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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.

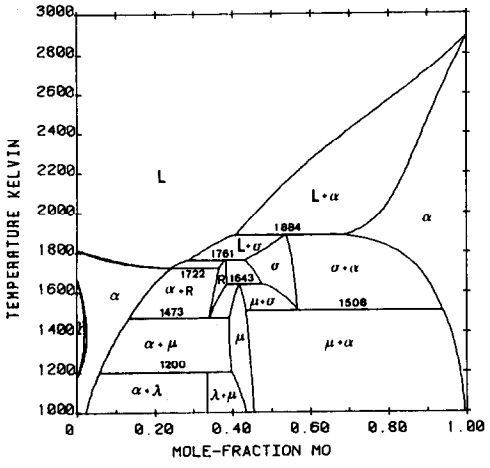


FIG. 1. The calculated phase diagram for the Fe-Mo system. Diagrams with only two components are of great interest for the assessment of data for the database (6).

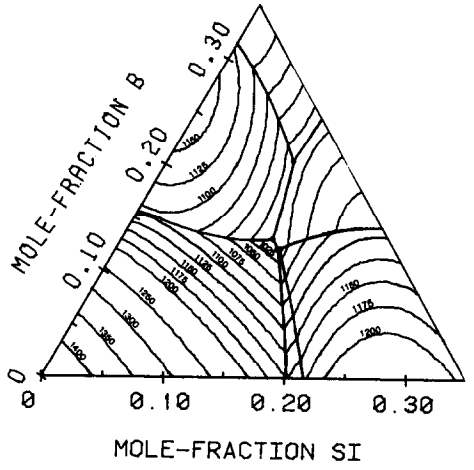


FIG. 2. The liquidus surface in the nickel rich corner of the Ni-Si-B system. This diagram was calculated in order to aid the selection of candidate alloys to be used for rapid solidification (7).

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.

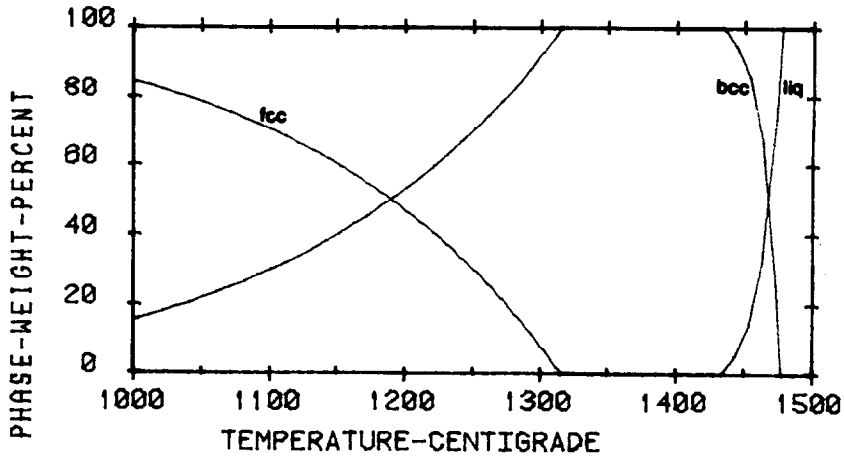


FIG. 3. The diagram shows how the relative amounts of the various phases vary with the temperature. Such information is a valuable guide in selecting the temperature for various kinds of heat treatment.

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.

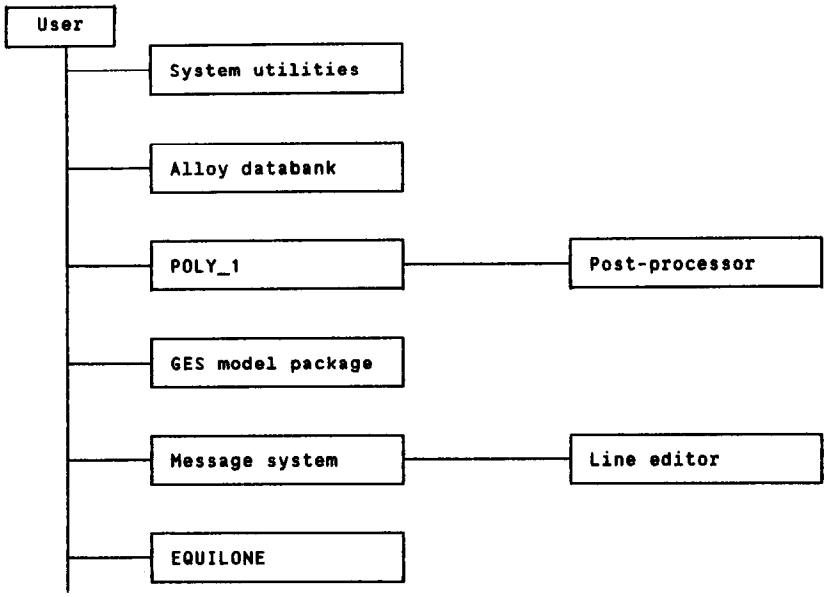


FIG. 4. The modular structure of Thermo-Calc. The postprocessor and the lined modules are local to the POLY_1 and MESSAGE module respectivly.

