

# Summary of features in OC version 3 including parallelization, assessments and some other stuff

Bo Sundman December 21, 2015

## 1 Background

The Open Calphad (OC) initiative started in 2010 when a group of scientists decided that there was a need of a high quality open source software to gain wider acceptance of computational thermodynamics (CT) as a useful tool in materials science. The use of thermodynamic calculations in many applications is severely restricted by the cost as well as the hardware and software limitations imposed by most proprietary thermodynamic software. Providing a free software would simplify such implementations and open a much larger market also for the high quality databases provided by the commercial vendors.

Another aim was to support the scientific interest in new thermodynamic models and improved algorithms for multicomponent thermodynamic calculations and a better software for thermodynamic assessments as described in the book by Lukas et al.[07Luk]. At present such developments can only be done by scientists who are affiliated to the commercial software companies.

The last version of the OC software is available on [<http://www.opencalphad.org>].

The last development version, less stable, is available on a repository called opencalphad at [<http://github.com>].

The OC software in its present state is mainly of interest for researchers, scientists and students with programming skills. It does not have any professional installation procedure and requires understanding of compilation and linking of software. It may be as stable as the commercial software in a few years time and it can be used for teaching computational thermodynamics and development of software using CT. There are two papers describing OC [15Sun1, 15Sun2].

This summary includes also the essential parts of the features of the previous versions.

## 2 Dependencies

To install OC a compiler for Fortran 95/08 like GNU gfortran 4.8 or later is required. For graphics the GNUPLOT software must be installed. For numerics the LAPACK/BLAS libraries are recommended but not necessary. If you need help to handle such things please

ask a local guru, the OC team provide this software for free and have no funding and cannot help with this.

### 3 Structure of the OC software

The software is divided into packages. There are well defined software interfaces between the packages that makes it possible to extend and change them independently.

- The General Thermodynamic Package. (GTP) which has data structures for storing model parameters, conditions and calculated results and code to calculate the Gibbs energy and its first and second derivatives of phase when the  $T$ ,  $P$  and constitution of the phase is known.

GTP includes also a number of general utility facilities needed by the other packages:

- The TP function package for storing and calculating functions that depend on  $T$  and  $P$ , including first and second derivatives.
  - The METLIB utility package mainly for use by the interactive user interface. Originally written in Fortran 77 and modified to the new Fortran standard but it includes features that are depreciated like ENTRY.
  - The command line user interface with a VAX/VMS flavour is part of the METLIB package.
  - The numlib routines for inverting a matrix and solving a system of linear equations. Currently very old and stable but rather inefficient routines are used. There is a LAPACK/BLAS version available.
- The HMS minimizer implementing the algorithm by Hillert[81Hil] for finding the equilibrium state in a multicomponent system for many different kinds of external conditions. It makes use of GTP for calculating the Gibbs energy and derivatives for each phase.
  - The step/map/plot (SMP) package for calculating and plotting diagrams. It uses HMS for calculating equilibria for conditions varying along the axis and the free software GNUPLOT for plotting on various devices.
  - A simple command line user interface with VAX/VMMS flavour. It provides macro facilities.
  - The OC-TQ software interface to integrate OC in general application software for various simulations. This has now been equipped with an iso-C binding which makes the data structures defined in the Fortran package available to programs in C++, java, phyton and other software langauges.

- There are no databases provided with OC except for the examples. To obtain high quality databases please contact a commercial vendor.

## 4 Features in version 1

The version 1 release of OC in 2013 could calculate multicomponent equilibria using Hillert's algorithm[81Hil] for models based on the Compound Energy Formalism (CEF)[01Hil, 07Luk]. It included a possibility to read unencrypted TDB files and a simple command interface with macro facilities to set conditions, calculate equilibria and list results. It had a grid minimizer to ensure finding the global minimum and detect miscibility gaps. There was also a limited application software interface called OC-TQ.

## 5 Features in version 2

The most important new facilities added was generating property and phase diagrams. However, these and many of the other features are still incomplete and fragile and may not work properly in some cases. Feedback from users (providing the data and a macro file reproducing the problem) is the best way to obtain a more stable and error free software.

A documentation of the code, a user guide and additional examples as macro files including graphics was also provided.

## 6 Features in version 3

The main aim of OC version 3 is to provide a stable and accurate calculation of single multicomponent equilibria for a very flexible set of conditions. It also includes parallelization using OpenMP on the equilibrium level and a possibility to assess model parameters.

Other important features like property and phase diagram are available in the same form as in version 2.

The main features and future ideas for OC are summarized below.

