

## THE THERMO-CALC DATABANK SYSTEM

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### ABSTRACT

A description is given of Thermo-Calc, a databank for thermochemistry and metallurgy developed at the division of Physical Metallurgy of the Royal Institute of Technology (KTH) in Stockholm. Using the facilities of Thermo-Calc one can tabulate thermodynamic data, calculate the heat change of chemical reactions and their driving force, evaluate equilibria for chemical systems and phase transformations and calculate various types of multicomponent phase diagrams by an automatic mapping procedure. The databank is quite general and can be applied to all systems where data assessed by a model implemented in the databank are available. The assessment procedure necessary to develop and extend the the databank is discussed. A brief description of the modules of Thermo-Calc is given and two examples are included which demonstrate how flexibly the calculations can be made. These examples will also show that the system is quite easy to use and that there are extensive on-line help facilities.

### Introduction

The knowledge of the equilibrium state of a system and how it is affected by various external factors is of great importance for the chemical and metallurgical industry. The experimental work to determine such equilibria is in many cases difficult because the number of components can be large and the external factors may be difficult to control. In such cases it may be interesting to predict the behaviour of a complex system by using extrapolations from systems that are easier to study experimentally. A thermochemical databank is an important tool in this work because the assessed data from binary, ternary and higher systems can be combined by a computer operated procedure and it is thus possible with very little effort to predict the equilibrium state for multicomponent systems. A number of computer programs for equilibrium calculations have been developed but these programs differ greatly in the choice of equilibrium conditions and thermochemical models and in the ease of handling. The Thermo-Calc databank system is an attempt to provide a single software system for all thermochemical calculations which is easy to learn and use.

Thermo-Calc is interactive and it is operated by sets of commands. It is a system composed of several application programs, modules, which cooperate through defined software interfaces and utilize a database of assessed thermochemical parameters. Each module has a specific purpose and the interfaces simplify addition of new modules and improvement of existing ones. The most important module at present is a very general and flexible program for the calculation of equilibria and a unique procedure to map stable equilibria and phase diagrams in multicomponent systems for one, two or three independent variables. As examples of important types of calculation one may mention:

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- constitution and amounts of various phases in equilibrium at selected temperatures, compositions and activities,
- phase diagrams in binary, ternary and higher-order systems under auxiliary conditions such as constant temperature or pressure, constant amount of some components or constant chemical activities,
- predominance area diagrams,
- liquidus surfaces,
- calculation of equilibria when the set of stable phases is prescribed,
- property diagrams where a dependent quantity is plotted versus an independent.

Much effort has gone into making Thermo-Calc a user-friendly system and to provide on-line help as well as extensive documentation (1-5). However, it should be understood that a databank to be used for calculations cannot be constructed in the same way as a retrieval system for bibliographic data. The user must know how to define his problem within the framework of the databank. For this purpose regular one-week courses are arranged for users.

Thermo-Calc is equipped with a post-processor for the final processing of the results of a calculation. With the post-processor the user can prepare tables and draw diagrams and by selecting relevant quantities and suitable scales he can present the result in various ways. Examples of diagrams generated by Thermo-Calc are shown in Fig. 1 to 3.

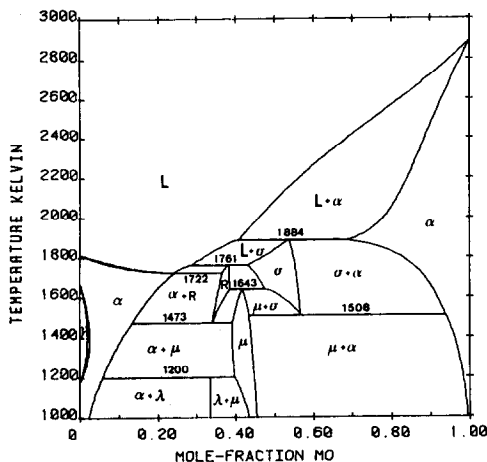


FIG. 1. The calculated phase diagram for the Fe-Mo system. Diagrams with only two components are of great interest for the assessment of data for the database (6).

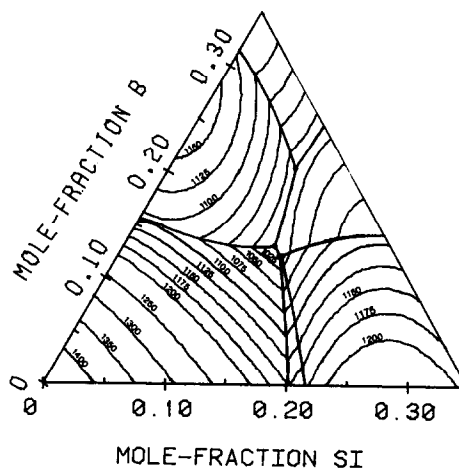


FIG. 2. The liquidus surface in the nickel rich corner of the Ni-Si-B system. This diagram was calculated in order to aid the selection of candidate alloys to be used for rapid solidification (7).

#### Thermochemical data

A large quantity of data concerning thermochemical quantities and chemical equilibria has been determined experimentally and is available in the literature. Nevertheless, it may still be difficult to find sufficient information for solving a particular problem. This is a consequence of the fact that the possible range of variation is so large that the experimental work can only cover a small fraction of all combinations. The missing data must therefore be estimated by some kind of extrapolation from the experimentally determined values. Such extrapolations require high skill.

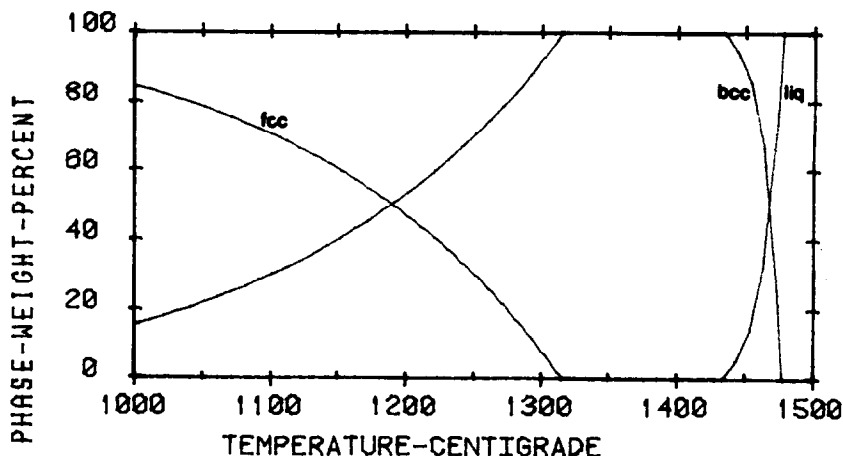


FIG. 3. The diagram shows how the relative amounts of the various phases vary with the temperature. Such information is a valuable guide in selecting the temperature for various kinds of heat treatment.

The Thermo-Calc databank has been designed to be useful both for the experts and for persons without the time or skill to make extrapolations from experimental data. This is achieved by applying the "Calphad method", i.e., the experimental data available in the literature are assessed by experts using mathematical models based on physical principles. From the models many relations can be derived between experimental data of various quantities and this makes it possible to use effectively scattered and incomplete experimental data. Special computer software has been developed to be used in such assessments (8-9). The results of the assessments are obtained as parameter values and these parameters are stored in the database together with a description of the mathematical model. These parameters describe not only the experimental data used in the assessment but can be used for reliable extrapolations. It thus makes no difference if a user asks for a value which has been determined experimentally or not. The value calculated from the parameters stored in the database is the best value available, according to the judgement of the assessor, provided it falls within the recommended range of validity of the assessment. From the models one may calculate many different quantities and their values are always mutually consistent.

The kernel of the Thermo-Calc system is a module for thermodynamic models which is written in such a general way that it can be used within many different fields of thermochemistry. For instance, the sublattice model (10), a model for magnetic ordering (11), a general model for liquids with ions (12) as well as the Pitzer model for aqueous solutions (13) are implemented. This thermodynamic module is coupled to the database where the various parameters are stored. Of course, the reliability of the calculations depends upon the quality of the assessments. In order to guarantee the highest possible quality the database must be developed through an international collaboration between researchers with long experience of assessment work in their respective field.

#### The modules in Thermo-Calc

The Thermo-Calc system consists of more than 600 subroutines and is divided into several modules. Most of the modules have an interactive monitor where the user decides the action to be taken by giving commands. Each module has its own prompt which is displayed whenever the system is expecting the user to give a new command. The modules currently connected to the Thermo-Calc system are:

SYSTEM_UTILITIES	General utilities
ALLOY_DATABANK	Data retrieval
POLY_1	Alloy calculations and post-processing
GIBBS_ENERGY_SYSTEM	The thermodynamic model package
MESSAGE_SYSTEM	Mail to manager and other users
EQUILONE	Equilibrium calculations with species
TEST_CALCULATIONS	Mainly for error checks
FILE_EDITOR	For text file editing

In Fig. 4 the modules are shown. The EQUILONE, TEST\_CALCULATION and FILE\_EDITOR modules will not be further described here.

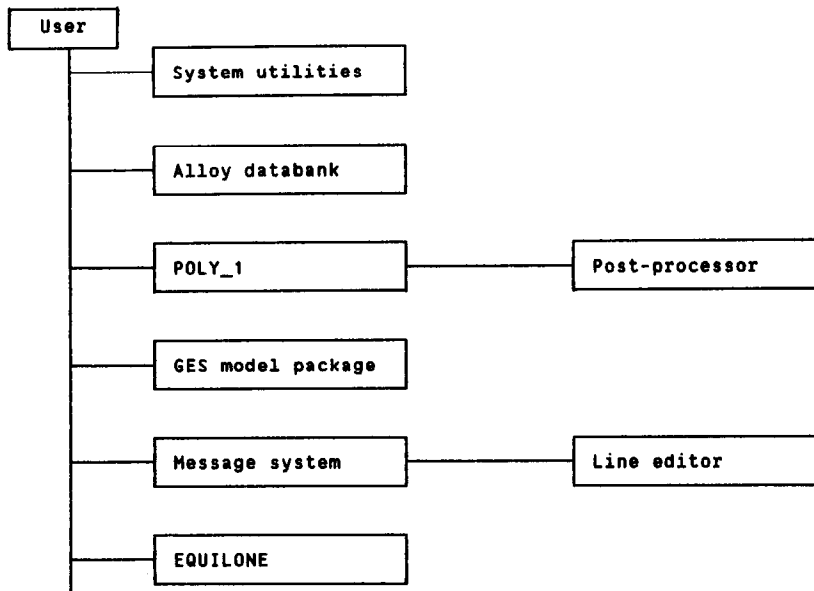


FIG. 4. The modular structure of Thermo-Calc. The postprocessor and the lined modules are local to the POLY\_1 and MESSAGE module respectively.

#### The SYSTEM UTILITY module

This is the module the program enters first. The commands in this module are used to set a number of global variables. Note that the commands are quite long and self-explanatory but a user can abbreviate the command and need only type so much that the command is unambiguous. If the command consists of several words these are connected with an underscore or hyphen. Each word in a command can be abbreviated separately as will be shown in the examples.

SYS> is the prompt in this module.

Commands that are available in this and most other modules are

HELP	INFORMATION
GOTO_MODULE	BACK
EXIT	

Useful commands in this module are

NEWS	SET_TIME_LIMIT
SET_TERMINAL	SET_LOG_FILE

Less frequently used commands are

OPEN_FILE	CLOSE_FILE
SET_COMMAND_UNITS	SET_ERROR_MESSAGE_UNIT
SET_INTERACTIVE_MODE	STOP_ON_ERROR

The following commands are for system debugging purpose only

```
PATCH          LIST_FREE_WORKSPACE
TRACE
```

HELP gives the list of commands or an explanation of any of the commands.

INFORMATION gives more extensive explanations of some features of the modules.

EXIT terminates the program.

GOTO transfer control to another module which must be specified.

BACK gives control back to the module used immediately before the present one.

The NEWS command gives a list of news messages.