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 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> 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.

SET_AXIS_VARIABLE must be given before using the automatic mapping procedure in order to calculate a property diagram, a phase diagram or a projection (of a three dimensional map). The degrees of freedom decrease by one for each axis.

CALPHAD is the command to activate the automatic stepping procedure. One must have at least one axis and must have given at least one start point before this command.

SET_WEIGHT_FRACTION and SET_MOLE_FRACTION must be used to inform POLY about whether the input is in weight (mass) fraction or mole fraction. Note that it is mass fraction and not mass percent. Mole fraction is the default.

SET_PHASE_STATUS can be used to SUSPEND a phase (i.e. to exclude it from the calculation), to FIX it (i.e. to force it to be included in the stable phase set, this decreases the degrees of freedom by one) or to set it to ENTERED which means that it will be included in the stable phase set if that will decrease the total Gibbs energy for the system. The ENTERED status is the default.

RESET_CONDITION will remove a condition set by the SET_CONDITION command.

SET_STORE_RESULT_FILE command has the effect that all results calculated by the CALPHAD command will be saved on the file. It must be given before the CALPAHD command. It must also be given before the first SAVE_ALL or READ_ALL command.

SAVE_ALL_WORKSPACES will save the current status on the store_result_file. This is useful if one has to finish a session and wishes to restart from the same point later on (e.g. after lunch).

READ_ALL_WORKSPACES will reset the POLY program to the point where it was when the last SAVE_ALL or CALPHAD command was given for the file defined by the command SET_STORE_RESULT_FILE.

POST_PROCESSOR shifts control to the post-processor where the result of a calculation can be presented graphically or in tables.

The post-processor

The post-processor is local to the POLY program. It can only be reached from the POLY module and you must go back to the POLY module in order to reach any other module.

```
POLY_1 POST PROCESSOR  VERSION 5.0

POST> is the prompt.

General commands are
BACK
EXIT                        HELP

The essential commands are
SET_DIAGRAM_AXIS            SET_SCALING_STATUS
SET_PLOT_FORMAT             PLOT_DIAGRAM

Tabular output is generated by the commands
LIST_ALL_AXIS_VALUES        LIST_ALL_EQUILIBRIA

Diagnostic commands are
LIST_PLOT_SETTINGS          LIST_SYSTEM_DEFINITION
```

```
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 interactivly 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 interactivly.

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 recieve 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 recieved 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 equlibrium fcc/bcc/cementite can be calculated directly. Finally a two-phase equlibrium 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>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>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>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>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>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 commad.

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 diffent 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                        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>INFO
WHICH SUBJECT /PURPOSE/: ?
   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 stucture 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: ?
      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 linearily 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-V
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
```

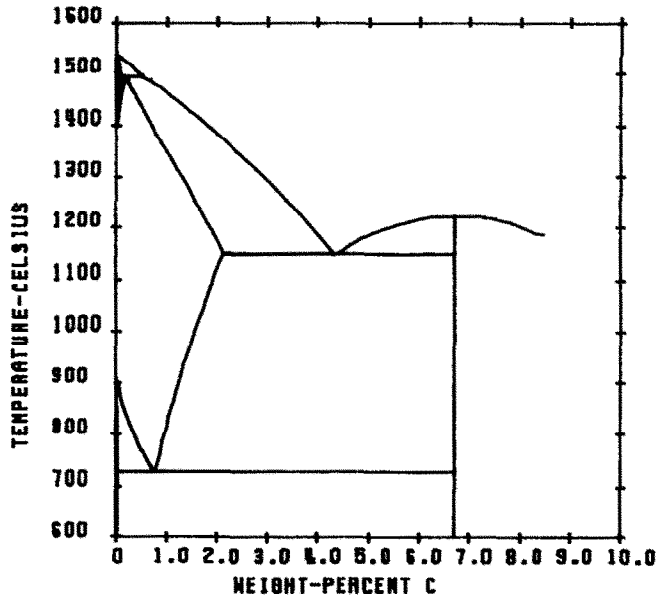
| The user needs help to interpret this output.

```
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 equlibrium. 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
```

