User Guide to the Open Calphad software package version 3.0

VERY PRELIMINARY DRAFT

Bo Sundman, August 5, 2015

This is a very preliminary version

1 Introduction

The Open Calphad software initiative aims to provide a hig quality software for thermodynamic calculations, including property and phase diagrams, for inorganic systems i.e. gases. liquids, alloys and other materials with many different crystalline phases.

It also provides a framwork to store many different composition dependent properties of materials and to assess model parameters using experimental and theoretical data.

2 Some general features

The command monitor has a menu of command and each of these usually has submenus and finally some questions may be asked like phase names, a value or an expression. At any level the user should be able to type a ? and get some help, usually an extract from this manual, a menue or possible answers.

2.1 Names and symbols

There are many symbols and names used in this package. A symbol or name MUST start with a letter A-Z. It usually can contain digits and the underscore character after the intitial letter. Some special symbols are also used:

- /- is used to denote the electron. /+ can be used for a psoitiv charge.
- # are used to identify composition sets after a phase name or sublattice after a constituent name.
- & are used in some parameter identifiers to specify the constituent for the parameter, mobilites.

2.2 Parameters

All data is organized relative to a phase and the phase is identified by a name. Each phase can have a different model for the composition dependence but the way to enter model parameters is the same for all models. However, the meaning of a model parameter may depend on the model of the phase.

Many types of data can be stored as explained in the section on parameter identifiers. The parameter also has a constituent specification explained in the constituent array section and possibly a degree, the meaning of which is model dependent.

The basic syntax of a parameter is

"identifier" ("phase name" , "constituent array" ; "degree") "expression" "reference"

These parts will now be explained in more detail.

2.2.1 Parameter Identifiers

The OC thermodynamic pacakage can handle any property that depend on composition using the composition models implemented. It is easy to extend the number of properties by declaring property identifiers in ths source code. The value of such identifiers can be obtained by the command "list symbol". If the parameters should have an influence on the Gibbs energy (like the Curie temperature) or a diffusion coefficient (like the mobility) the necessary code to calculate this must be added also.

The list here is tentative. Insensitive to case.

- G, the Gibbs energy or an interaction parameter.
- TC, the critical temperature for ferro or antiferro magnetic ordering using the Inden model.
- BMAGN, the avarage Bohr magneton number using the Inden model.
- CTA, the Curie temperature for ferromagnetic ordering using a modified Inden model.
- NTA, the Neel temperature for antiferromagnetic ordering using a modified Inden model.
- IBM&C, the individual Bohr magneton number for constituent C using a modified Inden model. For example IBM&FE(BCC,FE) is the Bohr magneton number for BCC Fe. The identifier IBM&FE(BCC,CR) means the Bohr magneton number of a single Fe atom in BCC Cr. An identifier IBM&FE(BCC,CR,FE) can be used to decribe the composition dependence of the Bohr magneton number for Fe in BCC.

- THET, the Debye or Einstein temperature.
- MOBQ&C, the logarithm of the mobility of constituent C
- RHO, the electrical resistivity
- MAGS, the magnetic suseptibility
- GTT, the glas transition temperature
- VISC, the viscosity
- LPAX, the lattic parameter in X direction
- LPAY, the lattic parameter in Y direction
- LPAZ, the lattic parameter in Z direction
- LPTH, the deviation from cubic structure
- EC11A, the elastic constrant C11
- EC12A, the elastic constrant C12
- EC44A, the elastic constrant C44

2.3 Constituent array and degrees

A constituent array specifies one or more constituent in each sublattice. A constituent must be entered as a species with fixed stoichiometry. Between constituents in different sublattices one must give a colon, ":", between interacting constituents in the same sublattice one must give a comma, ",". A constituent array with exactly one constituent in each sublattice is also called an "endmember" as it give the value for a "compound" with fixed stoichiometry. Constituent arrays with one or more interaction describe the composition dependence of the property, without such parameter the property will vary liearly between the endmembers.

If there are no sublattices, like in the gas, one just give the phase and the constituent

G(gas,C1O2)

If no degree is specified it is assumed to be zero. For endmembers the degree must be zero but it may sometimes be useful to specify the zero in order to distinguish the parameter from the expression for the chemical potential of a component. In the gas phase one normally assumes there are no interactions but it is possible to add such parameters. For an fcc phase with 4 sublattice for ordering and one for interstitials an endmember parameter is

G(fcc,AL:NI:NI:NI:VA)

This would be the Gibbs energy of an Al1NI3 compound.

An interaction between vacancies and carbon in the austenite is

G(fcc,Fe:C,VA;0)

For interaction one should always specify a degree but also in this case an omitted degree is interpreted as zero.