SET\_LOG\_FILE makes it possible to save everything the user types on a file.

SET\_TERMINAL makes it possible to turn on/off echo from the host.

The other commands in the system\_utility module are rather special and mainly intended for system support.

#### The ALLOY DATABANK module

This module usually presents itself with a message like:

```
THERMODYNAMIC ALLOY DATABANK RUNNING ON ND-500/KTH_MET
First version released 811012, Last update 830920
Current dataset: THERMO-CALC dataset ( prerelease )
```

TDB\_TC: is the prompt. Note that this prompt varies with the dataset.

General commands are

```
HELP          EXIT
BACK          GOTO_MODULE
INFORMATION
```

The essential commands are

```
DEFINE-SYSTEM GET_DATA
REJECT
```

The diagnostic commands are

```
LIST_DATASET LIST_SYSTEM
LIST_OPTIONS SET_OPTION
```

Less frequently used commands are

```
SWITCH_DATASET DATASET_INFORMATION
RESTORE
```

DEFINE\_SYSTEM is the command for selecting the components of the system.

GET\_DATA is the command that retrieves data from the database.

LIST\_SYSTEM lists the phases, constituents or species that are included in the defined system.

REJECT can be used to reject phases, constituents etc from the system listed with list\_system. It is advisable to reject all phases that one knows will not appear in the region where calculations are planned.

SWITCH\_DATASET makes it possible to select another set of data. Several datasets from various sources are available and they are kept separate because they are not consistent with each other. Users can have private datasets.

LIST\_DATASET lists the same as list\_system but for the whole dataset.

The module for phase diagram calculations

This module presents itself the first time with the following message

```
POLY_1 VERSION 5.0 RUNNING ON MD-500/KTH_MET
Developed by Bo Jansson at the Division of Physical Metallurgy
Royal Institute of Technology, Stockholm, Sweden
First version released 79.10.01, Last update 83.08.01
```

POLY\_1> is the prompt.

General commands are

```
BACK                EXIT
GOTO_MODULE         HELP
INFORMATION
```

The essential commands are

```
SET_CONDITION       RESET_CONDITION
SET_PHASE_STATUS   SET_AXIS_VARIABLE
START_VALUES       SET_STORE_RESULT_FILE
COMPUTE_PHASE_EQUIL CALPHAD
POST_PROCESSOR
```

Diagnostic commands are

```
LIST_FIX_SITE_FRACTIONS LIST_PHASE_EQUIL
LIST_PHASE_STATUS      LIST_START_POINTS
LIST_STORE_RESULT_FILE LIST_VARIABLE_STATUS
```

Less frequent commands are

```
SET_WEIGHT_FRACTION  SET_MOLE_FRACTION
SET_START_COMPOSITION REINITIATE_WORKSPACE
SAVE_WORKSPACES      READ_ALL_WORKSPACES
DELETE_ALL_START_POINTS DELETE_LAST_START_POINT
```

Special commands are

```
READ_POLY_WORKSPACE  SET_PRESSURE_LEVEL
SET_PRESENT_PHASE    RESET_PRESENT_PHASE
SET_BREAK_CONDITIONS PATCH_POLY_WORKSPACE
```

The commands in this module are used to define the conditions for which the user wants to calculate an equilibrium or a phase diagram. The most important of these are:

SET\_CONDITION to set a fixed composition, activity, temperature etc. The degrees of freedom is decreased by one for each condition and must be zero before any calculations can be made.

LIST\_VARIABLE\_STATUS informs the user which conditions he has set.

The command START\_VALUES will ask you for a start composition for all phases that are not suspended. This must be done before the first calculation is made.

COMPUTE\_PHASE\_EQUILIBRIUM computes a single equilibrium for the conditions set.

LIST\_PHASE\_EQUILIBRIUM lists the values of the state variables and the composition of each phase after a calculation.



Less frequently used commands are

SET_AXIS_LENGTH	SET_AXIS_PLOT_STATUS
SET_AXIS_TEXT_STATUS	SET_DIAGRAM_TYPE
SET_PLOT_SIZE	SET_RASTER_STATUS
SET_TIELINE_STATUS	SET_TITLE
DEFINE_FUNCTION	LIST_FUNCTIONS
REINITIATE_PLOT_SETTINGS	CHANGE_MY_SPEED

With SET\_DIAGRAM\_AXIS the quantity to plot on the axis is selected.

SET\_SCALING\_STATUS allows manual scaling of each axis.

SET\_PLOT\_FORMAT gives a choice of some graphical output units.

PLOT\_DIAGRAM generates the diagram.

LIST\_ALL\_AXIS\_VALUES generates a table with the same numeric values as would appear on the plot.

DEFINE\_FUNCTION makes it possible to define an arbitrary quantity, to be used as axis variable, in terms of state variables.

#### The thermodynamic model module

In this module a user can specify his system interactively or list and amend data he has read from the database. The module presents itself with the following message.

```
GIBBS ENERGY SYSTEM VERSION 5 RUNNING ON ND-500/KTH_MET
Developed by Bo Sundman at the Division of Physical Metallurgy
Royal Institute of Technology, Stockholm, Sweden
First version released 78.01.01, Last update 83.03.01
```

GES> is the prompt.

General commands are

BACK	EXIT
GOTO_MODULE	HELP
INFORMATION	

Commands to define a system interactively are

ENTER_ELEMENT	ENTER_PARAMETER
ENTER_PHASE	ENTER_SPECIES

Listing of data

LIST_DATA	LIST_PARAMETER
LIST_SYMBOLS	

Diagnostic commands are

LIST_CONSTITUTION	LIST_STATUS
-------------------	-------------

Less frequently used commands are

AMEND_ELEMENT_DATA	AMEND_PHASE_DESCRIPTION
AMEND_PARAMETER	AMEND_SYMBOL
CHANGE_COMPOSITION_SETS	CHANGE_STATUS
ENTER_SYMBOL	REINITIATE
SAVE_GES_WORKSPACE	READ_GES_WORKSPACE
SET_R_AND_P_NORM	



LIST\_DATA lists all thermochemical information read from the database or entered interactively.

LIST\_PARAMETER lists the expression for an individual parameter. Each parameter is an arbitrary function of temperature and pressure. The thermochemical model selected for a phase determines how the Gibbs energy of the phase depends on the parameter.

AMEND\_PARAMETER allows editing of the expression for a parameter.

ENTER\_PARAMETER will delete any previous expression and allow entering a new expression.

CHANGE\_STATUS can be used to hide an element, species or phase from other modules. No data are removed and a second CHANGE\_STATUS can be used to restore the previous system.

The ENTER commands makes it possible for a user to define his system and data at the terminal.

AMEND\_PHASE\_DESCRIPTION makes it possible to select the model for a phase.

#### The message module

This module has been developed in order to make it easy to communicate between remote users and the manager of the Thermo-Calc system. The manager should receive all messages concerning any problems you have and errors you find in the system. It is also possible to send messages between users.

MESS: is the prompt.

General commands are

HELP	EXIT
BACK	GOTO_PROGRAM
INFORMATION	

Essential commands are

NEWS	
SEND_MESSAGE	LIST_SENT_MESSAGES
LIST_ALL_MESSAGES	LIST_MESSAGES_UNREAD

Less frequently used commands are

RESEND_MESSAGE	LIST_USERS
CHANGE_PASSWORD	

NEWS lists the news file. It is the same as in the SYSTEM\_UTILITIES module.

LIST\_MESSAGES\_UNREAD lists new messages sent to the user. After each message the user can select whether he wants to delete the message, to print it on a file, continue to read the next one or to stop reading.

LIST\_ALL\_MESSAGES lists all messages that the user has received and not deleted.

LIST\_SENT\_MESSAGES lists all messages that the user has sent to other users.

LIST\_USERS lists the names of the users known to the message system.

By the command CHANGE\_PASSWORD the user can change his password for the Thermo-Calc system.

There is a line editor called LINED which is entered when one is entering a message. The commands there are simple and there is also on-line help available.

Example 1 of the use of THERMO-CALC

For this example we choose a simple binary system like the Fe-C system. The first part is an introductory exploration of the message and the databank module and a demonstration of the on-line help facilities. When we finally have obtained data for the system the phase diagram is calculated and plotted. A second plot with carbon activity instead of carbon fraction is also made. It is then shown how the three-phase equilibrium fcc/bcc/cementite can be calculated directly. Finally a two-phase equilibrium fcc/bcc at a fixed carbon activity is calculated.

```
| The text which follows shows exactly how the Thermo-Calc
| system interacts with the user. Nothing has been removed or
| added except some explanations written to the right of a
| vertical bar as this text. User input is underlined
```

THERMO CALC service on ND-500/KTH\_MET

USER NAME: DEMO  
PASSWORD:

Last news update 83.11.08  
Try the HELP, INFORMATION, NEWS and GOTO commands if you are a novice.

SYS><u>HELP

COMMAND:

BACK	CLOSE_FILE
EXIT	GOTO_MODULE
HELP	INFORMATION
LIST_FREE_WORKSPACE	NEWS
OPEN_FILE	PATCH
SET_COMMAND_UNITS	SET_ERROR_MESSAGE_UNIT
SET_INTERACTIVE_MODE	SET_LOG_FILE
SET_TERMINAL	SET_TIME_LIMIT
STOP_ON_ERROR	TRACE

SYS><u>HELP INFO

INFORMATION

This command gives information about the features of the system.

```
| The HELP command gives a list of the commands in the module.
| If a command is specified after HELP an explanation of the
| command is given. Note that the commands can be abbreviated.
```

SYS><u>INFO

WHICH SUBJECT /PURPOSE/: ?

```
| When the program asks a question the user can type a ? to
| obtain an explanation of the question. The default answer,
| which is taken if the user just presses the RETURN key,
| is displayed within slashes.
```

WHICH SUBJECT <subject>

Select any of the following subjects:

DATABANK MODELS ASSESSMENT MESSAGE\_SYSTEM GIBBS\_ENERGY\_SYSTEM  
POLY EQUILIBRIUM\_CALCULATIONS PHASE\_DIAGRAMS PURPOSE  
TABULATIONS CHEMICAL\_EQUATIONS

WHICH SUBJECT /PURPOSE/: DATABANK

**DATABANK**

The data used in the calculations are model parameters assessed from measured quantities. These parameters are stored in a dataset although at present it is necessary to have several different datasets because assessments are not always consistent. From the parameter values it is possible to recalculate the experimental data that were used in the assessment and to make interpolations and extrapolations. It is of great importance to be able to extrapolate outside the range of experimental data through the use of thermochemical models. That is the reason why the large effort going into the assessments is worth while.

WHICH SUBJECT //:

SYS><u>NEWS

SENT DATE 831213      FIRST READ DATE 831215      LAST READ DATE 831215  
FROM USER MANAGER

A number of minor bugs have been corrected in POLY. For example the SET-START-COMPOSITION works properly and SET-COND SITE-FRAC will work now.

CONTINUE (Yes/Print on file/Exit) : /Y/

SENT DATE 831026      FIRST READ DATE 831026      LAST READ DATE 831215  
FROM USER MANAGER

A large number of changes have been made in the THERMO-CALC system. The most important are:

- Complete revision of the commands in the ALLOY-DATABANK monitor.
- A small change in POLY\_1 monitor.
- Some changes in the POST-PROCESSOR of POLY\_1 and addition of a facility to plot functions of state variables e.g. heat capacities.

There is further news about this. Use the on-line help facility also but it may take a few days to update it correctly.

CONTINUE (Yes/Print on file/Exit) : /Y/EX

| The user now wants to send a message. He must then go to the  
| MESSAGE module.

SYS><u>GO

MODULE NAME: ?

MODULE NAME <name>

A list of available programs is given by hitting the RETURN key.