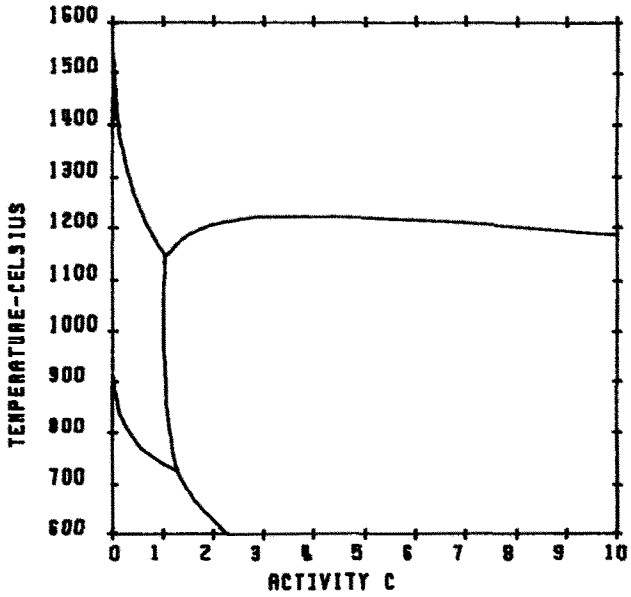
```
PHASE REGION BOUNDARY FOR THE FOLLOWING PHASES IS TO BE MAPPED
BCC                            1
LIQUID                         1
 4 ITS  X= 7.9499E-02  Y= 1.7673E+03
 ...
 9 ITS  X= 1.0000E-07  Y= 1.8108E+03

**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: ?

   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: W
ELEMENT NAME: C

POST>S-D-A
AXIS  (X, Y OR Z): Y
AXIS VARIABLE: T-C
```

```
POST>PLOT
PLOT FILE: /TERMINAL/:
```

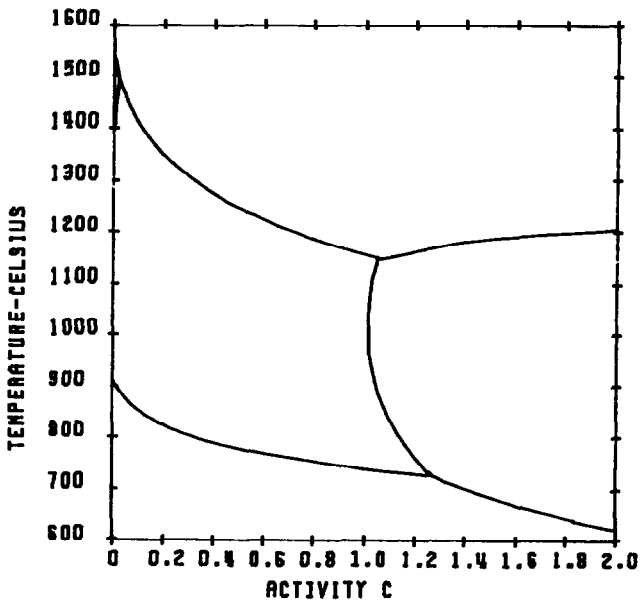


| Another way of presenting the results of the same
| calculation is to use the carbon activity as axis variable.

```
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 ND-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>INFO
WHICH SUBJECT /PURPOSE/: ?
   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-STATUS
PHASE NAME: FCC
STATUS: FIX
NUMBER OF MOLES: 1
POLY_1>S-P-S BCC FIX
NUMBER 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 0
POLY_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-
```

```
POLY_1>L-P-E,,,,

                | If the user knows the default values of the arguments
                | of a command and is satisfied with them he can avoid the
                | questions by giving commas after the command.

TEMP =  1.01252E+03    PRESSURE =  1.01325E+05      4 ITERATIONS
ELEMENT    X-FRACTION   POTENTIAL    ACTIVITY    REFERENCE STATE
VA          .00000E+00   .00000E+00  1.00000E+00 VACUUM
C          3.07547E-02   .00000E+00  1.00000E+00 GRAPHITE
FE         9.69245E-01 -3.03440E+02  9.64597E-01 FCC_PARAMAGNETIC

BCC                        1, STATUS=FIX
MOL FRACTION   .000E+00   PRESSURE   .000E+00   PRESSURE LEVEL   .000E+00
C -X-FRAC FE-X-FRAC
 .0009044  .9990956

CEMENTITE                  1, STATUS=ENTERED
MOL FRACTION   .000E+00   PRESSURE -1.890E+08   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
 .0307547  .9692453

LIQUID                     1, STATUS=ENTERED
MOL FRACTION   .000E+00   PRESSURE -3.921E+07   PRESSURE LEVEL   .000E+00
C -X-FRAC FE-X-FRAC
 .1093853  .8906147

POLY_1>EXIT

CPU TIME              106 SECONDS

                | This example is now finished. The total computer time
                | using a ND-500 computer was 106 seconds. The ND-500
                | computer is similar to a VAX11/780 in performance.
```