2.4 Macro files

The macro command is very useful for preparing complex calculations and to remember how you did them. A macro file is simplest to create staring from a log file (created by the SET LOG command).

You can insert stops in the macro file with "@&" at the beginning of a line.

You can insert comments in the macro file with "@$" at the beginning of the comment line.

A macro file should be terminated with the command set interactive which gives back control to the keyboard otherwise the program will terminate at the end of the macro.

A macro can start another macro file 5 levels deep.

3 All commands

The commands in alphabetica order as listed with the ?

ABOUT	ENTER	LIST	QUIT
AMEND	EXIT	MACRO	READ
BACK	FIN	MAP	SAVE
CALCULATE	HELP	NEW	SELECT
DEBUG	HPCALC	OPTIMIZE	SET
DELETE	INFORMATION	PLOT	STEP

Many of the commands have "subcommands" and usually there is a default (listed within slashes //) which is selected by pressing return. One can type commands and subcommands and other parameters on the same line if one knows the order, using a comma, "," to select the default.

There some options that can be set for the whole session or for just a single command. The options are idenfified by a - in front like -output=myfile.dat.

3.1 Option

These should be possible to specify directly after a command. But they are not yet implemented.

- -OUTPUT *file name*
- -ALL apply for all
- -FORCE override normal restrictions
- -VERBOSE write information while executing
- -SILENT do not write anything except fatal error messages

4 About

Some information about the software.

```
This is Open Calphad (OC), a free software for thermodynamic calculations
described in the open access journal:
Integrating Materials and Manufacturing Innovation (2015) 4:1
It is available for download at http://www.opencalphad.com

This software is protected by the GNU General Public License
You may freely distribute copies as long as you also provide the source code.
The software is provided "as is" without any warranty of any kind, either
expressed or implied.
The full license text is provided with the software or can be obtained from
the Free Software Foundation http://www.fsf.org

Copyright 2010-2015, several persons.
Contact person Bo Sundman, bo.sundman@gmail.com
This version linked 2015-08-05
```

5 Amend

Intended to allow changes of already entered data. Only some of the subcommands are implemented.

ALL_OPTIM_COEFF	CP_MODEL	PARAMETER	SYMBOL
BIBLIOGRAPHY	ELEMENT	PHASE	TPFUN_SYMBOL
COMPONENTS	EQUILIBRIUM	QUIT	
CONSTITUTION	GENERAL	SPECIES	

5.1 AMEND All optimizing cpefficients

The values of the optimizing coefficients, see section 25.16 can be rescaled (start values set to current values) or recovered (current values set to previous start values).

5.2 AMEND Bibliography

The bibliographic reference for a parameter can be amended.

5.3 AMEND Components

By default the elements are the components. Ths command can set any orthogonal set of species as components. The number of components cannot be changed.

Not implemented yet.

5.4 AMEND Constitution

The user can set a constitution of a phase before a calculation. This will be used as initial constitution for a calculation.

5.5 AMEND C_P model

The low temperature heat capacity model can be amendedd. Not implemented yet.

5.6 AMEND Element

Not implemented yet.

5.7 AMEND Equilirium

Not implemented yet.

5.8 AMEND General

A number of user specific settings for defaults can be made:

- The name of the system.
- The level of the user (beginner, frequent user, expert). This may affect the behaviour of the program (not implemented yet).
- Global minimization is allowed or not.
- Gridpoints in the same phase can be merged after global minimization.
- Automatic creation of composition sets not allowed.
- Redundant composition sets can be deleted automatically..

5.9 AMEND Parameter

The possible parameters are defined by the model of the phase. By specifying a parameter the user can change its expression. See the ENTER PARAMETER command. Not implemented yet but you can use the command ENTER PARAMETER to change the parameter.

5.10 AMEND Phase

You must first specify the phase name. If you want to amend something for a composition set you must specify the composition set number together with the phase name after a hash character (#) (like liquid#2). Then you can amend some of the properties of the phase:

COMPOSITION_SET	DISORDERED_FRACS	GLAS_TRANSITION	QUIT
DEBYE_CP_MODEL	EINSTEIN_CP_MDL	INDEN_WEI_MAGMOD	
DEFAULT_CONSTIT	ELASTIC_MODEL_A	MAGNETIC_CONTRIB	

5.10.1 AMEND PHASE Composition set

Each phase has by default a single composition set. If the same phase can exist as stable (or metastable) with two or more compositions (miscibility gaps or order/disorder transformations) you may have to amend the ohase by creating additional composition sets.

Composition sets may also be created automatically by the grid minimizer.