MODULE NAME:

NO SUCH MODULE, USE ANY OF THESE:

SYSTEM\_UTILITIES  
GIBBS\_ENERGY\_SYSTEM  
TEST\_CALCULATIONS  
EQUILONE  
MESSAGE\_SYSTEM  
POLY\_1  
ALLOY\_DATABANK  
FILE\_EDITOR

MODULE NAME: MESS

```
| In the message module the commands for this module is
| listed by the HELP command. Note that the prompt is
| different.
```

```
MESS: HELP
COMMAND:
HELP                EXIT
BACK               GOTO_PROGRAM
LIST_ALL_MESSAGES  LIST_MESSAGES_UNREAD
LIST_SENT_MESSAGES SEND_MESSAGE
RESEND_MESSAGE     NEWS
CHANGE_PASSWORD    LIST_USERS INFORMATION
```

```
MESS: SEND-MESS
TYPE IN YOUR MESSAGE, MAX 20 LINES
TERMINATE WITH TWO CARRIAGE RETURNS
Hello this is my first try.
```

```
LINED: HELP
COMMAND:
HELP                EXIT_AND_SEND_MESSAGE
SEND_MESSAGE        LIST_USERS
QUIT_DO_NOT_SEND_MESSAGE APPEND_LINES
INSERT_LINE         DELETE_LINE
RECOVER_DELETED_LINE LIST_LINE
EDIT_LINE           INFORMATION
TYPE_WHOLE_TEXT
```

```
LINED: EXIT
SEND MESSAGE TO USER: MANAGER
MESSAGE SENT TO USER MANAGER
```

```
| The user now, finally, goes to the ALLOY_DATABANK module to
| get the data for the Fe-C system.
```

```
MESS: GO
MODULE NAME: ALLOY
```

```
VA DEFINED
THERMODYNAMIC ALLOY DATABANK RUNNING ON ND-500/KTH_MET
First version released 811012, Last update 831027
Current dataset: THERMO-CALC dataset ( prerelease )
```

```
| Vacancies (VA) are by default defined as a component.
```

```
TDB_TC: HELP
COMMAND:
HELP                EXIT
BACK               GOTO_MODULE
SWITCH_DATASET     DATASET_INFORMATION
DEFINE-SYSTEM      INFORMATION
RESTORE            REJECT
LIST_DATASET       LIST_SYSTEM
LIST_OPTIONS       SET_OPTION
GET_DATA
```

**TDB\_TC: INFO**

This module of the THERMO-CALC system allows the user to define a system and get thermodynamic data for that system. A straight-forward way to do this will be described.

**SWITCH\_DATASET** is used to change the default dataset. The second part of the prompt **TDB\_???** indicates the present dataset.

**LIST\_DATASET ELEMENT** gives a list of elements known to the present dataset. The keyword **ELEMENT** can be substituted with **SPECIES**, **PHASE** or **CONSTITUENT**.

**DEFINE\_SYSTEM ELEMENT <list of elements>** The elements are combined together to form all possible species and phases.

**LIST\_SYSTEM CONSTITUENT** gives a list of the phases that can form from the defined system. The elements listed after each phase are the constituents of that phase. The keyword can be changed as in **LIST\_DATASET**.

**REJECT PHASE <list of phases>** tells the database not to retrieve any data for whichever phases you specify here. The keyword can be changed as previously mentioned. The new keyword **SYSTEM** can be used to reinitiate the database.

**RESTORE PHASE <list of phases>** acts as the reverse of **REJECT** except that the keyword **SYSTEM** cannot be used for this command.

**GET\_DATA** searches the database and enters the defined system to **GES5**. After executing this command it is possible to **GOTO POLY** for calculation of different equilibria.

Using these commands in this order together with appropriate parameters will enable an unexperienced user to enter thermodynamic data to **GES5**

**TDB\_TC: DEFINE-SYSTEM**

with **ELEMENT OR SPECIES: /ELEMENT/:**

**ELEMENT:FE\_C**

**FE DEFINED**

**C DEFINED**

**TDB\_TC: LIST-SYSTEM**

**ELEMENT, SPECIES, PHASE OR CONSTITUENT: /PHASES/: CONST**

**BCC :FE : VA C :**

**FCC :FE : VA C :**

**LIQUID :C FE : VA C :**

**CEMENTITE :FE : C :**

**M23C6 :FE : C :**

**M7C3 :FE : C :**

**HCP :FE : VA :**

**GRAPHITE :C :**

```
| For the Fe-C system the databank has data for the phases
| listed. After the phase name the possible constituents of
| the phase are listed. The colons are used to separate
| constituents in different sublattices. For carbon an
| interstitial model is used where carbon and vacancies (VA)
| mix on the interstitial sublattice.
```

```
| If the user by experience knows that some of the phases are
| metastable in the region where he wants to make calculations
| he can reject them. He can also reject a stable phase if he
| wants to calculate a metastable equilibrium. Note that phase
| names as well as commands can be abbreviated.
```

```
TDB_TC: REJECT
ELEMENT, SPECIES, PHASE, CONSTITUENT OR SYSTEM: /ELEMENT/: PHASE
PHASE:M23 M7 HCP GRA
M23C6 REJECTED
M7C3 REJECTED
HCP REJECTED
GRAPHITE REJECTED
```

```
TDB_TC: LI-SY
ELEMENT, SPECIES, PHASE OR CONSTITUENT: /CONSTITUENTS/:
BCC :FE : VA C :
FCC :FE : VA C :
LIQUID :C FE : VA C :
CEMENTITE :FE : C :
```

```
TDB_TC: GET
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
-OK-
TDB_TC: GO POLY
```

```
| The data have now been obtained from the database and the
| user goes to the module for phase diagram calculations.
```

POLY\_1 VERSION 5.0 RUNNING ON ND-500/KTH\_MET

Developed by Bo Jansson at the Division of Physical Metallurgy  
Royal Institute of Technology, Stockholm, Sweden  
First version released 79.10.01, Last update 83.08.01

POLY\_1>HELP

```
COMMAND:
BACK
COMPUTE_PHASE_EQUIL
DELETE_LAST_START_POINT
GOTO_MODULE
INFORMATION
LIST_PHASE_EQUIL
LIST_START_POINTS
LIST_VARIABLE_STATUS
POST_PROCESSOR
READ_POLY_WORKSPACE
RESET_CONDITION
SAVE_ALL_WORKSPACES
SET_BREAK_CONDITIONS
SET_MOLE_FRACTION
SET_PRESENT_PHASE
SET_START_COMPOSITION
SET_WEIGHT_FRACTION
CALPHAD
DELETE_ALL_START_POINTS
EXIT
HELP
LIST_FIX_SITE_FRACTIONS
LIST_PHASE_STATUS
LIST_STORE_RESULT_FILE
PATCH_POLY_WORKSPACE
READ_ALL_WORKSPACES
REINITIATE_WORKSPACE
RESET_PRESENT_PHASE
SET_AXIS_VARIABLE
SET_CONDITION
SET_PHASE_STATUS
SET_PRESSURE_LEVEL
SET_STORE_RESULT_FILE
START_VALUES
```

POLY\_1>INFO

WHICH SUBJECT /PURPOSE/: 2

WHICH SUBJECT

The subjects on which specific information is available are

1 PURPOSE	2 UNITS	3 LIMITATIONS
4 PHASE NAME	5 PHASE STATUS	6 CONDITIONS
7 SINGLE EQUILIBRIA	8 AXIS VARIABLES	9 MAPPING
10 DATA STORAGE	11 INITIATION	

WHICH SUBJECT /PURPOSE/:

PURPOSE

POLY is a computer program for equilibrium calculations in multi-component thermochemical systems. The equilibrium equations are generated by the program from conditions specified by the user. This gives a high flexibility and allows the program to be used for many different types of calculations. The POLY program can be used for single equilibrium calculations and for mapping of one-, two- or three-dimensional phase diagrams. POLY can handle systems only where the constituents in the phases are elements. It is thus suited for calculations in alloy systems but cannot handle, for example, a gas phase with molecules as constituents.

WHICH SUBJECT /PURPOSE/: MAPPING

MAPPING

A phase diagram is a geometrical representation of the variation of the state of equilibrium under consideration of some variable parameter. For a multi-component system the total phase diagram can be represented in a many-dimensional linear space. With the POLY program it is possible to map one-, two- and three-dimensional sections of the many-dimensional phase diagram. The topological structure of the sections of phase diagrams that is mapped by POLY are line segments joining in node points. The line segments and node points can be phase regions or phase region boundaries depending on the axis variables used in the mapping. The user must specify at least one start point, where the equilibrium state can be calculated, and a step direction in the diagram. The start points must be inside the diagram and not on the boundaries. At the start of the mapping POLY will step from the start point in the step direction to find a topological structure of the diagram that should be mapped. When a structure to be mapped is found all topologically connected structures will be mapped automatically. If the phase diagram consists of topological structures that are not connected the user must specify one start point for each topologically connected structure.

POLY\_1>HELP

COMMAND: LIST

LIST\_FIX\_SITE\_FRACTIONS

LIST\_PHASE\_EQUIL

LIST\_PHASE\_STATUS

LIST\_START\_POINTS

LIST\_STORE\_RESULT\_FILE

LIST\_VARIABLE\_STATUS

POLY\_1>LIST-VARIABLE-STATUS

TEMPERATURE	NOT-FIXED	PRESSURE	1.013E+05	
ELEMENT	FRACTION	ACTIVITY	POTENTIAL	REFERENCE STATE
C	NOT-FIXED	NOT-FIXED	NOT-FIXED	GRAPHITE
FE	NOT-FIXED	NOT-FIXED	NOT-FIXED	FCC_PARAMAGNETIC

NUMBER OF DEGREES OF FREEDOM : 3

ELEMENT FRACTION TYPE : MOLE FRACTION

POLY\_1>LIST-PHASE-STATUS

PHASE		STATUS	NO OF MOLES	PRESSURE LEVEL
BCC	1	ENTERED	.0000E+00	.0000E+00
CEMENTITE	1	ENTERED	.0000E+00	.0000E+00
FCC	1	ENTERED	.0000E+00	.0000E+00
LIQUID	1	ENTERED	.0000E+00	.0000E+00

| The digit 1 after each phase name indicates that the phase  
| has one set of fraction variables. Two sets of fractions  
| are needed when a miscibility gap shall be calculated.  
| (not demonstrated in this example).  
| The user now defines the axis variables he wants to use  
| in his calculation of the Fe-C phase diagram.

POLY\_1>SET-AXIS-VAR

AXIS (X, Y OR Z): /X/:

AXIS VARIABLE: 1

The user must specify an axis variable. In POLY the following axis variables are available:

TEMPERATURE  
PRESSURE  
ACTIVITY  
CHEMICAL POTENTIAL  
NORMALIZED FRACTION  
CLEAR

| If the explanation is insufficient more extensive help can  
| be obtained by typing two ??

AXIS VARIABLE: ??

AXIS VARIABLES

The axis variables must be specified in the order X,Y and Z. When an X axis variable is specified the Y and Z axis are cleared. When the Y axis is specified the Z axis is cleared. The following axis variables can be used for mapping phase diagrams.

TEMPERATURE  
PRESSURE  
ACTIVITY for an element  
CHEMICAL\_POTENTIAL for an element  
NORMALIZED\_FRACTION A linear combination of overall composition.

The user must give a start point and an end point in composition space for the axis. The normalized fraction will vary linearly from zero to one from the start point to the end point. If normalized fraction is used as axis variable on more than one axis, the same start point will be used, but different end points. The user can specify which and how many of the elements will take part in the linear combination of compositions.

CLEAR the axis specification will be cleared.

AXIS VARIABLE: NORM

START POINT, ELEMENT NAME: C

ELEMENT FRACTION: 0

END POINT, ELEMENT FRACTION FOR C : .3

MIN VALUE: /0/:

MAX VALUE: /1/:

MAX STEP INCREMENT: /.025/:



POLY\_1>INFO UNITS

## UNITS

The POLY program is mainly using SI units. The units for the following state variables should always be considered by the user.