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/: CON
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/: CONSTI
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 GES5 .....
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_CARBIDE            1    SUSPENDED
MC_HP_CARBIDE             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>SI-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>START-VALUE
START VALUES FOR COMPOSITIONS ( Y OR N): /N/: Y
AUSTENITE                    1
GIVE START VALUE FOR NUMBER OF MOLES: /0/: 1
GIVE 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: /.003306522198/:
GIVE SITE FRACTION FOR MO IN SUBLATTICE  1: /.03155682658/:
GIVE SITE FRACTION FOR SI IN SUBLATTICE  1: /.006467882591/:
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: /1/: .2
GIVE SITE FRACTION FOR FE IN SUBLATTICE  1: /1/: .2
GIVE SITE FRACTION FOR MN IN SUBLATTICE  1: /1/: .2
GIVE SITE FRACTION FOR MO IN SUBLATTICE  1: /1/: .2
GIVE SITE FRACTION FOR V  IN SUBLATTICE  1: /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: /1/: .05
GIVE SITE FRACTION FOR FE IN SUBLATTICE  1: /1/: .8
GIVE SITE FRACTION FOR MN IN SUBLATTICE  1: /1/: .01
GIVE SITE FRACTION FOR MO IN SUBLATTICE  1: /1/: .01
GIVE SITE FRACTION FOR SI IN SUBLATTICE  1: /1/: .01
GIVE SITE FRACTION FOR V  IN SUBLATTICE  1: /1/: .01
GIVE SITE FRACTION FOR C  IN SUBLATTICE  2: /1/: .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: /1/: .3
GIVE SITE FRACTION FOR FE IN SUBLATTICE  1: /1/: .3
GIVE SITE FRACTION FOR MN IN SUBLATTICE  1: /1/: .1
GIVE SITE FRACTION FOR MO IN SUBLATTICE  1: /1/: .2
M2C                          1
GIVE START VALUE FOR NUMBER OF MOLES: /0/:
GIVE SITE FRACTION FOR CR IN SUBLATTICE  1: /1/: .2
GIVE SITE FRACTION FOR FE IN SUBLATTICE  1: /1/: .2
GIVE SITE FRACTION FOR MO IN SUBLATTICE  1: /1/: .3
GIVE SITE FRACTION FOR V  IN SUBLATTICE  1: /1/: .2
M6C                          1
GIVE START VALUE FOR NUMBER OF MOLES: /0/:
GIVE SITE FRACTION FOR CR IN SUBLATTICE  1: /1/: .2
GIVE SITE FRACTION FOR FE IN SUBLATTICE  1: /1/: .2
GIVE SITE FRACTION FOR MO IN SUBLATTICE  1: /1/: .2
M7C3                         1
GIVE START VALUE FOR NUMBER OF MOLES: /0/:
GIVE SITE FRACTION FOR CR IN SUBLATTICE  1: /1/: .3
GIVE SITE FRACTION FOR FE IN SUBLATTICE  1: /1/: .2
MC_FCC_CARBIDE               1
GIVE START VALUE FOR NUMBER OF MOLES: /0/:
GIVE SITE FRACTION FOR CR IN SUBLATTICE  1: /1/: .2
GIVE SITE FRACTION FOR FE IN SUBLATTICE  1: /1/: .2
GIVE SITE FRACTION FOR MN IN SUBLATTICE  1: /1/: .1
GIVE SITE FRACTION FOR MO IN SUBLATTICE  1: /1/: .2
GIVE SITE FRACTION FOR V  IN SUBLATTICE  1: /1/: .2
MC_HP_CARBIDE                1
GIVE START VALUE FOR NUMBER OF MOLES: /0/:
GIVE SITE FRACTION FOR MO IN SUBLATTICE  1: /1/: .2
```

```
POLY_1>C-P-E

-OK-

POLY_1>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  1.85597E-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  .6869803

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: T

                  | 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: T
-OK-

                    | RESET means that the condition is removed.