More composition sets of a phase can be created or deleted. Phases with miscibility gaps or which can exist with different chemical ordering like A2 and B2 must be treated as different composition sets. The user can specify a prefix and suffix for the composition set. The composition set will always habe a suffix #digit where digiit is a number between 1 and 9. One cannot have more than 9 composition sets.

Composition sets can also be created automatically by the software. In such a case the composition set will have the suffix _AUTO,

In some cases it may be interesting to calculate metastable states inside miscibility gaps and one can prevent automatic creation of composition sets by AMEND GENERAL or for an individual phase by *SET PHASE BIT* phase *NO_AUTO_COMP_SET*

5.10.2 AMEND PHASE Debye C_P model

Not implemeneted yet.

5.10.3 AMEND PHASE Default Constitution

The default constitution of a phase can be set. This will be used when the first calculation with the phase is made and sometimes if there are convergence probems. Depending on the minimizing software used the initial consititution can be important to find the correct quilibrium if the phase has ordering or a miscibility gap.

5.10.4 AMEND PHASE Disordered fraction sets

For phases with several sublattices the Gibbs energy of the phase can be divided into two sets of fractions where the second or "disordered" set have only one or two sublattice and the fractions on these represent the sum of fraction on some or all of the first or "ordered" set of sublattices. This is particularly important for phases with ordering like FCC, BCC and HCP and for intermediate phases like SIGMA, MU etc.

5.10.5 AMEND PHASE Einstein C_P model

Not implemented yet.

5.10.6 AMEND PHASE Elastic model A

A contribution to the Gibbs energy due to elastic straing can be added. Requires also values of the elastic constants, see section 2.2.1. Requires code for calculating the elastic energy and it is not implemented yet.

5.10.7 AMEND PHASE Glas_Transition

A model for the heat capacity for undecooled liuqids can be added. Not implemented yet.

5.10.8 AMEND PHASE Inden-Wei Magnetic Model

An improved variant of the model for the magnetic contribution to the Gibbs energy can be set by this command. Requires individual Bohr magnetin numbers of the constituents of the phase. Not implemented yet.

5.10.9 AMEND PHASE Magnetic Contribution

The original Inden model for the magnetic contribution to the Gibbs energy can be set by this command.

5.10.10 AMEND PHASE Quit

Do not amend anything for the phase.

5.11 AMEND Quit

Do not amend anything.

5.12 AMEND Species

Not implemented yet.

5.13 AMEND Symbol

Not implemented yet.

5.14 AMEND Tpfun_Symbol

You can replace a TP function with a new expression.

This is somewhat dangerous if you have several equilibria because each equilibria has its own list of most recently calculated values of the function and they may not be aware of a change of the function and go on using the already calculated value unless

you change T or P, in each equilibrium, which will force recalculation. I am thinking of a way to handle this.

6 Back

Return back from the command monitor to the application program. In the OC software itself it means terminate the program.

7 Calculate

Different things can be calculated. The normal thing to calculate is **equilibrium**, the other things are special.

ALL_EQUILIBRIA	NO_GLOBAL	SYMBOL
EQUILIBRIUM	PHASE	TPFUN_SYMBOLS
GLOBAL_GRIDMIN	QUIT	TRANSITION

7.1 CALCULATE All equilibria

Intended for the assessment procedure. Not implemented yet.

7.2 CALCULATE Equilibrium

The normal command to calculate the equilibrium of a system for the current set of conditions and phase status. You can calculate a metastable equilibrium if some phases that should be stable have been set dormant or suspended or if automatic creation of composition sets is not allowed.

7.3 CALCULATE Global_Gridmin

Calculate with the global grid minimizer without using this result as a start point for the general minimizer. Used to debug the grid minimizer.

7.4 CALCULATE No_Global

Calculate the equilibrium with the current minimizer without using a global gid minimizer to generate start constitutions. The current equilibrium is used as start point. Can be quicker when just a small change of conditions made since previous calculation. It means no check of new miscibility gaps.

7.5 CALCULATE Phase

You must provide a phase name.

The Gibbs energy of a phase and possible derivatives are calculated. Mainly for debugging the implementation of models.

7.5.1 CALCULATE PHASE ... Only_G

The Gibbs energy and all T and P derivatives calculated and listed.

7.5.2 CALCULATE PHASE ... G_and_dGdy

The Gibbs energy, all T and P derivatives and all first derivatives with respect to constituents are calculated and listed.

7.5.3 CALCULATE PHASE ... All_Derivatives

The Gibbs energy, all T and P derivatives and all first and second derivatives with respect to constituents are calculated and listed.

7.6 CALCULATE Quit

Quit calculating.

7.7 CALCULATE Symbol

A state variable symbol or function is calculated using the results from the last equilibrium or grid minimizer calculation. It is used in particular for calculation of "dot derivatives" like H.T for the heat capacity.