1. The thermodynamic models include the Compound Energy Formalism (CEF) with up to 9 sublattices and allowing for molecules, ions and vacancies as constituents. For liquids with strong short range ordering the partially 2 sublattice ionic liquid model (I2SL) is implemented. For a detailed description of these (and other) models see the book [07Luk].
2. The Gibbs energy can be partitioned for phases with long range ordering (sublattices) in an ordered and a substitutional part. The implementation of this for phases with

order/disorder transformations, like A1/L1<sub>2</sub>/L1<sub>0</sub> has been revised and simplified.

3. The thermodynamic data can be entered interactively or read from a database. OC can read most database files following the TDB format defined by the SGTE organisation.
4. The equilibrium calculations follows the algorithm proposed by Hillert [81Hil] and recently explained in more detail by Sundman et al[15Sun2]. It allows a very flexible set of conditions on amounts or fractions of components, chemical potentials or activities, enthalpies, fix phases etc.

It is now possible to set condition on the enthalpy,  $H$  of a system or phase. For mole fractions one can also set an expression as condition like  $x_A^{\text{liquid}} - x_A^{\text{Laves}} = 0$  in order to calculate a congruent melting.

5. To ensure that the global equilibrium is calculated there is an initial grid minimizer described in the paper by Sundman et al[15Sun2]. The grid minimizer can automatically detect miscibility gaps, i.e. that a phase will be stable with two or more composition, called composition sets. It can optionally be turned off to speed up calculations.
6. Parallelization is possible on several levels in OC. For example one can calculate several equilibria with different sets of conditions in parallel using the OpenMP library. This is particularly important when OC is used for simulations, for example in a phase field software as the calculation time is divided by the number of CPU's available.
7. The STEP procedure for property diagram. Such diagrams are calculated with a single axis variable and the user can calculate and plot how various state variables or model properties depend on the axis variable. A primitive version of the step procedure was available also in version 1 but in the new version the exact value of the change of the set of stable phases is calculated.

There is also a “step separate” option for Gibbs energy curves and similar things when each phase is calculated separately along the axis.

8. The MAP procedure for phase diagrams. This calculates lines where the set of stable phases changes for different values of the axis variables. At present only two axis are allowed but in a future release up to 5 axis will be implemented.

As the mapping has some problems to calculate all lines it is possible to execute several map commands and append to the previous results. As an emergency one can remove lines that are wrong by editing the input file to GNUPLOT.

Mapping of binary systems is fairly stable although there are problems at the top of miscibility gaps and crossing congruent transformations. This can usually be handled by several start points.

Mapping of multicomponent system is possible but in general many lines are missing. There is an unresolved problem to exit from certain node points.

The present version of mapping will not discover miscibility gaps. The phase diagram for Cr-Fe looks horrible. Things like that will be taken care of in a future release.

During both MAP and STEP all calculated equilibria are saved and it is possible to plot various properties. All node points are saved as equilibria which can be inspected individually and it is also possible to copy equilibria along a line to a current equilibria and extract values.

The results from a STEP or MAP command can only be saved graphically. It is not possible to save the results on a file for later use but we are working on that. The user should create MACRO files for calculations he would like to repeat.

9. GNUPLOT version 4.6 or later is needed to generate the graphics. In the user interface of OC some additional graphics options, like a title and ranges of the x and y axis, has been added. It is also possible to edit the output files from OC to take advantage of all the graphics facilities of GNUPLOT.
10. The “dot derivative” method to calculate derivatives of state variables has been implemented. This allows calculation of properties like the heat capacity without resorting to numerical derivation. It makes use of the analytical first and second derivatives of the Gibbs energy for  $T, P$  and all constituent fractions implemented in the model package.

The implementation is not complete but derivatives of several state variables with respect to  $T$  are available.

11. For use in application software there is an interface following the TQ standard, OC-TQ. There are some examples to use this interface provided with the software, both for Fortran and C++.

A full Fortran/C++ application software interface including the use of compatible data structures has been implemented using the isoC binding. This means such software can directly access results from an Oc calculation without using calls to subroutines.

In the OC-TQ interface a new method has been introduced to identify phases called “phase tuples”. As many phases may have miscibility gaps and thus be stable with two or more different composition sets the software must have a way to specify this. The phase tuple is a Fortran 95 structure (TYPE) and in version 3 this has 4 integer values, one representing the original phase index, the second the composition set index and the third a link to the internal data structure for the phase. The 4th integer is currently unused. The user interface of OC also use phase tuples when listing phases and composition sets.

