITS, CPU TIME USED 1 SECONDS

POLY_3: **s-a-v 1 w(C) 0 .1**

Increment /.0025/:

POLY_3: **step**

Option? /NORMAL/:

No initial equilibrium, trying to add one 0

Phase Region from 0.100000E-01 for:

FCC_A1

M7C3

Calculated 6 equilibria

Phase Region from 0.175228E-01 for:

CEMENTITE

FCC_A1

```

M7C3
Calculated      5 equilibria

Phase Region from  0.232792E-01 for:
  CEMENTITE
  FCC_A1
Calculated      20 equilibria

Phase Region from  0.671716E-01 for:
  CEMENTITE
Error at first increment  6.719659241194829E-002
Calculated      2 equilibria

Phase Region from  0.671716E-01 for:
  CEMENTITE
  M7C3
Calculated      10 equilibria

Phase Region from  0.847372E-01 for:
  M7C3
Error at first increment  8.476220336147465E-002
Calculated      2 equilibria

Phase Region from  0.847372E-01 for:
  LIQUID
  M7C3
Calculated      10 equilibria

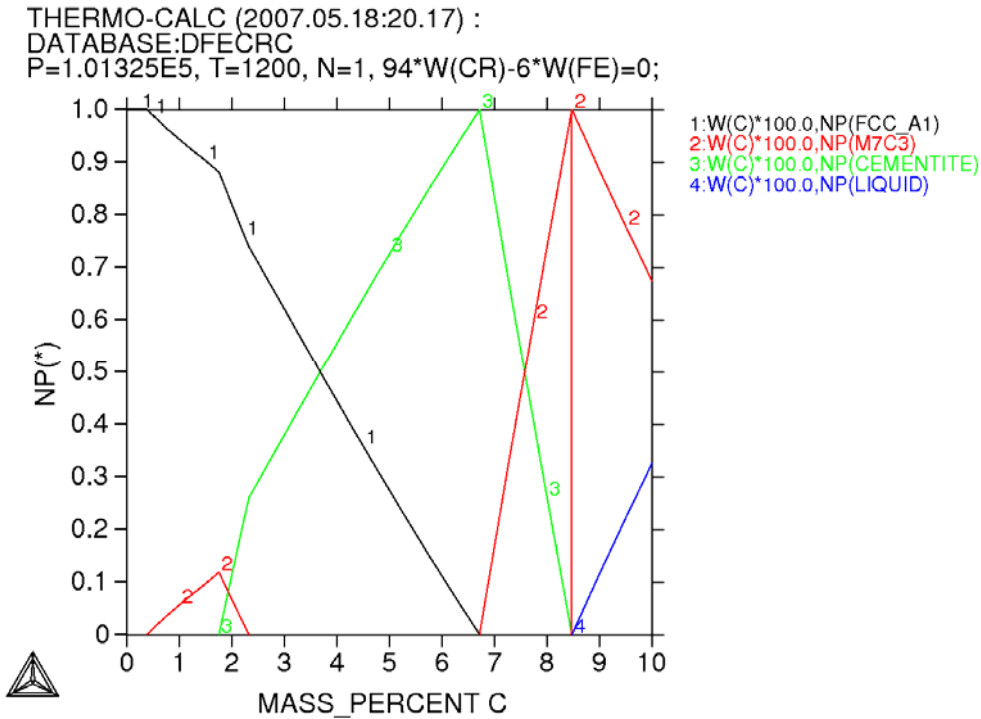
Phase Region from  0.100000E-01 for:
  FCC_A1
  M7C3
Calculated      5 equilibria

Phase Region from  0.387947E-02 for:
  FCC_A1
Calculated      5 equilibria
*** Buffer saved on file: USERPROFILE\RESULT.POLY3
POLY_3: post

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

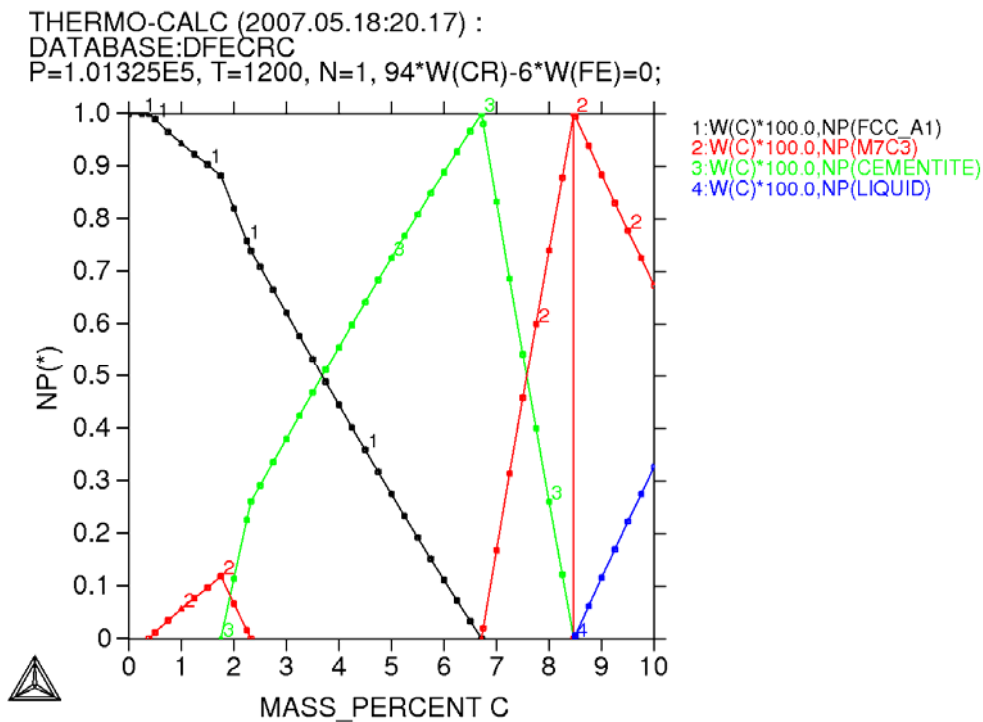
POST: s-d-a x w-p C
POST: s-d-a y Np(*)
COLUMN NUMBER /*/:
POST: set-lab f
POST: plot
OUTPUT TO SCREEN OR FILE /SCREEN/:

```



POST:

*) Sometimes POST will draw extra lines. In this case there is a vertical line without any number for identification. You can examine this further by including points representing the individual equilibria that were computed. Tick the box showing a curve with some points on it. You can find it in the toolbar at the upper left side of the Thermo-Calc area. There will be no points on such an extra line.



POST:

*) Now, make a diagram for cooling.

POST: **b**

POLY_3: **rein**

POLY_3: **ch-st p gra=sus**

POLY_3: **s-c P=101325 T=1800 N=1 w(C)=.05**

POLY_3: **s-c 94*w(Cr)-6*w(Fe)=0**

POLY_3: **c-e**

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 87413 grid points in 1 s

16 ITS, CPU TIME USED 1 SECONDS

POLY_3: **s-a-v 1 T 500 1900**

Increment /35/:

POLY_3: **step**

Option? /NORMAL/:

No initial equilibrium, trying to add one 0

Phase Region from 1800.00 for:

LIQUID

Calculated 6 equilibria

Phase Region from 1800.00 for:

LIQUID

Calculated 12 equilibria

Phase Region from 1473.37 for:

LIQUID

CEMENTITE

Calculated 4 equilibria

Phase Region from 1440.67 for:

LIQUID

CEMENTITE

FCC_A1

Calculated 3 equilibria

Phase Region from 1438.25 for:

CEMENTITE

FCC_A1

Calculated 15 equilibria

Phase Region from 1010.08 for:

BCC_A2

CEMENTITE

FCC_A1

Calculated 3 equilibria

Phase Region from 1009.86 for:

BCC_A2

CEMENTITE

Calculated 12 equilibria

Phase Region from 709.399 for:

BCC_A2

CEMENTITE

M3C2

Calculated 10 equilibria

*** Buffer saved on file: USERPROFILE\RESULT.POLY3

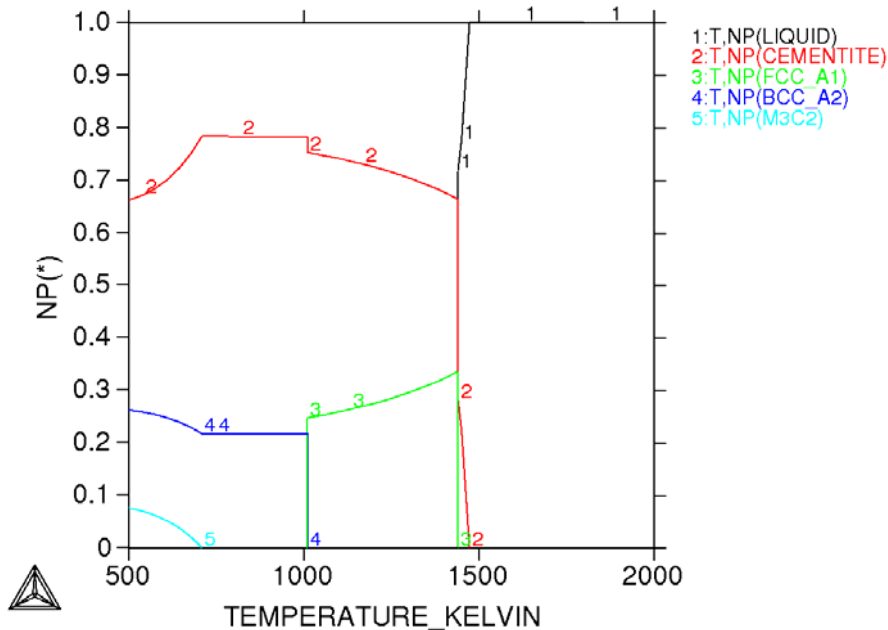
POLY_3: **post**

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

Setting automatic diagram axis

POST: **set-lab f**
 POST: **plot**
 OUTPUT TO SCREEN OR FILE /SCREEN/:

THERMO-CALC (2007.05.18:20.24) :
 DATABASE:DFECRC
 P=1.01325E5, N=1, W(C)=5E-2, 94*W(CR)-6*W(FE)=0;



POST: **b**
 POLY_3: **exit**
 CPU time 7 seconds

Comments

Here it is easy to see the invariant equilibria as revealed by vertical changes. Only the amounts of phases vary.

9.6. Topology of sectioned molar diagrams

Compute a zero-phase-fraction line of your own choice through the isopleth obtained in the first part of Problem 9.4. Plot this line in a diagram with the same axes as the isopleth.

Hint

Your data bank system should offer some method of requiring that a selected phase should take part in all the equilibria that are computed, but with zero amount.

Instructions for using T-C

In POLY this is done by defining the status of a phase.

Prompts, commands and responses

```
SYS: go da
THERMODYNAMIC DATABASE module running on PC/WINDOWS NT
Current database: TCS Demo Al-Mg-Si Alloys TDB v1
```

```
VA DEFINED
TDB_DALMGSI: sw DFeCrC
Current database: TCS Demo Fe-Cr-C Alloys TDB v1
```

```
VA DEFINED
TDB_DFECRC: def-el Fe C Cr
FE C CR
```

```
DEFINED
TDB_DFECRC: get
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
Rewind to read functions 100
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'
'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'
'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267 TRITA 0237 (1984);
C-FE'
'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92 TRITA 0270
(1986); CR-FE'
'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database, v1.2;
Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters at high temperatures.'
'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636 TRITA 0207 (1986);
C-CR-FE'
```

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

-OK-

```
TDB_DFECRC: go pol
```

```
POLY version 3.32, Aug 2001
```

```
POLY_3:
```

*) All phases offered by the database were accepted but you would not like graphite to take part in equilibria. You should thus suspend graphite.

```
POLY_3: ch-st p gra=sus
```

```
POLY_3:
```

*) You will soon step in C content and would then like the ratio between Fe and Cr to stay constant. Already when computing the single equilibrium you should prepare for this condition.

```
POLY_3: s-c P=101325 N=1 w(C)=.02 94*w(Cr)-6*w(Fe)=0
```

```
POLY_3:
```

*) You like liquid to take part in all the equilibria that will be computed, but with the amount zero.

```
POLY_3: ch-st p liq=fix 0
```

```

POLY_3: c-e
Normal POLY minimization, not global
Convergence problems, increasing smallest sitefraction from 1.00E-30
to hardware precision 2.00E-12. You can restore using SET-NUMERICAL-LIMITS
Testing POLY result by global minimization procedure
Calculated      87413  grid points in          1  s
260 ITS, CPU TIME USED  1 SECONDS
POLY_3: s-a-v 1 w(C)
Min value /0/:  0
Max value /1/:  .1
Increment /.0025/:
POLY_3: step
Option? /NORMAL/:
No initial equilibrium, trying to add one          0

Phase Region from  0.200000E-01 for:
LIQUID
FCC_A1
M7C3
Calculated      4 equilibria

Phase Region from  0.241703E-01 for:
LIQUID
CEMENTITE
FCC_A1
M7C3
Calculated      4 equilibria

Phase Region from  0.272434E-01 for:
LIQUID
CEMENTITE
FCC_A1
Calculated      19 equilibria

Phase Region from  0.671716E-01 for:
LIQUID
CEMENTITE
jump 10
Emergency fix  6.717159241194832E-002  6.842159241194833E-002
Calculated      2 equilibria

Phase Region from  0.684216E-01 for:
LIQUID
CEMENTITE
M7C3
Calculated      10 equilibria

Phase Region from  0.847372E-01 for:
LIQUID
M7C3
jump 2:          1611
*** Sorry cannot continue

Phase Region from  0.200000E-01 for:
LIQUID
FCC_A1
M7C3
Calculated      3 equilibria

Phase Region from  0.182539E-01 for:
LIQUID