7.8 CALCULATE Tpfun_Symbols

All or a specific TPFUN symbol is calculated for current values of T and P.

7.9 CALCULATE Transition

After calculating an equilibrium you can calculate directly when a phase will appear or disappear by releasing one of the conditions you have specified. Typically this is used to calculate the melting temperature of an alloy or a solubility limit.

You specify the phase name and the condition to be released. The program will set this phase as FIXED with zero amount and remove the condition you specified and calculate the equilibrium. The calculation may fail if the phase cannot be set stable with zero amount. If successful the removed condition will be set to the value calculated and the phase set stable with zero amount.

8 Debug

Several possibilities to trace calculations will be implemented in order to find errors. The only implemented feature is to stop the program whenever an error occurs. This is useful to find errors using macro files so the macro not just goes on doing other things.

8.1 DEBUG Elasticity

Not implemented.

8.2 DEBUG Free lists

Only for experts.

8.3 DEBUG Stop_on_Error

The program will stop at the command level after printing the error message if an error has occured when using macro file. This makes it easier to use macro files to find errors.

9 Delete

Not implemented yet and may never be, it is not so easy to allow deleting things when the data structure is so involved, it may be better to enter the data again without the data that should be deleted.

COMPOSITION_SET	EQUILIBRIUM	QUIT
ELEMENTS	PHASE	SPECIES

9.1 DELETE Composition set

The first composition set of a phase cannot be deleted. Otherwise usually no problem. Composition sets are created and deleted during normal equilibrium calculations to

detect miscibility gaps.

9.2 DELETE Element

Dangerous and will probably never be implemented.

9.3 DELETE Equilibrium

Dangerous but sometimes necessary. Done automatically for STEP and MAP commands when previous results are removed.

9.4 DELETE Phase

Dangerous and will probably never be implemented.

9.5 DELETE Quit

Nothing more to delete.

9.6 DELETE Species

Not implemented yet

10 Exit

Terminate the OC software.

11 Enter

In most cases data will be read from a database file. But it is possible to enter all thermodynamic data interactivly. This should normally start by entering all elements, then all species (the elements will automatically also be species) and then the phases.

A species have a fixed stoichiometry and possibly a charge. The species are the constituents of the phases.

A phase can have sublattices and various additions like magnetic or elastic (the latter not implemented yet).

TPFUN symbols can be used to describe common parts of model parameters.

Each parameter of a phase is entered separately. One may use TPFUN symbols which are already entered.

At present the multicomponent CEF model and the ionic 2-sublattice liquid model are the only one implemented. This includes the gas phase, regular solutions with Redlich-Kister Muggianu model and phases with up to 10 sublattices and magnetic contributions.

The subcommands are:

BIBLIOGRAPHY	EQUILIBRIUM	PHASE	TPFUN_SYMBOL
CONSTITUTION	EXPERIMENT	QUIT	
COPY_OF_EQUILIB	OPTIMIZE_COEFF	SPECIES	
ELEMENT	PARAMETER	SYMBOL	

11.1 ENTER Bibliography

Each parameter must have a reference. When entering a parameter a reference symbol is given and with this command one can give a full reference text for that symbol like a published paper or report.

11.2 ENTER Constitution

The constitution (fraction of all constituents) of a phase can be entered. This is a way to provide start values for a calculation or to calculate the Gibbs enegy for a specific phase at a specific constitution using **calculate phase**.

11.3 ENTER Copy of equilibrium

One can create a copy of an equilibrium with the same set of conditions and other data.

11.4 ENTER Element

The data for an element is entered. It consists of is symbol, name, reference state, mass, H298-H0 and S298. The latter two values are never used for any calculation.

11.5 ENTER Equilibrium

One can have several equilibria each with a unique set of conditions incuding phase status (dormant, suspended, fix or entered). This is useful for compare different states, to simulate transformations and to assess model parameters as each experimental or theoretical information represented as an equilibrium.

Each equilibrium is independent and they can be calculated in parallel.

11.6 ENTER Experiment

This is for assessment, experimental data can be specified.

11.7 ENTER Oprimize coefficient

The TP symbols for the coefficients to be optimized are entered. They have the names A00 to A99. They are used in model parameters and can be varied by the optimization procedure to minimize the difference between the experimental data and the same property calculated from the models of the phases.

11.8 ENTER Parameter

A parameter is definded by its identifier, the phase and constituent array. A parameter can be a constant or depend on T and P. The parameter will be multiplied with the fractions of the constituents given by its constituent array.

For example G(LIQUID,CR) is the Gibbs energy of liquid Cr relative to its reference state, normally the stable state of Cr at 298.15 K and 1 bar.