When a phase is entered it has one composition set with index 1 and a phase tuple is created with the same index as the phase and the composition set index equal to 1. When a new composition set is entered for a phase, either by the user or by the software itself, for example the grid minimizer, the phase tuple index for the new composition

set will be higher than any of the phases and have as values the phase number and a composition set number 2 or higher.

12. The user can enter several equilibria for the same system and have different conditions in each and calculate them separately and in parallel and transfer data between them. This facility is used also for storing step/map results and is a preparation for the software to assess model parameters from experimental data. Each equilibrium is independent and they be calculated in parallel.
13. The beginnings of an assessment procedure has been implemented is a straightforward least square fit of experimental data to the same data calculated by the model. The experimental data can be entered as equilibria (using the feature described in the previous item). In fact very little had to be done in the OC software for this purpose as we use as a free optimizing subroutine called LMDIF from the MINPACK software developed at Argonne National Lab 1980.

In OC some subroutines were added to allow this least square routine to change model parameters in the GTP package and to calculate the difference between the experimental data provided by the user and the same property calculated from the models of the phases. We would also like to develop additional statistical analysis of the results like estimating uncertainties using the assessment results for extrapolations.

A number of new commands had to be added for the user to set up and control the assessment process, these are described in section 9.

14. OC has a flexible way to handle properties like mobilities, elastic constants etc that may depend on the phase,  $T, P$  and the phase constitution. Some properties are predefined but a skilled programmer can easily add a specific property and a model to use it in a calculation. The values of such properties can be obtained interactively or by application software in the same way as thermodynamic state variables.
15. Minor things
  - The user can select the reference state of the elements for the thermodynamic properties. This should be done before the equilibrium calculation.
  - Reading TDB files is now less strict and it is possible to specify the elements to be selected from the database. With some editing of the TDB file it is also possible to read data for ordered phases modelled with the Thermo-Calc partitioned method.
  - It is possible to write parameter files in a TDB format but it may require editing to be read by other software.
  - Composition sets created automatically by the grid minimizer are normally be removed if they are not needed after the full equilibrium has been calculated.  
If the user has created composition sets for phases that may appear with specific constitutions, like the cubic MC carbide as a composition set of the FCC phase, the OC software will try to assign the correct composition to the appropriate composition set.

- Phases with order/disorder transformations like FCC ( $L1_2$  and  $L1_0$ ) modelled with 4 sublattices can have an “FCC\_PERMUTATION” bit set to simplify entering the parameters. With this bit set the user needs to enter each unique parameter only once, not all the permutations. All kinds of interaction parameters can be entered up to second order. For the BCC ordering permutations are more complicated and has not yet been implemented.

## 6.1 Known bugs and problems and missing features

Some things are problematic and from the long list of things we wanted to implement but did not manage this time, these are a few:

- Redefinition of the components to other species than the elements is still not possible.
- Some state variables like  $V$  cannot be used for conditions.
- Expressions as conditions are implemented only for mole fractions.
- There is a problem with the STEP procedure in a binary system using a composition as axis. The STEP will stop at a phase boundary and it does not take into account that nothing changes in a two-phase region except the amount of the phases.
- Ternary isothermal sections cannot be calculated.
- The corrected quasichemical model for liquids is not yet implemented.
- There is no check on miscibility gaps during a step or map command.
- Saving results from step and map on a file is not possible except graphically with GNUPLOT.
- The mapping is very fragile, lines are frequently missing or incomplete.
- Conditions are not restored after finished step/map.
- There is no plot of tie-lines.
- The Scheil-Gulliver solidification model is not implemented in OC but there is an application software provided written in C++ that can do this.
- The data structure is still volatile and likely to be changed in the next release.
- The application software interface (OC-TQ) will certainly be revised in the next release.

As OC is open source anyone who is interested to implement a particular feature is welcome to start working on it.

## 7 Long term goals for the OC software

Several of the long term software goals with the OC initiative has now been reached

- A model package open for the implementation of new models.
- A stable minimizer calculating equilibria for a flexible set of conditions.
- Calculation of property and phase diagrams with graphics output.
- An assessment package for fitting model parameters.
- A software interface to different applications.

All of this in an open software free for non-commercial applications. But there are still many bugs and features missing or not fully implemented.

The aim of OC is to open a rich field for testing new thermodynamic models and applications for anyone interested. It will also be interesting to implement other minimizers and optimizers and to improve the graphics.

## 8 Short description of all commands

See the ochelp3 file for additional documentation. There is also a description of the procedure and commands needed to perform an assessments in section 9

### 8.1 All top level commands

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

One restriction I have applied to commands and subcommands is that one should not need to type more than 3 characters to have a unique abbreviation.