TEMPERATURE	kelvin
PRESSURE	pascal
CHEMICAL POTENTIAL	joule/mole
AVERAGE COMPOSITION	mole fraction or mass fraction

WHICH SUBJECT //:

POLY\_1>S-A-Y

AXIS (X, Y OR Z): /Y/:

AXIS VARIABLE: I

MIN VALUE: 850

MAX VALUE: 1850

MAX STEP INCREMENT: /25/:

| The LIST-VARIABLE-STATUS command shows the conditions or  
| axis the user has set.

POLY\_1>L-V-S

TEMPERATURE	Y-AXIS	PRESSURE	1.013E+05
-------------	--------	----------	-----------

ELEMENT	FRACTION	ACTIVITY	POTENTIAL	REFERENCE STATE
C	X-AXIS	NOT-FIXED	NOT-FIXED	GRAPHITE
FE	DEPENDENT	NOT-FIXED	NOT-FIXED	FCC_PARAMAGNETIC

NUMBER OF DEGREES OF FREEDOM : 0

MAX NUMBER OF PHASES IN EQUIL : 2

ELEMENT FRACTION TYPE : MOLE FRACTION

| The user now gives a start point for the calculation. At the  
| start point he must make a crude guess of the constitution  
| of all non-suspended phases. Sublattice 2 is the  
| interstitial lattice for carbon and the carbon fraction  
| should be low. The selected step variable and direction  
| will be explained later.

POLY\_1>START-VALUE

X-AXIS VARIABLE IS NORMALIZED-FRACTION MAX= 1.00000E+00 MIN = .00000E+00

START VALUE FOR X-AXIS /0/: .1

Y-AXIS VARIABLE IS TEMPERATURE MAX= 1.85000E+03 MIN = 8.50000E+02

START VALUE FOR Y-AXIS /0/: 1800

STEP VARIABLE (X,Y,Z OR NONE) : Y

STEP DIRECTION (+1=POS, -1=NEG) : -1

START VALUES FOR COMPOSITIONS ( Y OR N): /N/: Y

BCC 1

GIVE START VALUE FOR NUMBER OF MOLES: /0/:

GIVE SITE FRACTION FOR C IN SUBLATTICE 2: /1/: .01

CEMENTITE 1

GIVE START VALUE FOR NUMBER OF MOLES: /0/:

FCC 1

GIVE START VALUE FOR NUMBER OF MOLES: /0/:

GIVE SITE FRACTION FOR C IN SUBLATTICE 2: /1/: .01

LIQUID 1

GIVE START VALUE FOR NUMBER OF MOLES: /0/: 1

GIVE SITE FRACTION FOR C IN SUBLATTICE 1: /1/: .01

GIVE SITE FRACTION FOR C IN SUBLATTICE 2: /1/: .01

DO YOU WANT TO STORE START VALUES AS A START POINT ( Y OR N): /N/: Y

-OK- START POINT STORED

| POLY has calculated and stored the result as a start point.  
| The result can be listed by the next command.

```

POLY_1>L-P-E
FILE NAME: /TERMINAL/:
SITE FRACTIONS LISTED (Y OR N) /N/:
TEMP = 1.80000E+03    PRESSURE = 1.01325E+05    8 ITERATIONS
ELEMENT  X-FRACTION  POTENTIAL  ACTIVITY  REFERENCE STATE
VA      .00000E+00  .00000E+00  1.00000E+00  VACUUM
C       3.00000E-02 -5.60477E+04  2.36343E-02  GRAPHITE
FE      9.70000E-01 -5.04707E+02  9.66838E-01  FCC_PARAMAGNETIC

BCC      1, STATUS=ENTERED
MOL FRACTION  .000E+00  PRESSURE -4.801E+07  PRESSURE LEVEL  .000E+00
C -X-FRAC FE-X-FRAC
  .0057688  .9942312

CEMENTITE 1, STATUS=ENTERED
MOL FRACTION  .000E+00  PRESSURE -3.404E+07  PRESSURE LEVEL  .000E+00
C -X-FRAC FE-X-FRAC
  .2500000  .7500000

FCC      1, STATUS=ENTERED
MOL FRACTION  .000E+00  PRESSURE -3.518E+07  PRESSURE LEVEL  .000E+00
C -X-FRAC FE-X-FRAC
  .0100811  .9899189

LIQUID   1, STATUS=ENTERED
MOL FRACTION  1.000E+00  PRESSURE  .000E+00  PRESSURE LEVEL  .000E+00
C -X-FRAC FE-X-FRAC
  .0300000  .9700000

```

| The user needs help to interpret this output.

```

POLY_1>HELP L-P-E
LIST_PHASE_EQUIL

```

All relevant information concerning the equilibrium stored in the POLY workspace will be listed by this command.

The list starts with the values of the global quantities in the system, i.e. the temperature and pressure and for each component its overall composition, activity and potential. The reference state for the components is also listed.

For each phase that is not suspended the list will contain - the amount, - the pressure, - the pressure level, - the composition.

A phase which is not stable has the amount zero, of course. The pressure of a phase is the negative of the driving force for precipitation divided by the molar volume of the phase. For a stable phase this is zero, for a dormant phase which should be stable the pressure is positive and for an unstable phase it is negative. The pressure level of a phase is set by a separate command. The composition of a dormant or unstable phase is calculated by POLY using the condition that the partial Gibbs energies of the components of the phase should be equal to the potentials for the calculated equilibrium but for a constant value, i.e. the driving force for precipitation.

```

POLY_1>HELP CALPHAD
CALPHAD

```

This command will map the specified phase diagram. The start points stored in the workspace will be used in the search. If a STORE RESULT FILE is specified the workspaces will be saved before the mapping starts. During the mapping the axis variable values for all calculated equilibria will be written on the terminal. All data for the equilibria calculated will be stored in a buffer space. When the buffer space is full or the mapping is completed it is written in binary format on the store result file. If no store result file is specified the mapping will be terminated when the buffer is full.

POLY\_1>CALPHAD

PHASE REGION FOR THE FOLLOWING PHASES IS TO BE MAPPED

LIQUID 1

PHASE REGION BOUNDARY FOR THE FOLLOWING PHASES IS TO BE MAPPED

FCC 1

LIQUID 1

3 ITS X= 1.0000E-01 Y= 1.7579E+03

| This output is only to inform the user that the program  
| is running smoothly. 3 ITS means that 3 iterations were  
| needed to calculate the equilibrium. Superfluous output  
| during this command has been suppressed from this example.

...

4 ITS X= 5.7678E-01 Y= 1.4208E+03

PHASE REGION BOUNDARY FOR THE FOLLOWING PHASES IS TO BE MAPPED

CEMENTITE 1

FCC 1

| The eutectic equilibrium has already been found (the  
| metastable one as graphite has been excluded). The program  
| continues with a connected two-phase region.

4 ITS X= 3.0491E-01 Y= 1.4208E+03

...

6 ITS X= 1.1553E-01 Y= 1.0000E+03

PHASE REGION BOUNDARY FOR THE FOLLOWING PHASES IS TO BE MAPPED

BCC 1

CEMENTITE 1

6 ITS X= 3.2327E-03 Y= 1.0000E+03

...

5 ITS X= 6.7845E-04 Y= 8.5000E+02

PHASE REGION BOUNDARY FOR THE FOLLOWING PHASES IS TO BE MAPPED

BCC 1

FCC 1

5 ITS X= 1.1553E-01 Y= 1.0000E+03

...

4 ITS X= 1.5721E-10 Y= 1.1851E+03

PHASE REGION BOUNDARY FOR THE FOLLOWING PHASES IS TO BE MAPPED

CEMENTITE 1

LIQUID 1

4 ITS X= 5.7678E-01 Y= 1.4208E+03

...

4 ITS X= 1.0000E+00 Y= 1.4571E+03

PHASE REGION BOUNDARY FOR THE FOLLOWING PHASES IS TO BE MAPPED

FCC 1

LIQUID 1

4 ITS X= 1.0000E-01 Y= 1.7579E+03

...

8 ITS X= 7.9499E-02 Y= 1.7673E+03

PHASE REGION BOUNDARY FOR THE FOLLOWING PHASES IS TO BE MAPPED

BCC 1

FCC 1

8 ITS X= 2.5374E-02 Y= 1.7673E+03

...

4 ITS X= 2.5137E-11 Y= 1.6669E+03

PHASE REGION BOUNDARY FOR THE FOLLOWING PHASES IS TO BE MAPPED

```
BCC                1
LIQUID             1
 4 ITS  X= 7.9499E-02  Y= 1.7673E+03
...
 9 ITS  X= 1.0000E-07  Y= 1.8108E+03
```

\*\*NO MORE START-POINTS\*\*

| The post-processor is entered to draw a diagram.

POLY\_1>POST

POLY\_1 POST PROCESSOR VERSION 5.0

POST>HELP

COMMAND:

BACK	CHANGE_MY_SPEED
DEFINE_FUNCTION	EXIT
HELP	LIST_ALL_AXIS_VALUES
LIST_ALL_EQUILIBRIA	LIST_FUNCTIONS
LIST_PLOT_SETTINGS	LIST_SYSTEM_DEFINITION
PLOT_DIAGRAM	REINITIATE_PLOT_SETTINGS
SET_AXIS_LENGTH	SET_AXIS_PLOT_STATUS
SET_AXIS_TEXT_STATUS	SET_DIAGRAM_AXIS
SET_DIAGRAM_TYPE	SET_PLOT_FORMAT
SET_PLOT_SIZE	SET_RASTER_STATUS
SET_SCALING_STATUS	SET_TIELINE_STATUS
SET_TITLE	LIST_FUNCTIONS

POST>SET-DIAGRAM-AXIS

AXIS (X, Y OR Z): X

AXIS VARIABLE: T

#### AXIS VARIABLE

The user must specify which state variable is to be used as diagram axis. The default axis variable is the variable which has been used for the mapping. When a new axis variable is set the scaling status is set to automatic scaling. The following axis variables are defined in the Post\_Processor.

TEMPERATURE-KELVIN	
TEMPERATURE-CELSIUS	
PRESSURE-PASCAL	
ACTIVITY	for an element
CHEMICAL-POTENTIAL	for an element
NORMALIZED-FRACTION	an axis defined for the mapping
MOLE-FRACTION	for an element
WEIGHT-PERCENT	for an element
SITE-FRACTION	for an element (in a sublattice)
PHASE-MOLE-FRACTION	for a phase
PHASE-WEIGHT-PERCENT	for a phase
IN-PHASE-MOLE-FRACTION	for an element in a phase
IN-PHASE-WEIGHT-PERCENT	for an element in a phase
IN-PHASE-SITE-FRACTION	for an element (sublattice) in a phase
FUNCTION	an defined function
CLEAR	to clear the axis

AXIS VARIABLE: H

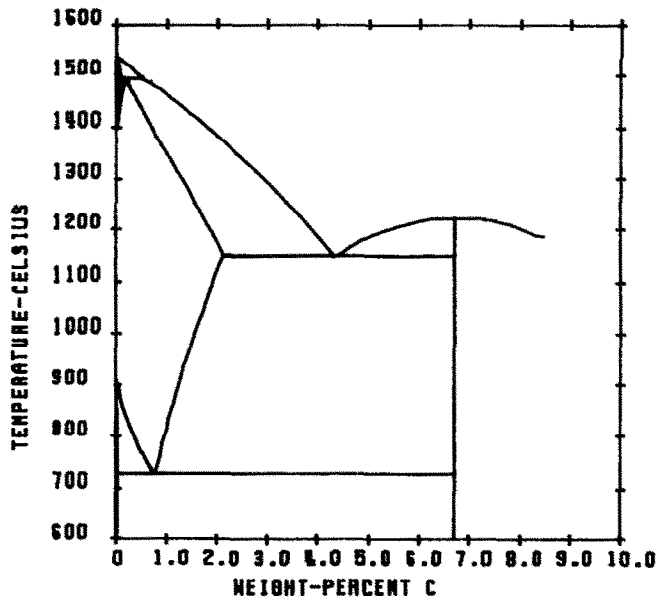
ELEMENT NAME: C

POST>S-D-A

AXIS (X, Y OR Z): Y

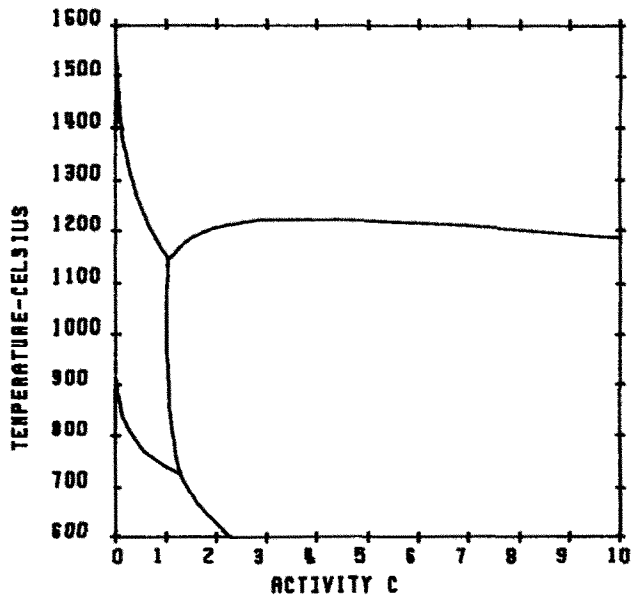
AXIS VARIABLE: T-C

POST>PLOT  
 PLOT FILE: /TERMINAL/:



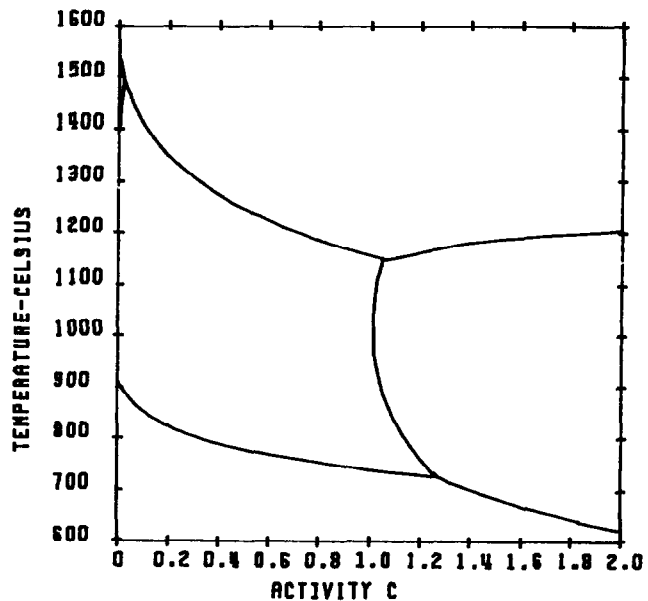
| Another way of presenting the results of the same  
 | calculation is to use the carbon activity as axis variable.

POST>S-D-A  
 AXIS (X, Y OR Z): X  
 AXIS VARIABLE: ACT  
 ELEMENT NAME: C  
 POST>PLOT  
 PLOT FILE: /TERMINAL/:



| If the automatic scaling gives a poor diagram it is  
| possible to set the scaling manually

POST>SET-SCALING  
 AXIS (X, Y OR Z): X  
 AUTOMATIC SCALING (Y OR N): /N/:  
 MIN VALUE: 0  
 MAX VALUE: 2  
 POST>PLOT  
 PLOT FILE: /TERMINAL/:



POST>BACK  
 POLY\_1 VERSION 5.0 RUNING ON NO-500/KTH\_MET

| The user now wants to calculate the equilibrium where the  
| phases fcc, bcc and cementite can coexist. First he must  
| reinitiate.

POLY\_1>REINITIATE  
 -OK-  
 POLY\_1>LIST-VARIABLE-STATUS

TEMPERATURE	NOT-FIXED	PRESSURE	1.013E+05	
ELEMENT	FRACTION	ACTIVITY	POTENTIAL	REFERENCE STATE
C	NOT-FIXED	NOT-FIXED	NOT-FIXED	GRAPHITE
FE	NOT-FIXED	NOT-FIXED	NOT-FIXED	FCC_PARAMAGNETIC

NUMBER OF DEGREES OF FREEDOM : 3  
 ELEMENT FRACTION TYPE : MOLE FRACTION

POLY\_1>LIST-PHASE-STATUS

PHASE	STATUS	NO OF MOLES	PRESSURE LEVEL
BCC	1 ENTERED	.0000E+00	.0000E+00
CEMENTITE	1 ENTERED	.0000E+00	.0000E+00
FCC	1 ENTERED	.0000E+00	.0000E+00
LIQUID	1 ENTERED	.0000E+00	.0000E+00

POLY\_1&gt;INFO

WHICH SUBJECT /PURPOSE/: 1

WHICH SUBJECT

The subjects on which specific information is available are

1 PURPOSE	2 UNITS	3 LIMITATIONS
4 PHASE NAME	5 PHASE STATUS	6 CONDITIONS
7 SINGLE EQUILIBRIA	8 AXIS VARIABLES	9 MAPPING
10 DATA STORAGE	11 INITIATION	

WHICH SUBJECT /PURPOSE/: PHASE-STATUS

PHASE STATUS

The status of a phase tells POLY how to treat a phase in the equilibrium calculations. The following status specifications are available.

**ENTERED** The phase will be considered at the equilibrium calculations. The amount of the phase is allowed to vary. For an entered phase that does not take part in an equilibrium a hypothetical driving force, expressed as a pressure, that would bring the phase in equilibrium with the system, and the most favourable composition is calculated. This is the default status of all phases at the initiation of POLY.

**FIX** The phase must take part in the equilibria and the number of moles of formula unit of the phase is prescribed. This status can only be used for calculation of single equilibria. For each fix phase in the system the degrees of freedom will decrease with one unit.

**DORMANT** The phase will not take part in any equilibria even if that would give a more stable equilibrium. The driving force and the composition of the phase will be calculated. A positive driving force indicates that the phase would take part in the equilibrium if it was entered.

**SUSPENDED** The phase will not be considered in an equilibrium calculation.

WHICH SUBJECT //:

POLY\_1>SET-PHASE-STATUSPHASE NAME: FCCSTATUS: FIXNUMBER OF MOLES: 1POLY\_1>S-P-S BCC FIXNUMBER OF MOLES: 0

```
| A novice user of Thermo-Calc can always be prompted for the
| arguments of a command by pressing RETURN after each value.
| As the user becomes more skilled he usually types more and
| more on the same line.
```

POLY\_1>S-P-S CEM FIX 0POLY\_1>L-V-S

TEMPERATURE NOT-FIXED PRESSURE 1.013E+05

ELEMENT	FRACTION	ACTIVITY	POTENTIAL	REFERENCE STATE
C	NOT-FIXED	NOT-FIXED	NOT-FIXED	GRAPHITE
FE	NOT-FIXED	NOT-FIXED	NOT-FIXED	FCC_PARAMAGNETIC

NUMBER OF DEGREES OF FREEDOM : 0

MAX NUMBER OF PHASES IN EQUIL : 3

ELEMENT FRACTION TYPE : MOLE FRACTION

POLY\_1>L-P-S

PHASE	STATUS	NO OF MOLES	PRESSURE LEVEL
BCC	1 FIX	.0000E+00	.0000E+00
CEMENTITE	1 FIX	.0000E+00	.0000E+00
FCC	1 FIX	1.0000E+00	.0000E+00
LIQUID	1 ENTERED	.0000E+00	.0000E+00

POLY\_1>ST-V

GIVE START VALUE FOR TEMPERATURE: /0/: 700

START VALUES FOR COMPOSITIONS ( Y OR N): /N/: N

| Start values for compositions are usually needed only once.  
| The last calculated equilibrium from the mapping will now be  
| used as start values. To calculate a single equilibrium the  
| command is COMPUTE-PHASE-EQUIL.

POLY\_1>C-P-E

-OK-

| The user can now list the results by the LIST-PHASE-EQUIL  
| command. Separate commands to set, calculate and list gives  
| the user a large flexibility in his use of the program.

POLY\_1>L-P-E

FILE NAME: /TERMINAL/:

SITE FRACTIONS LISTED (Y OR N):

TEMP =	1.00001E+03	PRESSURE =	1.01325E+05	8 ITERATIONS
ELEMENT	X-FRACTION	POTENTIAL	ACTIVITY	REFERENCE STATE
VA	.00000E+00	.00000E+00	1.00000E+00	VACUUM
C	3.46603E-02	1.92227E+03	1.26011E+00	GRAPHITE
FE	9.65340E-01	-3.45075E+02	9.59346E-01	FCC_PARAMAGNETIC

BCC		1, STATUS=FIX		
MOL FRACTION	.000E+00	PRESSURE	.000E+00	PRESSURE LEVEL .000E+00
C -X-FRAC	FE-X-FRAC			
	.0009698			.9990302

CEMENTITE		1, STATUS=FIX		
MOL FRACTION	.000E+00	PRESSURE	.000E+00	PRESSURE LEVEL .000E+00
C -X-FRAC	FE-X-FRAC			
	.2500000			.7500000

FCC		1, STATUS=FIX		
MOL FRACTION	1.000E+00	PRESSURE	.000E+00	PRESSURE LEVEL .000E+00
C -X-FRAC	FE-X-FRAC			
	.0346603			.9653397

LIQUID		1, STATUS=ENTERED		
MOL FRACTION	.000E+00	PRESSURE	-3.838E+07	PRESSURE LEVEL .000E+00
C -X-FRAC	FE-X-FRAC			
	.1180408			.8819592

| Note that the carbon activity is 1.26 relative to graphite  
| for this three-phase equilibrium. To find the stable  
| three-phase equilibrium with graphite we can instead set a  
| condition that the carbon activity should be unity. The  
| cementite must have its status changed first, otherwise the  
| degrees of freedom will not be zero.

POLY\_1>S-P-S CEM ENT 0

POLY\_1>SET-COND

STATE\_VARIABLE: ACT

ELEMENT NAME: C

VALUE: /1.26010862/: 1

POLY\_1>C-P-E

-OK-





Example 2 of the use of THERMO-CALC

In this example the stable phases in a high-speed steel between 1300 and 600 Celsius is calculated. The steel contains C, Si, Mn, Cr, Mo, W, and V.

First a single equilibrium is calculated for a fixed temperature and composition. This calculation shows how to obtain a start point. For any calculation but especially in multicomponent alloys it is important to have an idea about the stable phase set and the constitution of the phases at some point. In this example the alloy must consist of austenite and some carbides at 1200 °C. Thus a calculation with only austenite is made first. Then the other phases are entered and a new equilibrium is calculated. The unstable phases have their most favourable constitution calculated in order to make it possible to determine when they can become stable, e.g. during an automatic mapping calculation.

An automatic mapping calculation in temperature is then started and all equilibria from 1573 K to 873 K are calculated. The stable phase set changes during this stepping calculation according to the stabilities of the phases. After the calculation the variation of the carbon activity is plotted vs temperature. A second plot of the amount of carbides vs temperature is also made.

The normal amount of erroneous input that a skilled user will make is included in the example. A minimum of on-line help is used.

THERMO CALC service on ND-500/KTH\_MET

USER NAME: DEMO  
PASSWORD:

Last news update 83.11.08

Try the HELP, INFORMATION, NEWS and GOTO commands if you are a novice.