For a gas molecule G(GAS,C1O2) is the Gibbs energy of the C1O2 molecule relative to the reference states of C (carbon) and O (oxygen).

For phases with sublattices the constituents in each sublattice are separated by a semicolon, ":" and interacting constituents in the same sublattice by a comma, ",". For example

G(FCC,FE:C,VA) is the interaction between C (carbon) and VA (vacant interstitial sites) in the FCC phase.

One can store many different types of data in OC using the parameter identifier. A description of the identifiers currently implemeneted are given in the introduction. Here is a short list.

- G, the Gibbs energy or an interaction parameter

- TC, the critical temperature for ferro or antiferro magnetic ordering
- BMAGN, the avarage Bohr magneton number
- CTA, the Curie temperature for ferromagnetic ordering
- NTA, the Neel temperature for antiferromagnetic ordering
- IBM&C, the individual Bohr magneton number for constituent C
- THETA, the Debye or Einstein temperature
- MOBQ&C, the logarithm of the mobility of constituent C
- RHO, the electrical resistivity
- MAGS, the magnetic suseptibility
- GTT, the glas transition temperature
- VISC, the viscosity
- LPAX, the lattice parameter in X direction
- LPTH, the deviation from cubic structure
- EC11A, the elastic constrant C11
- EC12A, the elastic constrant C12
- EC44A, the elastic constrant C44

The current list can be obtained by the command LIST PARAMETER_ID.

11.9 ENTER Phase

All thermodynamic data are connected to a phase as defined by its parameters, see **enter parameter**. A phase has a name with can contain letters, digits and the underscore character.

A phase can have 1 or more sublattices and the user must specify the number of sites on each. He must also specify the constituents on each sublattice. For some models, like the ionic liquid model, the number of sites may change with composition.

By default the model for a phase is assumed to be the Compound Energy Formalism (CEF). If any onther model should be used that is set by the **amend** or **set phase bit** commands.

11.10 ENTER Quit

Quit entering things.

11.11 ENTER Species

A species consists of a name and a stochiometric formula. It can have a valence or charge. The name is often the stoichiometric formula but it does not have to be that. Examples:

- enter species water h2o
- enter species c2h2cl2_trans c2h2cl2
- enter species c2h2cl2_cis c2h2cl2
- enter species h+ h1/- -1

There can be a problem with ambiguety with a species name like h2o if there is also a species h2o2. In such cases use a final unity, i.e. h2o1.

Single letter element names must be followed by a stocichiometric factor unless it is the last element when 1 is assumed. Two-letter element names have by default the stoichiometric factor 1.

- enter species carbonmonoxide c1o1
- enter species cobaltoxide coo
- enter species carbondioxide c1o2

The species name is important as it is the name, not the stoichiometry, that is used when referring to the species elsewhere like as constituent. It is of course convenient to choose a species name similar to its stoichiometric formula but as shown above, that is not always sufficient.

11.12 ENTER Symbol

The OC package has both "symbols" and "tpfun_symbols", the latter has a very special syntax and can be used when entering parameters.

The symbols are designed to handle relations between state variables, one can define expressions like

enter symbol K = X(LIQUID,CR)/X(BCC,CR);

where K is set to the partition of the Cr mole fractions between liquid and bcc.

The symbols also include "dot derivatives" like H.T which is the temperature derivative of the enthalpy for the current system at the given set of conditions, i.e. the heat capacity.

11.13 ENTER Tpfun_Symbol

This symbol is an expression depending on T and P that can be used when entering parameters. A TPfun can refer to another TPfun.

TPFUNS have a strict syntax because the software must be able to calculate first and second derivatives with respect to T and P.

12 Exit

Terminate the OC software in Swedish.

13 Fin

Terminate the OC software in French.

14 Help

Can give a list if commands or subcommands or parts of this help text.

15 HPCALC

A reverse polish calculator.

16 Information

Not implemeneted yet.

17 List

Many things can be listed. Output is normally on the screen unless it is redirected by the -output option.

AXIS	EQUILIBRIA	PARAMETER	SHORT
BIBLIOGRAPHY	LINE_EQUILIBRIA	PHASE	STATE_VARIABLES
CONDITIONS	MODEL_PARAM_ID	QUIT	SYMBOLS
DATA	OPTIMIZATION	RESULTS	TPFUN_SYMBOLS

17.1 LIST Axis

Lists the axis set by the user.

17.2 LIST Bibliography

List the bibliographic references for the data.

17.3 LIST Conditions

Lists the conditions set by the user.

17.4 LIST Data

Lists all thermodynamic data. The deafult is on screen but you can also choose among the options, LaTeX, macro, ODB and TDB

17.4.1 LIST DATA LaTeX

The thermodynatic data will be formatted according to LaTeX for later inclusion in publications. Not implemented.

