User Guide to the
Open Calphad software package
version 3.0

VERY PRELIMINARY DRAFT

Bo Sundman, December 22, 2015

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Contents

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, like for 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" "bib.ref."

These parts will now be explained in more detail.

2.2.1 Parameter Identifiers

The OC thermodynamic package can handle any phase property that depend on T, P and the constitution of the phase using the models implemented. It is easy to extend the number of properties by declaring property identifiers in ths source code. 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.

The list below is tentative and insensitive to case.

- G, the Gibbs energy parameter for an endmember or an interaction. G(LIQUID,FE;0) is the Gibbs energy for pure liquid Fe. Note that the parameter will be used also below the melting temperature of Fe for a liquid phase containg Fe. G(LIQUID,CR,FE;0) is the regular parameter for Cr and Fe in the liquid.

- TC, a parameter for the critical temperature for ferro or antiferro magnetic ordering using the Inden model.

- BMAGN, a parameter for the avarage Bohr magneton number using the Inden model.

- CTA, a parameter for the Curie temperature for ferromagnetic ordering using a modified Inden model.

- NTA, a parameter for the Neel temperature for antiferromagnetic ordering using a modified Inden model.

- IBM&C, a parameter for 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.

- THETA, a parameter for the Debye or Einstein temperature.

- MQ&C, a parameter for the logarithm of the mobility of constituent C

- RHO, a parameter for the electrical resistivity

- MSUS, a parameter for the magnetic suseptibility

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- GTT, a parameter for the glas transition temperature

- VISCA, a parameter for the viscosity

- LPX, a parameter the lattic parameter

- EC11A, a parameter for the elastic constrant C11

- EC12A, a parameter for the elastic constrant C12

- EC44A, a parameter for the elastic constrant C44

The current value of any of these parameter identifiers can be obtaind by the command LIST STATE_VARIABLE using the identifier and appropriate phase and component specifiers.

2.2.2 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.

2.2.3 Expression and bibliographic reference

The expression for a parameter can be a single value or a function of T and P. It must start with a low temperaure limit, usually 298.15 K and must finish with a high temperature limit. These expressions as well as their first an second derivatives will be calculated by the TP-fun package. To simplify that there is a strict syntax for the expression. A term in the expression is

"numeric value" * "name of TP function" *T** "power" *P** "power"

You can construct very complex expression by referring to other functions. If "power" is zero the corresponding *T** or *P** can be ignored. If it is negative it must be surrounded by parenthesis like (-1). If it is unity the **1 can be skipped.

Several terms, seperateb by signs, forms an expression and it must be terminated by a semicolon, ";". After the semicolon there must be a high temperature limit or a breakpoint in temperature. A breakpoint must be followed by the letter "Y" and then a new expression for temperatures above the breakpoint.

It is the responsability of the user to ensure the expression is continuous at the breakpoint. If there are jumps in the value at a breakpoint strange things can happen when calculating equilibria.

After the high temperature limit the letter "N" must be given followed by a bibliographic reference for the parameter. Use the commands AMEND or ENTER BIBLIOGRAPIC to give the reference.

Always add a bibliographic reference even if it is just your name and date. This avoids people to misstake a value inspired by your experience as a carefully validated parameter.

A term can be used inside a natural logarithm, LN, or exponential, EXP. And the LN or EXP can be multiplied with a term. On the other hand you are not allowed to have any parenthesis, except around powers or arguments to LN and EXP. A valid expression is

```
 298.15 -8856.94+157.48*T-26.908*T*LN(T)+.00189435*T**2
         -1.47721E-06*T**3+139250*T**(-1); 2180 Y
         -34869.344+344.18*T-50*T*LN(T)-2.88526E+32*T**(-9); 6000 N 91Din
```

where 91Din is the reference to the SGTE unary database.

2.3 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). See the macros directory for examples.

You can insert stops in the macro file with "@&" at the beginning of a line. It can be useful to inspect output. The macro continues after pressing RETURN key. If you plot the program will automatically stop and you must use the mouse to click on the figure to continue.

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.

3.1   Options

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.

The options can be specifies directly after a command. Only a few are implemented.