SYS>GO ALLOY

VA DEFINED  
THERMODYNAMIC ALLOY DATABANK RUNNING ON ND-500/KTH\_MET  
First version released 811012, Last update 831027  
Current dataset: THERMO-CALC dataset ( prerelease )

TDB\_TC: SWITCH  
Use one of these datasets

- 1) THERMO-CALC dataset ( prerelease )
- 2) FE\_base Parameters by Uhrenius, Waldenstroem and Jarl
- 3) Kaufman Parameters Published in Calphad
- 4) Substance dataset
- 5) Userdefined dataset

Dataset number: /1/: 2

VA DEFINED  
THERMODYNAMIC ALLOY DATABANK RUNNING ON ND-500/KTH\_MET  
First version released 811012, Last update 831027  
Current dataset: FE\_base Parameters by Uhrenius, Waldenstroem and Jarl

TDB\_FE:LI-DATA

ELEMENT, SPECIES, PHASE OR CONSTITUENT: /PHASES/: COM  
 AUSTENITE 2 SUBLATTICES, SITES 1.00: 1.00:  
 SI P V CR MN FE CO NI CU MO W: VA C N:  
 FERRITE 2 SUBLATTICES, SITES 1.00: 3.00:  
 SI P V CR MN FE CO NI CU MO W: VA C N:  
 LIQUID 2 SUBLATTICES, SITES 1.00: 1.00:  
 SI P CR MN FE NI W: VA C:  
 CEMENTITE 2 SUBLATTICES, SITES 1.00: .33:  
 V CR MN FE NI MO W: C:  
 M23C6 2 SUBLATTICES, SITES 1.00: .26:  
 CR MN FE NI MO W: C:  
 M7C3 2 SUBLATTICES, SITES 1.00: .43:  
 CR MN FE NI: C:  
 M6C 2 SUBLATTICES, SITES 1.00: .17:  
 CR FE CO MO W: C:  
 MC\_HP\_CARBIDE 2 SUBLATTICES, SITES 1.00: 1.00:  
 MO W: C:  
 MC\_FCC\_CARBIDE 2 SUBLATTICES, SITES 1.00: 1.00:  
 V CR MN FE CO NI MO W: C:  
 GRAPHITE C:  
 M2C 2 SUBLATTICES, SITES 1.00: .50:  
 V CR FE MO W: C:  
 FE3W2 2 SUBLATTICES, SITES .60: .40:  
 FE: W:  
 EPSILON 2 SUBLATTICES, SITES 2.00: 1.00:  
 CR FE: VA N:  
 CRN 2 SUBLATTICES, SITES 1.00: 1.00:  
 FE CR: N:

TDB\_FE:DEFINE-SYSTEM

with ELEMENT OR SPECIES: /ELEMENT/:  
 ELEMENT:FE C SI MN CR MO W V

FE DEFINED  
 C DEFINED  
 SI DEFINED  
 MN DEFINED  
 CR DEFINED  
 MO DEFINED  
 W DEFINED  
 V DEFINED

TDB\_FE:LI-SYS

ELEMENT, SPECIES, PHASE OR CONSTITUENT: /PHASES/: CONSI  
 AUSTENITE :SI V CR MN FE MO W : VA C :  
 FERRITE :SI V CR MN FE MO W : VA C :  
 LIQUID :SI CR MN FE W : VA C :  
 CEMENTITE :V CR MN FE MO W : C :  
 M23C6 :CR MN FE MO W : C :  
 M7C3 :CR MN FE : C :  
 M6C :CR FE MO W : C :  
 MC\_HP\_CARBIDE :MO W : C :  
 MC\_FCC\_CARBIDE :V CR MN FE MO W: C :  
 GRAPHITE :C :  
 M2C :V CR FE MO W : C :  
 FE3W2 :FE : W :  
 EPSILON :CR FE : VA :

TDB\_FE:REJECT  
 ELEMENT, SPECIES, PHASE, CONSTITUENT OR SYSTEM: /ELEMENT/: PHASE  
 PHASE:LIQ\_EPS  
 LIQUID REJECTED  
 EPSILON REJECTED  
 TDB\_FE:GO POLY

\*\*\* You have not executed the GET\_DATA command

POLY\_1 VERSION 5.0 RUNNING ON ND-500/KTH\_MET

Developed by Bo Jansson at the Division of Physical Metallurgy  
 Royal Institute of Technology, Stockholm, Sweden  
 First version released 79.10.01, Last update 83.08.01

| The user was reminded that he has not made any GET  
 | command and thus has no data. He can directly go BACK  
 | to the databank module and correct this mistake.

POLY\_1>BACK  
 TDB\_FE:GET  
 REINITIATING GESS .....  
 ELEMENTS .....  
 SPECIES .....  
 PHASES .....  
 PARAMETERS ...  
 -OK-  
 TDB\_FE:BACK

POLY\_1 VERSION 5.0 RUNNING ON ND-500/KTH\_MET

POLY\_1>LIST-VARIABLE-STATUS

TEMPERATURE	NOT-FIXED	PRESSURE	1.013E+05	
ELEMENT	FRACTION	ACTIVITY	POTENTIAL	REFERENCE STATE
C	NOT-FIXED	NOT-FIXED	NOT-FIXED	GRAPHITE
CR	NOT-FIXED	NOT-FIXED	NOT-FIXED	BCC
FE	NOT-FIXED	NOT-FIXED	NOT-FIXED	AUSTENITE
MN	NOT-FIXED	NOT-FIXED	NOT-FIXED	FCC
MO	NOT-FIXED	NOT-FIXED	NOT-FIXED	BCC
SI	NOT-FIXED	NOT-FIXED	NOT-FIXED	DIAMOND
V	NOT-FIXED	NOT-FIXED	NOT-FIXED	BCC
W	NOT-FIXED	NOT-FIXED	NOT-FIXED	FCC

NUMBER OF DEGREES OF FREEDOM : 9

ELEMENT FRACTION TYPE : MOLE FRACTION

POLY\_1>LIST-PHASE-STATUS

PHASE		STATUS	NO OF MOLES	PRESSURE LEVEL
AUSTENITE	1	ENTERED	.0000E+00	.0000E+00
CEMENTITE	1	ENTERED	.0000E+00	.0000E+00
FE3W2	1	ENTERED	.0000E+00	.0000E+00
FERRITE	1	ENTERED	.0000E+00	.0000E+00
GRAPHITE	1	ENTERED	.0000E+00	.0000E+00
M23C6	1	ENTERED	.0000E+00	.0000E+00
M2C	1	ENTERED	.0000E+00	.0000E+00
M6C	1	ENTERED	.0000E+00	.0000E+00
M7C3	1	ENTERED	.0000E+00	.0000E+00
MC_FCC_CARBIDE	1	ENTERED	.0000E+00	.0000E+00
MC_HP_CARBIDE	1	ENTERED	.0000E+00	.0000E+00

| The overall composition of the alloy is set as conditions.

POLY\_1>SET-COND  
STATE\_VARIABLE: ?

STATE VARIABLE

The user must specify the type of the state variable which is to be assigned a value. The following state variables are defined in POLY:

TEMPERATURE  
PRESSURE  
ACTIVITY  
CHEMICAL\_POTENTIAL  
ELEMENT\_FRACTION  
SITE\_FRACTION

STATE\_VARIABLE: ELEMENT  
ELEMENT NAME: C  
VALUE: /0/: .009

| The user must specify that input is to be taken as weight  
| fractions rather than mole fractions.

POLY\_1>SET-WEIGHT  
-OK-  
POLY\_1>SET-COND EL SI .003  
POLY\_1>S-C EL MN .003  
POLY\_1>S-C EL CR .04  
POLY\_1>S-C EL W .08  
POLY\_1>S-C EL MO .05  
POLY\_1>L-V-S

TEMPERATURE	NOT-FIXED	PRESSURE	1.013E+05	
ELEMENT	FRACTION	ACTIVITY	POTENTIAL	REFERENCE STATE
C	9.000E-03	NOT-FIXED	NOT-FIXED	GRAPHITE
CR	4.000E-02	NOT-FIXED	NOT-FIXED	BCC
FE	NOT-FIXED	NOT-FIXED	NOT-FIXED	AUSTENITE
MN	3.000E-03	NOT-FIXED	NOT-FIXED	FCC
MO	5.000E-02	NOT-FIXED	NOT-FIXED	BCC
SI	3.000E-03	NOT-FIXED	NOT-FIXED	DIAMOND
V	NOT-FIXED	NOT-FIXED	NOT-FIXED	BCC
W	8.000E-02	NOT-FIXED	NOT-FIXED	FCC

NUMBER OF DEGREES OF FREEDOM : 2  
ELEMENT FRACTION TYPE : WEIGHT FRACTION

POLY\_1>S-C EL V .02  
POLY\_1>SET-PHASE-STATUS  
PHASE NAME: ?

PHASE NAME

The name of the phase for which the status is to be changed. To specify that the status of all phases is to be changed type an asterisk '\*'.  
PHASE NAME: \*

STATUS: SUS  
POLY\_1>S-P-S AUSTENIT ENTERED 1

| All phases but austenite have been suspended.

```

POLY_1>L-P-S
PHASE                                STATUS      NO OF MOLES  PRESSURE LEVEL

AUSTENITE                            1  ENTERED    1.0000E+00   .0000E+00
CEMENTITE                             1  SUSPENDED
FE3W2                                 1  SUSPENDED
FERRITE                                1  SUSPENDED
GRAPHITE                               1  SUSPENDED
M23C6                                  1  SUSPENDED
M2C                                    1  SUSPENDED
M6C                                    1  SUSPENDED
M7C3                                   1  SUSPENDED
MC_FCC_CARBIIDE                       1  SUSPENDED
MC_HP_CARBIIDE                         1  SUSPENDED
POLY_1>START-VALUE

```

```

*** ERROR 127 IN POLY_1
*** DEGREES OF FREEDOM NOT EQUAL TO ZERO

```

```

POLY_1>SET-COND T 1473

```

```

| The user was too eager, no temperature had been set.
| The start value command must be used to set a composition
| of the austenite even if it is the only phase.

```

```

POLY_1>ST-V
START VALUES FOR COMPOSITIONS ( Y OR N): /N/: Y
AUSTENITE 1
GIVE START VALUE FOR NUMBER OF MOLES: /1/:
GIVE SITE FRACTION FOR CR IN SUBLATTICE 1: /1/: .05
GIVE SITE FRACTION FOR FE IN SUBLATTICE 1: /1/: .8
GIVE SITE FRACTION FOR MN IN SUBLATTICE 1: /1/: .001
GIVE SITE FRACTION FOR MO IN SUBLATTICE 1: /1/: .05
GIVE SITE FRACTION FOR SI IN SUBLATTICE 1: /1/: .001
GIVE SITE FRACTION FOR V IN SUBLATTICE 1: /1/: .02
GIVE SITE FRACTION FOR C IN SUBLATTICE 2: /1/: .01

```

```

POLY_1>C-P-E

```

```

-OK-

```

```

POLY_1>L-P-E

```

```

FILE NAME: /TERMINAL/:

```

```

SITE FRACTIONS LISTED (Y OR N):

```

```

TEMP = 1.47300E+03  PRESSURE = 1.01325E+05  7 ITERATIONS
ELEMENT  W-FRACTION  POTENTIAL  ACTIVITY  REFERENCE STATE
VA       .00000E+00  .00000E+00  1.00000E+00  VACUUM
C        9.00000E-03  -2.83157E+04  9.90581E-02  GRAPHITE
CR       4.00000E-02  -3.24180E+04  7.08626E-02  BCC
FE       7.95000E-01  -2.10164E+03  8.42313E-01  AUSTENITE
MN       3.00000E-03  -8.59482E+04  8.95712E-04  FCC
MO       5.00000E-02  -2.54893E+04  1.24772E-01  BCC
SI       3.00000E-03  -1.40821E+05  1.01460E-05  DIAMOND
V        2.00000E-02  -7.66367E+04  1.91586E-03  BCC
W        8.00000E-02  -2.72526E+04  1.08041E-01  FCC

```

```

AUSTENITE 1, STATUS=ENTERED
WEIGHT FRACTION 1.000E+00  PRESSURE .000E+00  PRESSURE LEVEL .000E+00
C -W-FRAC CR-W-FRAC FE-W-FRAC MN-W-FRAC MO-W-FRAC SI-W-FRAC V -W-FRAC W -W-FRAC
.0090000 .0400000 .7950000 .0030000 .0500000 .0030000 .0200000 .0800000

```

```

POLY_1>S-P-S * ENT 0

```

```

| All phases entered again and need start values. A
| very crude guess is sufficient.