17.4.2 LIST DATA Macro

The thermodynamic data will be written as a macro file that can later be read back into the OC software. Not implemented.

17.4.3 LIST DATA ODB

A variant of the TDB file format suitable of OC.

17.4.4 LIST DATA TDB

A variant of the TDB file format with Thermo-Calc flavour.

17.5 LIST Equilibria

Lists the equilibria entered (not the result ...).

17.6 LIST Line equilibria

Lists the equilibria entered during STEP or MAP commands

17.7 LIST Model parameter identifiers

Lists the model parameter identifiers implemented in the current version of OC, see section 2.2.1.

17.8 LIST Optimization

Lists results of an optimization, sereval suboptions will be implemented but currently there is a short version only.

17.9 LIST Parameter

List a specific parameter.

17.10 LIST Phase

You must first specify the phase name. Then you can specify if you want the constitution, data or model.

17.10.1 LIST PHASE ... Constitution

List the constitution of the phase.

17.10.2 LIST PHASE ... Data

List the model and thermodynamic data.

17.10.3 LIST PHASE ... Model

List some model data for example if there is a disordered fraction set.

17.11 LIST ... Quit

You did not really want to list anyting.

17.12 LIST Results

List the results of an equilibrium calculation. This is the most frequent list command. The listing will contain the current set of conditions, a table with global data, a table with component specific data and then a list of stable phases with amounts, compositions and possibly constitutions. It is possible to list also unstable phases.

There are 9 options for the formatting:

1. Output in mole fractions, phase constituents in value order (constituent with highest fraction first)
2. As 1 but include also the phase constitution (sublattices and their fractions)
3. As 1 with the phase composition in alphabetical order (do not work)
4. As 1 with mass fractions
5. As 4 with the phase composition in alphabetical order (do not work)
6. As 4 and also include the phase constitutions
7. All phases will be listed with composition in mass fractions and in alphabetical order of the elements. A negative driving force for a phase means the phase is not stable.
8. All phases will be listed with composition in mole fraction in value order and driving force, negative driving force means the phase is not stable.
9. All phases will be listed with composition and constitutions in alphabetical order of the elements and the driving force.

For each phase the name, status and driving force (in dimensionless units) is given on the first line.

The second line has the amount of the phase in moles and mass of components (zero if not stable) and its volume (zero if no pressure data).

The third line has the number of formula units of the phase (zero if not stable) and the moles of atoms per formula unit. The first value on the third line multiplied with the second will be the first value on the second line. The gas phase and phases with interstitials have a varying amount of moles of atoms per formula units.

17.13 LIST Short

The A option list a single line for each element, species and phase with some essential data.

The P option lists only the phases order in decreasing order of stability.

17.14 LIST State_Variables

Values of individual state variables like G, HM(LIQUID), X(LIQUID,CR) etc. can be listed. Terminate the command by an empty line. Note that the values of symbols and TP functions cannot be listed here, they are calculated by the CALCULATE SYMBOL or CALCULTE TP command.

17.15 LIST Symbols

All state variable symbols listed but not their values, they are calculated by the CALCULATE SYMBOL command.

17.16 LIST Tpfun_Symbols

All TPFUN expressions listed, their values are calculated with the CALCULATE TP command.

18 Macro

By specifying a file name commands will be read from that file. The default extention is OCM. A macro file can open another macro file (max 5 levels). When a mcro file finish with SET INTERACTIVE the calling macro file will continue.

19 Map

For phase diagram calculations. One must first ste two axis with state variables also set as conditions.

If one gives several MAP commands one can erase or keep the previous results.

During mapping each calculated equilibria is saved and then different kinds of state vaiables can be used for plotting.

20 New

To remove all data so a new system can be entered. Fragile

21 Plot

Plot the result from a STEP or MAP calculation. A simple interface to gnuplot has been implemented.

You must forst specify the state variable on the horisontal (xaxis) and vertical (yaxis) axis. Then you can give several of the options below, finish with RENDER or QUIT.

GIBBS_TRIANGLE	POSITION_OF_KEYS	TITLE	YRANGE
GRAPHICS_FORMAT	QUIT	XRANGE	YTEXT
OUTPUT_FILE	RENDER	XTEXT	

21.1 (PLOT xaxis yaxis) Gibbs triangle

Not implemented yet

21.2 (PLOT xaxis yaxis) Graphics format

Screen, PNG and Postscript possible.

21.3 (PLOT xaxis yaxis) Output file

By default plotting will generate a ocgnu.DAT and ocgnu.PLT files for GNUPLOT. You can specify other name here. If you plot on other device than screen there will be additionally an ocgnu.PNG or ocgnu.PS file.