- /OUTPUT=*file name* open a file and write

- /APPEND=*file name* append output to a file

- /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 by B Sundman, U R Kattner, M Palumbo and S G Fries,
Integrating Materials and Manufacturing Innovation (2015) 4:1

It is available for download at http://www.opencalphad.org or
the opencalphad repository at http://www.github.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 2015-12-22
```

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 coefficients

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 text for bibliographic reference identifier can be amended. The reference identifier is case insensitive.

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 by this command. Not implemented yet.

5.4 *amend* Constitution

The program will ask for a phase name and the user can set the amount and constitution of the phase. This will be used as initial constitution for a calculation unless the grid minimizer is used.

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).

- If global minimization is allowed or not.

- If gridpoints in the same phase can be merged after global minimization.

- If automatic creation of composition sets is allowed or not.

- If 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. As this is not yet implemented you must use the command ENTER PARAMETER to change the parameter expression.

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 phase by creating additional composition sets.

Composition sets can also be created automatically by the grid minimizer during an equilibrium calculation. In such a case the composition set will have the suffix _AUTO,

Composition sets of a phase can be created and 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. Extra composition sets will always habe a suffix #digit where digiit is a number between 2 and 9. One cannot have more than 9 composition sets.

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 for the first calculation with the phase 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.

For each consititent you can spefify a minimum > or maximum < fraction or give NONE if there are no default.

If a phase has miscibility gaps and the user has created composition sets with default constitutions the grid minimzer will try to select the composition set with a composition closeset to the default for a stable phase.

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. Calcullates all equilibra with non-zero weight indicated by the SET RANGE command.

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 for the specified phase for current T, P and its current composition.

7.5.2 *calculate phase ...* G_and_dGdy

The Gibbs energy, all T and P derivatives and all first derivatives with respect to constituents for the specified phase for current T, P and its current composition 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 for the specified phase for current T, P and its current composition 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 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	

10.1 *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.

10.2 *enter* Constitution

The constitution (fraction of all constituents) of a phase can be entered. This is a way to provide start values for an equilibrium calculation (when not using grid minimmizer) or to calculate the Gibbs energy for a specific phase at a specific constitution using **calculate phase**.

10.3 *enter* Copy of equilibrium

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

10.4 *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.

10.5 *enter* Equilibrium

One can have several equilibria each with a unique set of conditions incuding phase status (dormant, suspended, fix or entered) but with the same components. 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.

10.6 *enter* Experiment

This is for assessments, experimental data can be specified for an equilibrium.

10.7 *enter* Optimizing 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.

10.8 *enter* Parameter

A model 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. See the documentation of the GTP model package or the book by Lukas et al[07Luk] for more information about thermodynamic models.

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, and called an endmember.

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

For interaction parameters the components are separated by a comma ",", like in G(LIQUID,CR,FE).

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.

The only excess model implemented in OC is the Redlish-Kiter Muggianu

$$L_{A,B} = \sum_{\nu=0}^{n} (y_A - y_B)^\nu \, {}^\nu L_{A,B}$$

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and the degree, ν, of the interaction parameter is specified after a semicolon, L(phase,A,B;ν).

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 endmember 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

- MQ&C, the logarithm of the mobility of constituent C

- RHO, the electrical resistivity

- MSUS, the magnetic suseptibility

- GTT, the glas transition temperature

- VISCA, the viscosity

- LPX, the lattice parameter in X direction

- 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. All of them can be composition dependent. Some cannot depend on T or P or both.

Many parameters of the parameters are available but the models to handle them are not yet implemented.

10.9 *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. It must start with a letter.

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 so the number specified is irrelevant.

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.

10.10 *enter* Quit

Quit entering things.

10.11 *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.

10.12 *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.

10.13 *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 fastly calculate first and second derivatives with respect to T and P during equilibrium calculations.

11 Exit

Terminate the OC software in Swedish, Ha en bra dag.

12 Fin

Terminate the OC software in French, Au revoir.

13 Help

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

14 HPCALC

A Start the reverse polish calculator.

15 Information

Not implemeneted yet.

16 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