```

```

FCC_A1
jump 13
Emergency fix 2.499999999999989E-003 1.249999999999989E-003
Calculated 10 equilibria

```

```

Phase Region from 0.125000E-02 for:
LIQUID
BCC_A2
FCC_A1
Calculated 3 equilibria

```

```

Phase Region from 0.998406E-03 for:
LIQUID
BCC_A2
Calculated 4 equilibria
*** Buffer saved on file: USERPROFILE\RESULT.POLY3
POLY_3: post

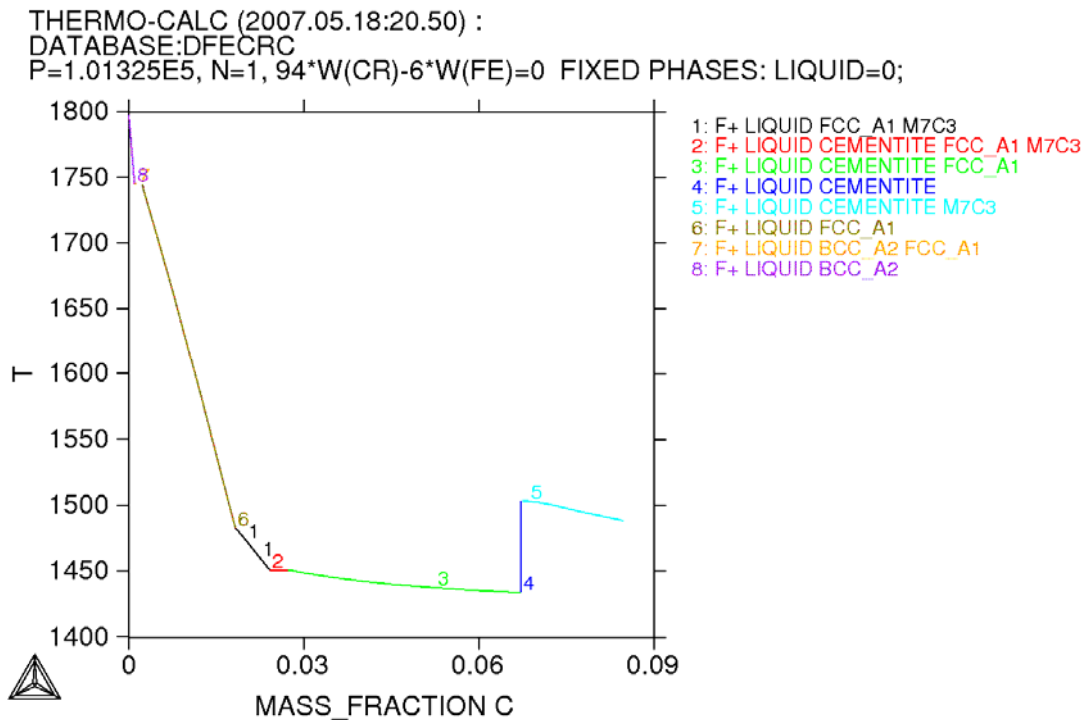
```

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

```

POST: s-d-a x w-f C
POST: s-d-a y T
POST: set-lab e
POST: plot
OUTPUT TO SCREEN OR FILE /SCREEN/:

```



```

POST: exit
CPU time 2 seconds

```

Comments

You can find all the pieces of the computed zero-phase-fraction line in the isopleth of Problem 9.4.

All the phase boundaries, in phase diagrams represent zero fraction of some phase. The concept of "zero-phase-fraction line" does not make sense until one combines those pieces into one line.

The zero-phase-fraction line for liquid was obtained here simply because of the condition "ch-st p liq = fix 0" for the single equilibrium in the beginning.