21.4 (PLOT xaxis yaxis) Position of keys

Tje identification of the labels of the curves can be positioned with this command. See GNUPLOT for information.

21.5 (PLOT xaxis yaxis) Quit

No plot generated.

21.6 (PLOT xaxis yaxis) Render

Finally plot.

21.7 (PLOT xaxis yaxis) Title

Title on top of the figure.

21.8 (PLOT xaxis yaxis) Xrange

Scaling (range) of the hoisontal axis, the min and max values.

21.9 (PLOT xaxis yaxis) Xtext

Text on thee horisontal axis

21.10 (PLOT xaxis yaxis) Yrange

Scaling (range) of the verical axis, the min and max values.

21.11 (PLOT xaxis yaxis) Ytext

Text on thee vertical axis

21.12 Quit

Terminate the OC software in English.

22 Read

At present there a very limited SAVE command implemented in OC as it is difficult to do that before the datastructure is well defined.

It is possible to read a (non-encrypted) TDB file but it should be not too different from what is generated by the LIST_DATA command in TC.

DIRECT	QUIT	UNFORMATTED
EXPERIMENT_DATA	TDB	

22.1 READ Direct

In the future it will be possible to save results on a random access (DIRCT) file.

22.2 READ Experimental data

Equilibra with experimental data for assessments can be read from this file.

22.3 READ Quit

You did not really want to read anything.

22.4 READ TDB

A TDB file (with extention TDB) should be specified. The TDB file must not deviate very much from the output of Thermo-Calc.

22.5 READ Unformatted

For use to read a file created with a SAVE UNFORMATTED command. It will not always work as the datastructure is not fixed.

23 Save

There are several forms of save, three forms write a text file that can be read and modified with a normal editor. Two forms are unformatted, either on a sequential file or a direct (random access) file.

DIRECT QUIT TDB UNFORMATTED

23.1 SAVE Direct

It will eventually be possible to save the result of STEP and MAP commands on a random access file for later processing.

23.2 SAVE Quit

You dod not want to save anything

23.3 SAVE Unformatted

The intention is that one will be able to save the current status of the calculations on a file and then reassume the calculations by reading this file. A tentative version is implemented.

24 Select

There are a few things that can be selected, most important which equilibrium the commands will operate on.

24.1 SELECT Equilibrium

As the user can enter several equilibria with different conditions this command allows him to select the current eqilibria.

24.2 SELECT Graphics

Only GNUPLOT available.

24.3 SELECT Minimizer

Only one implemented.

25 Set

Many things can be set. Things to be “set” and “amended” sometimes overlap.

ADVANCED	FIXED_COEFF	OPTIMIZING_COND	STATUS
AS_START_EQUILIB	INPUT_AMOUNTS	PHASE	UNITS
AXIS	INTERACTIVE	QUIT	VARIABLE_COEFF
BIT	LEVEL	RANGE_EXP_EQUIL	VERBOSE
CONDITION	LOG_FILE	REFERENCE_STATE	WEIGHT
ECHO	NUMERIC_OPTIONS	SCALED_COEFF	

25.1 SET Advanced

Not implemented yet

25.2 SET As start equilibrium

The current equilibrium will be copied to the list of start equilibria for STEP and MAP commands.

25.3 SET Axis

A condition can be set as an axis variable with a low and high limit and a maximum increement. With 2 or more axis one will calculate a phase diagram, i.e. lines where the set of stable phases changes.

With one axis one calculates the set of stable phases and their properties while changing the axis variable.

25.4 SET Bit

Only for those who who what it means.

25.5 SET Condition

A condition is a value assigned to a state variable or an expression of state variables (the latter not yet implemented). By setting the status of a phase to fix one has also set a condition.

25.6 SET Echo

This is useful command in macro files.

25.7 SET Fixed coefficient

An optimizing coefficient is assigned a fixed value.

25.8 SET Input_Amounts

This allows the user to specify a system by giving a redundant amount of various species in the system. The software will tranform this to conditions on the amounts of the components.

25.9 SET Interactive

The usual end of a macro file. Gives command back to the keyboard of the user, or to the calling macro file. Without this the program will just terminate.

25.10 SET Level

I am no longer sure what this should do and if it is needed ...

25.11 SET Log_File

A useful command to save all interactive input while running OC. The log file can easily be transformed to a macro file. All bug reports should be accompanied by a log file which reproduces the bug.

25.12 SET Numeric_Options

Some numeric option can be set.

25.13 SET Optimizing conditions

A few variables used to guide the optimization of model parameters can be set.

25.14 SET Phase

You must specify a phase name. Some phase specific things can be set, also for the model.