POLY_1>S-A-V
AXIS (X, Y OR Z): /X/:
AXIS VARIABLE: T
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.

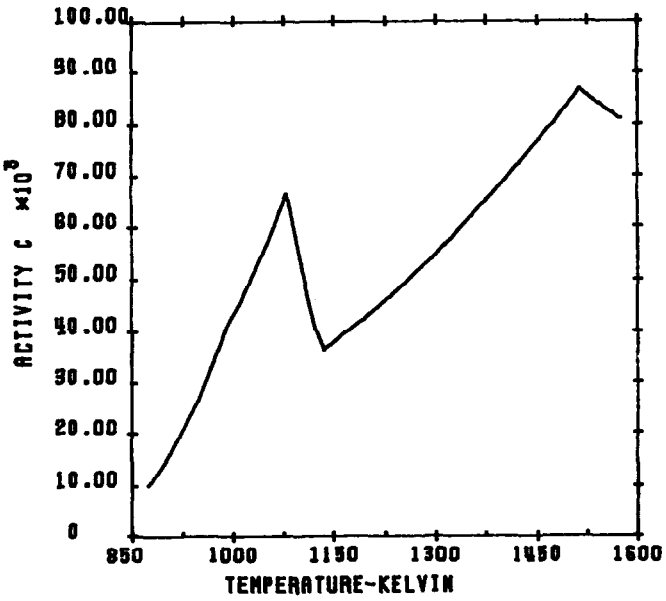
```
POLY_1>SET-STORE-RESULT
FILE NAME: (PAGE)SPEED-STEEL:POLY

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.

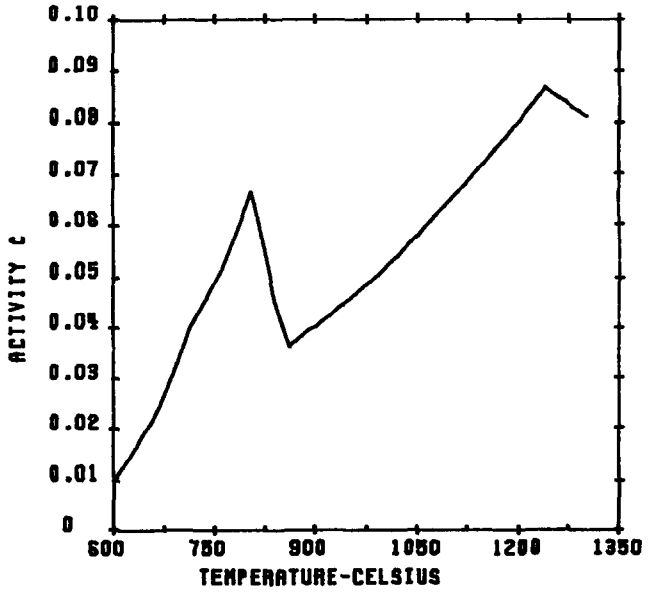
```
POLY_1>POST

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: ?
   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/:
```



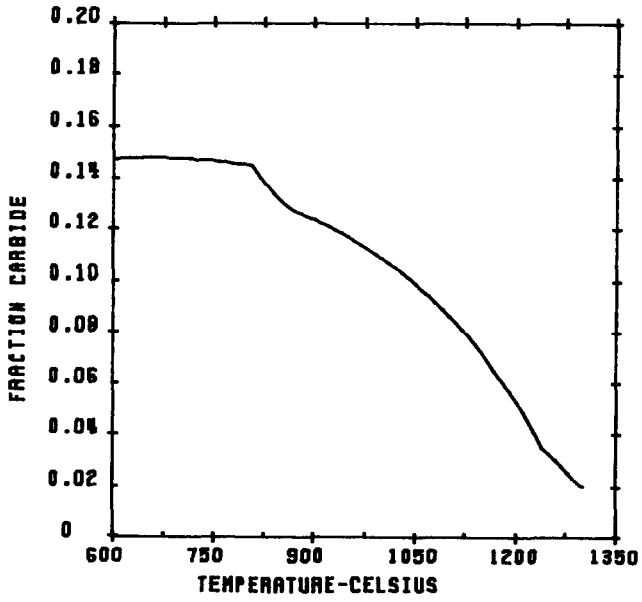
| The irregular shape of the activity curve is due to the
| changes of the set of stable phases with the temperature.

```
POST>S-D-A
AXIS  (X, Y OR Z): X
AXIS VARIABLE: T-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 universites 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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