Welcome to

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Problems to be solved on the Thermo-Calc data bank system

Based on the textbook by Mats Hillert:

Phase Equilibria, Phase Diagrams and Phase Transformations
2nd edition, Cambridge University Press, 2007

These Problems and their computerized solutions are open to anyone for reading and studying. However, in order to produce your own solution by following those presented in this document you at least need a free-of charge licence to the Thermo-Calc DEMO package. You may apply for a licence on
http://www.thermocalc.com/PEPDPT/PEPDPT.html
It may take a few days to be given a licence.
The licence is for a limited time but may be renewed.

The present collection of problems was not designed to make a general instruction to the use of the Thermo-Calc package but will introduce the student to features essential for solving the special questions raised by the problems. Often these problems are not of the kinds of interest to the ordinary customers and Thermo-calc may not always be designed to give the most direct way of finding the answer to such questions. On the other hand, a more detailed path to a solution may be instructive for the student and may give her/him a deeper insight in how thermodynamics works.

The problems are designed as exercises to various sections in the textbook and are collected Chapter-wise. The student is advised first to study the **General instructions for using the Thermo-Calc System.** Later on it may also be useful to be familiar with the **Index of special features**.

1. General Instructions for Using the Thermo-Calc System

Introduction

Even though you may gain some experience in the use of the special free-of-charge version of the Thermo-Calc software and databank system, the main purpose of this instructions and in connection with the present set of Problems is to help you to understand those particular solutions. If trying to modify a problem, you may run into difficulties that require a deeper insight in the facilities offered by Thermo-Calc (T-C). Much more detailed instructions can be obtained by turning to the download area at www.thermocalc.com but they may require a substantial effort.

General structure of T-C

T-C is composed of modules. It operates with prompts and commands. When ":" appears at the end of a text, you are prompted to give a command. The command will be executed when you press "return".

When you type your response to a prompt, it generally does not matter if you use upper or lower case characters. You may thus type fe for Fe and t for T.

Your response to a prompt may contain a main command and further information (arguments). Both the main command and arguments may be abbreviated as long as it can be distinguished from all other legal options.

A list of the optional commands can always be inspected by typing **?** or **help**. The content of the list depends on where in the program you are.

Often a default argument is given within / / just before ":". You can accept the default by simply pressing "return".

Often you are required to give several arguments to a command. You may type them on the same line if you know what will be required. Otherwise, simply press "return", you will be prompted to type the arguments one by one.

The main command may consist of several words. They are connected by hyphens or underscores. They may be abbreviated by omitting a word completely or by abbreviating each word but keeping the hyphens or underscores. Arguments are separated by a blank space or by a comma and a blank space.

The prompt "SYS:" indicates that you have accessed the T-C system. You can go to any module with the command **goto <name of module>**.

The command **set-log <name of a file>** will allow you to save the commands used in the whole session into a file. You can run the created file as a macro by simply changing the file extension from "LOG" to "TCM" and then dragging-and-dropping the file to your T-C icon. If you want to modify your commands and arguments for similar calculations you may edit the macro file by using any simple editor (e.g. notepad, wordpad, emacs),

Units and symbols

T-C uses and requires SI units, e.g. pascal Pa (1 bar=1E5 Pa, 1 atm=1.01325E5 Pa), kelvin K (=^{o}C+273.15) and meter m for setting conditions and internal calculations. *Exception*: Mass (weight) must be expressed in gram, not kg. During post-processing of calculation results, non-SI units can be used for plotting some properties, for example temperature in Celsius or Fahrenheit.

The formula unit depends on the model used in the database. It could be $CaCO_3$ or $(Fe,Mn)_1(Va,C)_1$ or (H_2, O_2, H_2O) for a gas.

The symbol for mass is B but the symbol for mass (weight) fraction is W. Weight% or mole % is not used in calculations. They can be used in plots of results.

N is the symbol for the number of moles of components (usually atoms) in the system.
NP(phase) is the number of moles of a phase present in the system.
N(species) is the number of moles of the species in the system. Notice that this works only for species that have been defined as component.
N(phase,species) is the number of moles of the species in a phase.

If Z is an extensive property, whether for the whole system or for a phase, then
ZM is per mole of components (usually atoms)
ZW is per mass (in gram)
ZV is per volume (in m^3)
ZF is per mole of formula unit of a phase.

T-C uses the symbol A for Helmholtz energy instead of F.

Composition and constitution

The components of a system are usually the elements. This can be changed only by a special command.

The composition of the system is given by the mole fractions or mass fractions of components, e.g. x(C) or w(C). The composition of a phase is given by x(phase,C) or w(phase,C).

The constitution of a system or of a phase is defined as the distributions of the species among the phases and within each phase.

The constitution of a phase with sublattices, e.g. the fcc phase $(Fe,Mn)_1(Va,C)_1$, is given by the site fractions of the species, e.g. y(fcc,C#2) where C is a species in sublattice 2.

Species is any unit of matter used in the model of a phase stored in the database, e.g. H_2 in the gas phase.

Constituent is a species in a specified sublattice.

Save, print and plot options

When using the **step** or **map** commands in POLY the calculation results will automatically be saved on a file. The file will be stored in the default directory USERPROFILE, which is usually "C:\Documents and Settings\xxx", where xxx is your login user name. The file name will be RESULT.POLY3. At the end of a **step/map** calculation the following line will thus appear:

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

However, it is possible (and recommended) to use the command SAVE just before the **step/map** command. This will enable you to use different file names for different calculations. The file may be uploaded using the command **read** in POLY.

A diagram that has been plotted in the POST-processor may also be printed on paper. The command in POST is **print_diagram**. It is available under Windows NT/2000/XP and Windows 95/98/ME environments.

The command **set_label_curve_option** may be used to identify the curves drawn in the post-processor by marking each curve with a digit and then list the meaning of these digits beside the plot. The options used in the Problems are:

E – lists stable phases along a line (color)
F – lists axis quantity (color)

Databases

There are several free databases accompanying this special version of Thermo-Calc. Some of them contain no data on molar volumes and others contain only rough values. High quality information on molar volumes may be found in a few databases.

All databases are not completely consistent with each other, depending on their special purposes.

One may append data from another database after having obtained data from a database.

The following list of databases available with the special free-of-charge version of T-C can always be obtained by typing **?** after **switch** when in the database module. It should be emphasized that the special version of T-C allows the use of information involving only three elements at a time. Once you have selected a database you may type the command **database_information** to get a description for the selected database.

```
DALMGSI =  TCS Demo Al-Mg-Si Alloys TDB v1
DFECRC  =  TCS Demo Fe-Cr-C Alloys TDB v1
PURE4   =  SGTE Unary (Pure Elements) TDB v4
PSUB    =  TCS Public Pure Substances TDB v1
PBIN    =  TCS Public Binary Alloys TDB v1
PKP     =  Kaufman Binary Alloys TDB v1
PCHAT   =  Chatenay-Malabry Binary Alloys TDB v1
PTERN   =  TCS Public Ternary Alloys TDB v1
PG35    =  G35 Binary Semi-Conductors TDB v1
PION    =  TCS Public Ionic Solutions TDB v2
PAQ2    =  TCS Public Aqueous Solution TDB v2
PGEO    =  Saxena Pure Minerals Database v1
PFRIB   =  Fridberg Dilute Fe-Alloys MDB v1
```

2. Index of special features

3. Problems

All problems are available for download one by one from
http://www.thermocalc.com/PEPDPT/PEPDPT.html