25.14.1 SET PHASE ... Amount

One can specify the amount of the phase which is used as initial value for an equilibrium calculation.

25.14.2 SET PHASE ... Bits

Some of the models and data storage depend on the bits of the phase. These are

- FCC_PERMUTATIONS is intended for the 4 sublattice CEF model for fcc ordering. Setting this bit means that only unique model parameters needs to be entered, the software will take care of all permutations. HCP permutations is also handelled by this bit as they are identical in the 4 sublattice model.
- BCC_PERMUTATIONS is intended for the 4 sublattice CEF model for BCC ordering. The BCC tetrahedron is unsymmetric which makes it a bit more complicated. Not implemented yet.
- IONIC_LIQUID_MDL. By setting this bit the phase is treated with the 2 sublattice paritally ionic liquid model. It must have been entered with 2 sublattices and only cations in the first sublattice and only anions, vacancy and neutrals in the second.
- AQUEOUS_MODEL. Not implemented yet.
- QUASICHEMICAL. Is intended for the classical quasichemical model for crystalline phases. Not implemented yet.
- FCC_CVM_TETRADRN. Is intended for the CVM tetrahedron model. Not implemented yet.
- FACT_QUASICHEMCL. Is intended for one for the FACT modified quasichemical liquid models. Not implemented yet.
- NO_AUTO_COMP_SET. This makes it possible to prevent that a specific phase has automatic composition set created during calculations.
- ELASTIC_MODEL_A. This should specify the elastic model to be used. Not implemented yet.

25.14.3 SET PHASE ... CONSTITUTION

This is the same as **amend phase constitution**.

25.14.4 SET PHASE ... DEFAULT_CONSTITU

Same as **amend phase default_constit**.

25.14.5 SET PHASE ... Quit

You did not want to set anything for the phase.

25.14.6 SET PHASE ... STATUS

A phase can have 4 status

- entered, this is the default. The phase will be stable if that would give the most stable state for the current conditions. The user can give a tentative amount.
- suspended, the phase will not be included in any calculations.
- dormant, the phase will be included in the calculations but will not be allowed to become stable even if that would give the most stable equilibrium. In such a case the phase will have a positive driving force.
- fixed means that it is a condition that the phase is stable with the specified amount. Note that for solution phases the composition is not known.

25.15 SET Quit

You did not really want to set anything.

25.16 SET Range of experimental equilibria

For an assessment several consquetive equilibria with experimental data must be entered. This command specifies the first and last of those equilibria. It possible to add more equilibria later one by one (not yet though).

The equilibria is assigned weight one by default. This can be changed with the SET WEIGHT command.

25.17 SET Reference_State

For each component (also when not the elements) one should be able to specify a phase at a given temperature and pressure as reference state. The phase must exist for the pure component.

25.18 SET Scaled coefficient

A coefficient for optimization can be specified with a start value, scaling factor and a minimum and maximum value. The SET VARIABLE command sets the scaling factor equal to the start value and have no min or max values.

25.19 SET Status

The status of a phase can be changed. The other options are not yet implemented.

25.19.1 SET STATUS Constituent

A constituent of a phase can be suspended. Not yet implemented.

25.19.2 SET STATUS Element

An element can be ENTERED or SUSPENDED. If an element is suspended all species with this element is automatically suspended. Not yet implemented.

25.19.3 SET STATUS Phase

A phase can have 4 status as described for the SET PHASE STATUS command above. Changing the pase status does not affect anything except the phase itself. It is the same as SET PHASE STATUS.

25.19.4 SET STATUS Species

A species can be ENTERED or SUSPENDED. If a species is suspended all phases that have this as single constituent in a sublattice will be automatically suspened. Not yet implemented.

25.20 SET Units

For each property the unit can be specified like Kelvin, Farenheit or Celsius for temperature. Not implemented yet.

25.21 SET Variable coefficient

A coefficient for optimization is assiged a start value.

25.22 SET Verbose

Not implemented yet.

25.23 SET Weight

Intended for assessments. A weight is zero or a positive value. Equilibria with weight zero will be ignored in an optimization.

You can specify the current equilibrium or give an abbreviation that will set the weight of all equilibria for which the abbreviation fots.

26 Step

Requires that a single axis is set.

26.1 STEP Contitional

A specified symbol is evaluated at each step. Can be used for Scheil-Gulliver solidification simulation when implemented.

26.2 STEP Normal

Calculates equilibria from the low axis limit to the high at each increment.

26.3 STEP Quit

You did not want to STEP.

26.4 STEP Separate

Calculates each phase separately. Can be used to calculate Gibbs energy curves.

27 Summary

That's all and I hope enough (when all is implemented).