```

## POLY\_1&gt;START-VALUE

START VALUES FOR COMPOSITIONS ( Y OR N): /N/: Y

AUSTENITE

1

GIVE START VALUE FOR NUMBER OF MOLES: /0/: 1GIVE SITE FRACTION FOR CR IN SUBLATTICE 1: /./: .04658145922/GIVE SITE FRACTION FOR FE IN SUBLATTICE 1: /./: .8619663517/GIVE SITE FRACTION FOR MN IN SUBLATTICE 1: /./: .003306522196/GIVE SITE FRACTION FOR MO IN SUBLATTICE 1: /./: .03155682658/GIVE SITE FRACTION FOR SI IN SUBLATTICE 1: /./: .006467802591/GIVE SITE FRACTION FOR V IN SUBLATTICE 1: /./: .02377285272/GIVE SITE FRACTION FOR C IN SUBLATTICE 2: /./: .04537183828/

CEMENTITE

1

GIVE START VALUE FOR NUMBER OF MOLES: /0/:

GIVE SITE FRACTION FOR CR IN SUBLATTICE 1: /./: .2GIVE SITE FRACTION FOR FE IN SUBLATTICE 1: /./: .2GIVE SITE FRACTION FOR MN IN SUBLATTICE 1: /./: .2GIVE SITE FRACTION FOR MO IN SUBLATTICE 1: /./: .2GIVE SITE FRACTION FOR V IN SUBLATTICE 1: /./: .2

FE3W2

1

GIVE START VALUE FOR NUMBER OF MOLES: /0/:

FERRITE

1

GIVE START VALUE FOR NUMBER OF MOLES: /0/:

GIVE SITE FRACTION FOR CR IN SUBLATTICE 1: /./: .05GIVE SITE FRACTION FOR FE IN SUBLATTICE 1: /./: .8GIVE SITE FRACTION FOR MN IN SUBLATTICE 1: /./: .01GIVE SITE FRACTION FOR MO IN SUBLATTICE 1: /./: .01GIVE SITE FRACTION FOR SI IN SUBLATTICE 1: /./: .01GIVE SITE FRACTION FOR V IN SUBLATTICE 1: /./: .01GIVE SITE FRACTION FOR C IN SUBLATTICE 2: /./: .01

GRAPHITE

1

GIVE START VALUE FOR NUMBER OF MOLES: /0/:

M23C6

1

GIVE START VALUE FOR NUMBER OF MOLES: /0/:

GIVE SITE FRACTION FOR CR IN SUBLATTICE 1: /./: .3GIVE SITE FRACTION FOR FE IN SUBLATTICE 1: /./: .3GIVE SITE FRACTION FOR MN IN SUBLATTICE 1: /./: .1GIVE SITE FRACTION FOR MO IN SUBLATTICE 1: /./: .2

M2C

1

GIVE START VALUE FOR NUMBER OF MOLES: /0/:

GIVE SITE FRACTION FOR CR IN SUBLATTICE 1: /./: .2GIVE SITE FRACTION FOR FE IN SUBLATTICE 1: /./: .2GIVE SITE FRACTION FOR MO IN SUBLATTICE 1: /./: .3GIVE SITE FRACTION FOR V IN SUBLATTICE 1: /./: .2

M6C

1

GIVE START VALUE FOR NUMBER OF MOLES: /0/:

GIVE SITE FRACTION FOR CR IN SUBLATTICE 1: /./: .2GIVE SITE FRACTION FOR FE IN SUBLATTICE 1: /./: .2GIVE SITE FRACTION FOR MO IN SUBLATTICE 1: /./: .2

M7C3

1

GIVE START VALUE FOR NUMBER OF MOLES: /0/:

GIVE SITE FRACTION FOR CR IN SUBLATTICE 1: /./: .3GIVE SITE FRACTION FOR FE IN SUBLATTICE 1: /./: .2

MC\_FCC\_CARBIDE

1

GIVE START VALUE FOR NUMBER OF MOLES: /0/:

GIVE SITE FRACTION FOR CR IN SUBLATTICE 1: /./: .2GIVE SITE FRACTION FOR FE IN SUBLATTICE 1: /./: .2GIVE SITE FRACTION FOR MN IN SUBLATTICE 1: /./: .1GIVE SITE FRACTION FOR MO IN SUBLATTICE 1: /./: .2GIVE SITE FRACTION FOR V IN SUBLATTICE 1: /./: .2

MC\_HP\_CARBIDE

1

GIVE START VALUE FOR NUMBER OF MOLES: /0/:

GIVE SITE FRACTION FOR MO IN SUBLATTICE 1: /./: .2

POLY\_1&gt;C-P-E

-OK-

POLY\_1&gt;L-P-E

```

TEMP = 1.47300E+03    PRESSURE = 1.01325E+05    18 ITERATIONS
ELEMENT  W-FRACTION  POTENTIAL  ACTIVITY  REFERENCE STATE
VA       .00000E+00  .00000E+00  1.00000E+00  VACUUM
C        9.00000E-03  -3.09421E+04  7.99380E-02  GRAPHITE
CR       4.00000E-02  -3.11112E+04  7.88419E-02  BCC
FE       7.95000E-01  -1.59896E+03  8.77604E-01  AUSTENITE
MN       3.00000E-03  -8.48266E+04  9.81614E-04  FCC
MO       5.00000E-02  -3.56298E+04  5.45157E-02  BCC
SI       3.00000E-03  -1.45557E+05  6.89227E-06  DIAMOND
V        2.00000E-02  -7.70257E+04  1.8597E-03   BCC
W        8.00000E-02  -3.78833E+04  4.53535E-02  FCC

AUSTENITE 1, STATUS=ENTERED
WEIGHT FRACTION 8.715E-01  PRESSURE .000E+00  PRESSURE LEVEL .000E+00
C -W-FRAC CR-W-FRAC FE-W-FRAC MN-W-FRAC MO-W-FRAC SI-W-FRAC V -W-FRAC W -W-FRAC
.0062720 .0421197 .8766157 .0034421 .0194131 .0034424 .0185286 .0301665

CEMENTITE 1, STATUS=ENTERED
WEIGHT FRACTION .000E+00  PRESSURE -3.377E+07  PRESSURE LEVEL .000E+00
C -W-FRAC CR-W-FRAC FE-W-FRAC MN-W-FRAC MO-W-FRAC SI-W-FRAC V -W-FRAC W -W-FRAC
.0659056 .2074262 .5881497 .0034720 .0450552 .0000000 .0647088 .0252825

FE3W2 1, STATUS=ENTERED
WEIGHT FRACTION .000E+00  PRESSURE -6.372E+07  PRESSURE LEVEL .000E+00
C -W-FRAC CR-W-FRAC FE-W-FRAC MN-W-FRAC MO-W-FRAC SI-W-FRAC V -W-FRAC W -W-FRAC
.0000000 .0000000 .3130197 .0000000 .0000000 .0000000 .0000000 .8869803

FERRITE 1, STATUS=ENTERED
WEIGHT FRACTION .000E+00  PRESSURE -1.698E+08  PRESSURE LEVEL .000E+00
C -W-FRAC CR-W-FRAC FE-W-FRAC MN-W-FRAC MO-W-FRAC SI-W-FRAC V -W-FRAC W -W-FRAC
.0015398 .0388725 .8691024 .0027290 .0242904 .0049651 .0201367 .0383641

GRAPHITE 1, STATUS=ENTERED
WEIGHT FRACTION .000E+00  PRESSURE -2.527E+07  PRESSURE LEVEL .000E+00
C -W-FRAC CR-W-FRAC FE-W-FRAC MN-W-FRAC MO-W-FRAC SI-W-FRAC V -W-FRAC W -W-FRAC
1.0000000 .0000000 .0000000 .0000000 .0000000 .0000000 .0000000 .0000000

M23C6 1, STATUS=ENTERED
WEIGHT FRACTION .000E+00  PRESSURE -3.215E+07  PRESSURE LEVEL .000E+00
C -W-FRAC CR-W-FRAC FE-W-FRAC MN-W-FRAC MO-W-FRAC SI-W-FRAC V -W-FRAC W -W-FRAC
.0504988 .1944845 .6403037 .0034533 .0487694 .0000000 .0000000 .0624904

M2C 1, STATUS=ENTERED
WEIGHT FRACTION .000E+00  PRESSURE -4.247E+07  PRESSURE LEVEL .000E+00
C -W-FRAC CR-W-FRAC FE-W-FRAC MN-W-FRAC MO-W-FRAC SI-W-FRAC V -W-FRAC W -W-FRAC
.0760119 .1148487 .0439726 .0000000 .4474503 .0000000 .2303468 .0873697

M6C 1, STATUS=ENTERED
WEIGHT FRACTION 1.223E-01  PRESSURE .000E+00  PRESSURE LEVEL .000E+00
C -W-FRAC CR-W-FRAC FE-W-FRAC MN-W-FRAC MO-W-FRAC SI-W-FRAC V -W-FRAC W -W-FRAC
.0203780 .0260509 .2537476 .0000000 .2665651 .0000000 .0000000 .4332584

M7C3 1, STATUS=ENTERED
WEIGHT FRACTION .000E+00  PRESSURE -5.355E+07  PRESSURE LEVEL .000E+00
C -W-FRAC CR-W-FRAC FE-W-FRAC MN-W-FRAC MO-W-FRAC SI-W-FRAC V -W-FRAC W -W-FRAC
.0866988 .3671536 .5390169 .0071307 .0000000 .0000000 .0000000 .0000000

MC_FCC_CARBIDE 1, STATUS=ENTERED
WEIGHT FRACTION 6.217E-03  PRESSURE .000E+00  PRESSURE LEVEL .000E+00
C -W-FRAC CR-W-FRAC FE-W-FRAC MN-W-FRAC MO-W-FRAC SI-W-FRAC V -W-FRAC W -W-FRAC
.1676090 .0172415 .0005673 .0000328 .0778272 .0000000 .6196737 .1170484

MC_HP_CARBIDE 1, STATUS=ENTERED
WEIGHT FRACTION .000E+00  PRESSURE -1.566E+08  PRESSURE LEVEL .000E+00
C -W-FRAC CR-W-FRAC FE-W-FRAC MN-W-FRAC MO-W-FRAC SI-W-FRAC V -W-FRAC W -W-FRAC
.0703034 .0000000 .0000000 .0000000 .1597985 .0000000 .0000000 .7698981

```



POLY\_1>SET-AXIS-VARIABLE

AXIS (X, Y OR Z): /X/:

AXIS VARIABLE: I

| The user now wants to calculate the stable equilibria for  
| this alloy from 1300 to 600 degree Celsius. He then  
| tries to set the temperature as axis variable but must first  
| reset the condition that the temperature should be constant.

\*\*\* ERROR 120 IN POLY\_1

\*\*\* ALREADY SET CONSTANT

POLY\_1>HELP

COMMAND:

BACK	CALPHAD
COMPUTE_PHASE_EQUIL	DELETE_ALL_START_POINTS
DELETE_LAST_START_POINT	EXIT
GOTO_MODULE	HELP
INFORMATION	LIST_FIX_SITE_FRACTIONS
LIST_PHASE_EQUIL	LIST_PHASE_STATUS
LIST_START_POINTS	LIST_STORE_RESULT_FILE
LIST_VARIABLE_STATUS	PATCH_POLY_WORKSPACE
POST_PROCESSOR	READ_ALL_WORKSPACES
READ_POLY_WORKSPACE	REINITIATE_WORKSPACE
RESET_CONDITION	RESET_PRESENT_PHASE
SAVE_ALL_WORKSPACES	SET_AXIS_VARIABLE
SET_BREAK_CONDITIONS	SET_CONDITION
SET_MOLE_FRACTION	SET_PHASE_STATUS
SET_PRESENT_PHASE	SET_PRESSURE_LEVEL
SET_START_COMPOSITION	SET_STORE_RESULT_FILE
SET_WEIGHT_FRACTION	START_VALUES

POLY\_1>RESET-COND

STATE\_VARIABLE: I

-OK-

| RESET means that the condition is removed.