Directly after the top level command the user can give some options preceeded by a slash like /output=filename or /append=filename. The output that would normally appear on the screen will instead be listed on this file with extention DAT. The output option will delete any previous content on the file but the append will add the new output at the end of the file. The output is reset to the screen after the command.

A frequent Thermo-Calc user must disable his tendency to put hyphens or underscore characters between the command and subcommand.



## 8.2 Commands without subcommands

- ABOUT the software
- BACK to calling software (or exit) after confirmation
- EXIT, terminate the software (in Swedish) after confirmation
- FIN, terminate the software (in French) without confirmation
- HELP gives explanations about a (few) commands from the user guide
- HPCALC starts the inverse polish calculator
- INFORMATION is not implemented yet
- MACRO asks for name of macro file and executes it. A macro file can call another macro five levels deep.
- MAP a phase diagram with 2 or more independent axis.  
If the user already given a MAP command he is asked if he wants to keep the previous results.
- NEW asks for confirmation and if so removes all data.
- OPTIMIZE asks for the maximum number of iterations and then use a least square routine to obtain the best fit to experimental data by varying the set of model parameters specified by the user.
- QUIT terminates the software (in English) after confirmation

## 8.3 Commands with subcommands

Many subcommands are not implemented, I have indicated some but not all.

- AMEND should change something already entered or set. But sometimes it creates something so one should be careful if it should be an ENTER or SET command.
  - ALL\_OPTIM\_COEFF means you can rescale or recover previous set of the optimizing coefficients.
  - BIBLIOGRAPHY asks for a bibliographic id and amends its text.
  - COMPONENTS changes the set of components (not implemented).
  - CONSTITUTION asks for a phase and the user can amend the amount and current constitution of a phase. I have put this here and not as part of AMEND PHASE to avoid confusion with adding a composition set.

- CP\_MODEL not implemented and probably redundant.
- ELEMENT amends data for an element (not implemented).
- EQUILIBRIUM is not implemented yet and probably redundant.
- GENERAL can name of current equilibrium, the user can specify if he is a beginner (the software can provide more help (not implemented)), or expert, if global gridminimizer should be used and if it can merge composition sets, if composition sets can be created automatically and if redundant composition set can be deleted after an equilibrium calculation. The latter questions are mainly interesting for debugging.
- PARAMETER amends a parameter expression for a phase (not implemented, use ENTER PARAMETER to change it).
- PHASE (default) asks for phase name and amends data for this phase like:
  - \* COMPOSITION\_SET (default) adds or deletes a composition set. Composition sets are needed for miscibility gaps when a phase can be stable with two or more compositions. A composition set can be identified with a hash symbol “#” followed by a number or by a user specified prefix or suffix. Deleting a set will always be the one with the highest number. When adding a set the user can provide a prefix and suffix and the default constitution for this set.
  - \* MAGNETIC\_CONTRIB adds an Inden-Hillert magnetic model.
  - \* DISORDERED\_FRACS adds a disordered fraction set for an ordered phase. This replaces AMEND ... DISORDERED\_PART in Thermo-Calc.
  - \* GLAS\_TRANSITION adds a glas transition model (not implemented).
  - \* QUIT You did not want to amend anything for the phase
  - \* DEFAULT\_CONSTIT amends the default constitution for a composition set of the phase. Same as SET PHASE “name” DEFAULT\_CONSTITU.
  - \* DEBYE\_CP\_MODEL adds a Debye Cp model (not implemented).
  - \* EINSTEIN\_CP\_MDL adds a Einstein Cp model (not implemented).
  - \* INDEN\_WEI\_MAGMOD adds a magnetic model according to Wei (not implemented).
  - \* ELASTIC\_MODEL\_A adds an elastic model (not implemented). Note the LIST MODEL\_PARAM\_ID how to enter  $T$ ,  $P$  and composition dependent elastic constants and lattice parameters.
- QUIT you did not want to amend anything.
- SPECIES amends data for a species (not implemented).
- SYMBOL the user can specify if the symbol can only be calculated when explicitly named (usually all symbols are evaluated when any symbol is evaluated as they can depend on each other). This is needed for symbols used as conditions. The user can also specify that a symbol should be local to a specific equilibrium. In

this way one can store the value of a symbol from one equilibrium and calculate differences with respect to other equilibria.

- TPFUN\_SYMBOL amends a TPfun expression.

- CALCULATE various things like:

- ALLEQUILIBRIA all equilibria within the range set for experimental equilibria with non-zero weight are calculated. This is useful for testing if there are any problems before optimizing.