16.1 *list* Axis

Lists the axis set by the user.

16.2 *list* Bibliography

List the bibliographic references for the data.

16.3 *list* Conditions

Lists the conditions set by the user.

16.4 *list* Data

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

16.4.1 *list data* LaTeX

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

16.4.2 *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.

16.4.3 *list data* ODB

A variant of the TDB file format suitable of OC. Not implemented.

16.4.4 *list data* TDB

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

16.5 *list* Equilibria

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

16.6 *list* Line quilibria

Lists the equilibria entered during STEP or MAP commands

16.7 *list* Model parameter identifiers

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

16.8 *list* optimization result

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

16.9 *list* Parameter

List a specific parameter.

16.10 *list* Phase

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

16.10.1 *list phase ...* Constitution

List the constitution of the phase.

16.10.2 *list phase ...* Data

List the model and thermodynamic data.

16.10.3 *list phase ...* Model

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

16.11 *list* Quit

You did not really want to list anyting.

16.12 *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) in value order.

3. As 1 with the phase composition in alphabetical order

4. Output in mass fractions, phase composition in value order.

5. As 4 with the phase composition in alphabetical order.

6. As 4 and also include the phase constitutions in value order.

7. Output all phases will with composition in mass fractions and in value order. Unstable phases will have a negative driving force.

8. Output all phases will with composition in in mole fraction in value order. Unstable phases will have a negative driving force.

9. As 8 including constitutions in value order.

For each phase the name, status (S/D/E/F), moles (or mass), volume, number of formula units, atoms per formula units and driving force (in dimensionless units) is given on one line.

The moles of a phase is the number of formula unit multiplied with atoms per formula units. The gas phase and phases with interstitials and vacancies have a varying amount of moles of atoms per formula units. The composition of the phase can be in value order or alphabetical order.

16.13   *list* Short

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

The P option lists one line for each stable phase and then one line for each remaining phase in decreasing order of stability.

16.14   *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.

The current values of parameter identifiers, see section 2.2.1 can be listed with the command, like TC(BCC) will give the calculated Curie temperature for BCC. A symbol like MQ&FE(FCC) will give the logarithm of the mobility of Fe in the FCC phase.

16.15 *list* Symbols

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

16.16 *list* Tpfun Symbols

All TPFUN expressions listed. To obtain their values use the **calculate TP** command.

17 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 or the user can continue interactivly.

18 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 choose to erase or keep the previous results.

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

19 New

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

20 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	

20.1 *plot xaxis yaxis* Gibbs triangle

Not implemented yet

20.2 *plot xaxis yaxis* Graphics format

Screen, PNG and Postscript possible.

20.3 *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 a file with extention PNG or PS.

20.4 *plot xaxis yaxis* Position of keys

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

20.5 *plot xaxis yaxis* Quit

No plot generated.

20.6 *plot xaxis yaxis* Render

Finally plot.

20.7 *plot xaxis yaxis* Title

Title on top of the figure.

20.8 *plot xaxis yaxis* Xrange

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

20.9 *plot xaxis yaxis* Xtext

Text on the horisontal axis

20.10 *plot xaxis yaxis* Yrange

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

20.11 *plot xaxis yaxis* Ytext

Text on the vertical axis

21 Quit

Terminate the OC software in English, have a nice day.

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 (DIRECT) file.

22.2 *read* Quit

You did not really want to read anything.

22.3 *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.

22.4 *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* TDB

Saves current set of model parameters and functions on a file in TDB format. Same as the command **list data tdb**.

23.4 *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. Note that most of them are set automatically by the software and changing them with this command may not have the expected effect. The bits 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

Use the SET STATUS PHASE command to set the status of several phases. 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.

40

- 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 are assigned weight one by default. The weight 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 component as pure.

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 elements, constituents, species or phases can be changed. Only phases are 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 with a name for which the abbreviation fits.

26 Step

Requires that a single axis is set. If a second step command is given you have the choice of deleting or keeping the previous results.

26.1 *step* Conditional

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. The exact axis value for any phase changes is calculated.

26.3 *step* Quit

You did not want to *step*.

26.4 *step* Separate

Calculates each phase separately. It calculates equilibria for each phase separately. It can be used to calculate Gibbs energy curves.

27 Summary

That's all and I hope enough (when all is implemented). Have fun and report all errors or problems providing a macro file and the necessary data.

References

[07Luk] H L Lukas, S G Fries and B Sundman, Computational Thermodynamics, Cambridge Univ Press 2007.