POLY\_1>S-A-V

AXIS (X, Y OR Z): /X/:

AXIS VARIABLE: I

MIN VALUE: 873

MAX VALUE: 1573

MAX STEP INCREMENT: /17.5/: 10

POLY\_1>ST-V

X-AXIS VARIABLE IS TEMPERATURE

MAX= 1.57300E+03 MIN = 8.73000E+02

START VALUE FOR X-AXIS /0/: 1573

STEP VARIABLE (X,Y,Z OR NONE) : X

STEP DIRECTION (+1=POS, -1=NEG) : -1

START VALUES FOR COMPOSITIONS ( Y OR N): /N/:

DO YOU WANT TO STORE START VALUES AS A START POINT ( Y OR N): /N/: Y

-OK- START POINT STORED

POLY\_1>L-P-S

PHASE		STATUS	NO OF MOLES	PRESSURE LEVEL
AUSTENITE	1	ENTERED	9.4426E-01	.0000E+00
CEMENTITE	1	ENTERED	.0000E+00	.0000E+00
FE3W2	1	ENTERED	.0000E+00	.0000E+00
FERRITE	1	ENTERED	.0000E+00	.0000E+00
GRAPHITE	1	ENTERED	.0000E+00	.0000E+00
M23C6	1	ENTERED	.0000E+00	.0000E+00
M2C	1	ENTERED	.0000E+00	.0000E+00
M6C	1	ENTERED	5.5736E-02	.0000E+00
M7C3	1	ENTERED	.0000E+00	.0000E+00
MC_FCC_CARBIDE	1	ENTERED	.0000E+00	.0000E+00
MC_HP_CARBIDE	1	ENTERED	.0000E+00	.0000E+00

```
| The LIST-PHASE-STATUS command gives a condensed summary of
| the stable phase set. Note that at the start point at 1573 K
| only the austenite and the M6 carbide are stable. The user
| now defines a file where the program shall store the result
| of the calculation. It is necessary to set a result file if
| the user wants to save the results to another occasion or if
| he expects that the results of the calculation will exceed
| the available buffer.
```

POLY\_1>SET-STORE-RESULT

FILE NAME: (PAGE)SPEED-STEEL:POLY

POLY\_1>CALPHAD

PHASE REGION FOR THE FOLLOWING PHASES IS TO BE MAPPED

```
AUSTENITE          1
M6C                 1
1 ITS X= 1.5730E+03
```

The output during the mapping has been compressed.

```
...
3 ITS X= 1.5136E+03
```

PHASE REGION FOR THE FOLLOWING PHASES IS TO BE MAPPED

```
AUSTENITE          1
M6C                 1
MC_FCC_CARBIDE     1
3 ITS X= 1.5136E+03
```

```
...
4 ITS X= 1.1366E+03
```

PHASE REGION FOR THE FOLLOWING PHASES IS TO BE MAPPED

```
AUSTENITE          1
FERRITE            1
M6C                 1
MC_FCC_CARBIDE     1
4 ITS X= 1.1366E+03
```

```
...
4 ITS X= 1.0799E+03
```

PHASE REGION FOR THE FOLLOWING PHASES IS TO BE MAPPED

```
FERRITE            1
M6C                 1
MC_FCC_CARBIDE     1
4 ITS X= 1.0799E+03
```

```
...
7 ITS X= 9.8855E+02
```

PHASE REGION FOR THE FOLLOWING PHASES IS TO BE MAPPED

```
FERRITE          1
M23C6           1
M6C             1
MC_FCC_CARBIDE  1
```

7 ITS X= 9.8855E+02

...

5 ITS X= 8.7300E+02

## MUST STORE BUFFER ON FILE. ##

## BUFFER STORED ON FILE. ##

\*\*NO MORE START-POINTS\*\*

```
| At the end of the mapping the program saves the results on
| the store file. In the post-processor the user can now
| obtain diagrams that show how a number of quantities have
| varied during the change in temperature.
```

POLY\_1>POST

POLY\_1 POST PROCESSOR VERSION 5.0

POST>HELP

COMMAND:

```
BACK                CHANGE_MY_SPEED
DEFINE_FUNCTION     EXIT
HELP                LIST_ALL_AXIS_VALUES
LIST_ALL_EQUILIBRIA LIST_FUNCTIONS
LIST_PLOT_SETTINGS LIST_SYSTEM_DEFINITION
PLOT_DIAGRAM        REINITIATE_PLOT_SETTINGS
SET_AXIS_LENGTH     SET_AXIS_PLOT_STATUS
SET_AXIS_TEXT_STATUS SET_DIAGRAM_AXIS
SET_DIAGRAM_TYPE    SET_PLOT_FORMAT
SET_PLOT_SIZE       SET_RASTER_STATUS
SET_SCALING_STATUS  SET_TIELINE_STATUS
SET_TITLE
```

POST>SET-DIA-AXIS

AXIS (X, Y OR Z): Y

AXIS VARIABLE: T

AXIS VARIABLE

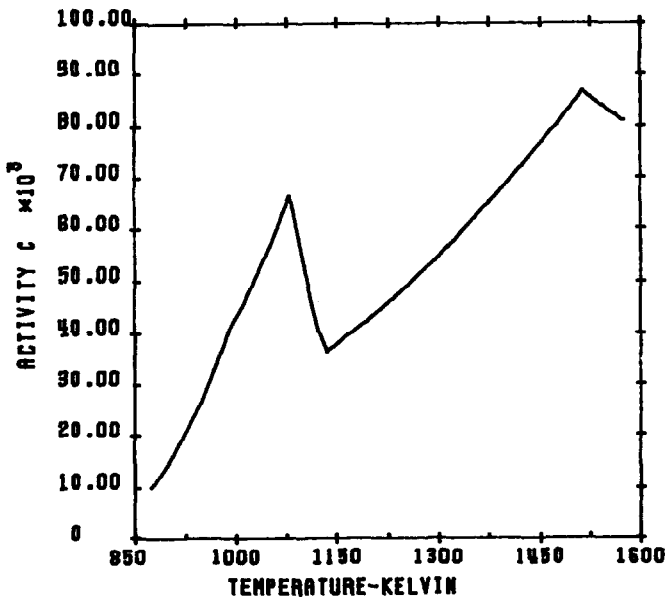
The user must specify which state variable is to be used as diagram axis. The default axis variable is the variable which has been used for the mapping. When a new axis variable is set the scaling status is set to automatic scaling. The following axis variables are defined in the Post\_Processor.

```
TEMPERATURE-KELVIN
TEMPERATURE-CELSIUS
PRESSURE-PASCAL
ACTIVITY                for an element
CHEMICAL-POTENTIAL     for an element
NORMALIZED-FRACTION    an axis defined for the mapping
MOLE-FRACTION          for an element
WEIGHT-PERCENT         for an element
SITE-FRACTION          for an element (in a sublattice)
PHASE-MOLE-FRACTION    for a phase
PHASE-WEIGHT-PERCENT   for a phase
IN-PHASE-MOLE-FRACTION for an element in a phase
IN-PHASE-WEIGHT-PERCENT for an element in a phase
IN-PHASE-SITE-FRACTION for an element (sublattice) in a phase
FUNCTION                an defined function
CLEAR                  to clear the axis
```

AXIS VARIABLE: ACT

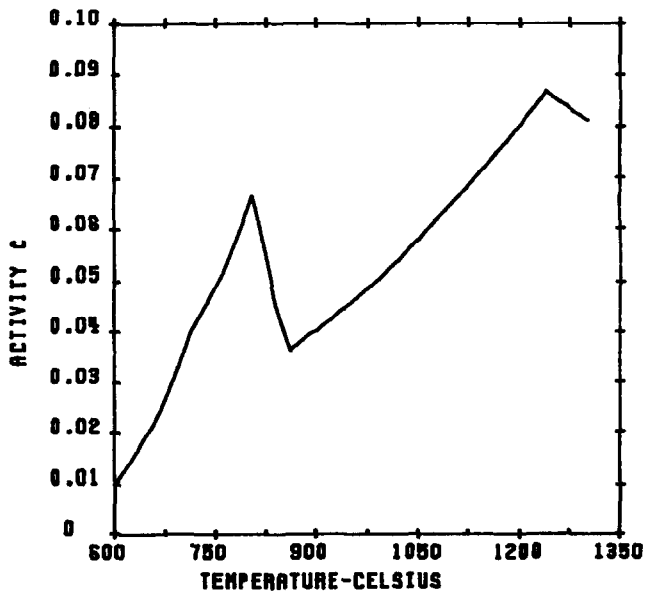
ELEMENT NAME: C

POST>PLOT  
PLOT FILE: /TERMINAL/:



| The irregular shape of the activity curve is due to the  
| changes of the set of stable phases with the temperature.

POST>S-D-A  
AXIS (X, Y OR Z): X  
AXIS VARIABLE: I-C  
POST>SET-SCAL  
AXIS (X, Y OR Z): Y  
AUTOMATIC SCALING (Y OR N): /N/  
MIN VALUE: 0  
MAX VALUE: .1  
POST>PLOT  
PLOT FILE: /TERMINAL/:



| The user now uses the facility to define a function as an  
 | expression of state variables. Such state variables are the  
 | constitution and amounts of the phases, the activities or  
 | potentials of the components or thermodynamic quantities as  
 | the entropy, enthalpy etc. The program has symbols for these  
 | variables and the symbol NP used below is the amount of a  
 | phase. The function gives how much of the system that is  
 | neither austenite or ferrite, i.e. the amount of carbides.

POST>DEFINE-FUNCTION FCARB  
PARAMETER NA=NP(AUST),NF=NP(FERR):

1-NA-NF:

;

POST>S-D-A Y FUN

FUNCTION: FCARB

POST>SET-AXIS-TEXT

AXIS (X, Y OR Z): Y

AUTOMATIC AXIS TEXT (Y OR N): /N/: N

AXIS TEXT: FRACTION CARBIDE

POST>SET-SCAL

AXIS (X, Y OR Z): Y

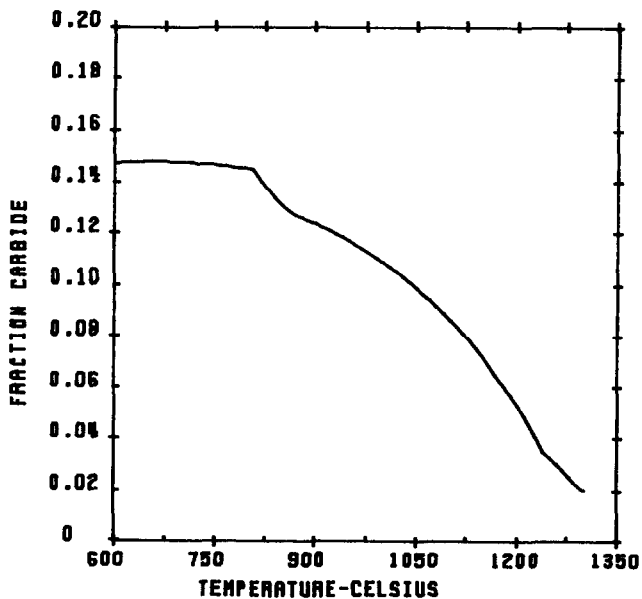
AUTOMATIC SCALING (Y OR N): /N/:

MIN VALUE: 0

MAX VALUE: .2

POST>PLOT

PLOT FILE: /TERMINAL/:



POST>EXIT  
 CPU TIME

875 SECONDS

#### Final remarks

Thermo-Calc is a thermochemical databank with powerful software for various kinds of complex thermochemical calculations. At present it operates on a number of specific databases. In the future, the new thermochemical database being developed in collaboration with SGTE (Scientific Group Thermodata Europe) will be available. Thermo-Calc is already used on-line in research and by the industry and also for a consultancy service for calculations on behalf of customers. It is possible for universities and other research organisations to lease a copy of the databank and the assessment software for implementation on a VAX or ND-500 computer. Thermo-Calc is a large program consisting of more than 600 subroutines and 30000 lines of code written in standard Fortran 77.

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