If you are running the version compiled with OpenMP the equilibria will be calculated in parallel. Additional experimental or other symbols and properties can be calculated.

- EQUILIBRIUM (default) is the normal equilibrium calculation command which first calls the grid minimizer (if the conditions allow) and then the iterative minimizer.
- GLOBAL\_GRIDMIN Only the grid minimizer is called to find the gridpoints that represent the lowest Gibbs energy. These are normally used by the iterative minimizer to find the real equilibrium. If followed by COMPUTE NO\_GRIDMIN one will have the same result as COMPUTE EQUILIBRIUM.
- NO\_GLOBAL calculates the equilibrium for the current set of conditions starting from the current set of stable phases and their constitutions. No grid minimizer called.
- PHASE ask for phase name, amount and constitution and at current  $T$  and  $P$  calculates either:
  - \* ONLY\_G Gibbs energy and first and second derivatives with respect to  $T$  and  $P$ .
  - \* G\_AND\_DGDY calculates also all first derivatives with respect to the phase constituents.
  - \* ALL\_DERIVATIVES Also all second derivatives with respect to the phase constituents.
  - \* CONSTITUTION\_ADJUST will calculate  $G$  and all derivatives after adjusting the constitution of the phase to have the minimum Gibbs energy for the same overall composition as the original constitution. It is only interesting when one or more components are parts of several constituents (not implemented).
- QUIT if you did not really want to calculate anything.
- SYMBOL Calculate the value of one or all symbols at the current equilibrium.
- TPFUN\_SYMBOLS all TP functions values and their first and second derivatives with respect to  $T$  and  $P$  (6 values).

- TRANSITION asks for a phase to be stable with zero amount and a condition to be released to calculate the equilibrium. The phase must not have the FIX status. After the calculation the phase is set to be entered and the released condition set to the calculated value. If calculation fails the status is not reset (sorry I have not had time to do all). No grid minimizer called.
- DEBUG Nothing of this works
  - FREE\_LISTS
  - STOP\_ON\_ERROR
  - ELASTICITY
- DELETE Only composition sets and equilibria can be deleted. To delete a parameter you can amend its expression to be zero.
  - PHASE (default) but not allowed
  - ELEMENTS not allowed
  - SPECIES not allowed
  - QUIT you did not want to delete anything
  - COMPOSITION\_SET The highest set is deleted (one cannot delete the first). Must be used with great care.
  - EQUILIBRIUM must be used with great care.
- ENTER is the main command to enter data interactively. Note that in most cases data are read from a TDB file.
  - BIBLIOGRAPHY enter a bibliographic reference id and text.
  - COMMENT enter a text that is saved and listed with the equilibrium.
  - CONSTITUTION to enter the constitution of a phase (same as AMEND CONSTITUTION).
  - COPY\_OF\_EQUILIB the current equilibrium is copied to a new one with a name specified by the user.
  - ELEMENT an element with data.
  - EQUILIBRIUM an equilibrium record with the specified name is created. Each equilibrium record has an independent set of conditions. Will be used for assessments and is already used to store node points during step and map.
  - EXPERIMENT data for assessments. These are a state variable of symbol followed by an equal sign, =, larger than, >, or lesser than, <, and a value and uncertainty separated by a colon. For example:  
 experiment t<sub>l</sub>1200:1 x(liq,mo)=.2:.01 hm(fcc)=-30000

- MANY\_EQUILIBRIA allows the user to enter a table with conditions for many equilibria with similar conditions. It is intended for assessments but can be used also to calculate various properties that for a range of conditions not suitable for a STEP calculation. The user must give a general “head” of the table specifying phase status and all conditions including some that are different in the different equilibria. For those familiar with Thermo-Calc it replaces the POP file in assessments but is more flexible.
  - \* This command will first ask Table head::  
and the user must specify conditions and other things for the table. The user can refer to values (or text) in the table by giving an “@” character followed by a digit. In the examples below user input is **in bold**.  
By default all phases are suspended for the equilibria so the user must specify the phases that should not be suspended.  
Table head:: **entered 0** \* *all phases should be entered*  
Table head:: **fix 0 liquid** *liquid should be fix with 0 moles*  
Table head:: **fix 1 @2** *the phase in column 2 should be fix with 1 moles*
  - \* The conditions can be given using the @ character to indicate values that are given in the specified column in table to follow.  
Table head:: **condition t=@1 p=1e5 n=1 w(cr)=@3 w(mo)=@4**
  - \* Optional calculations of entered symbols  
Table head: **calculate cp**
  - \* Optional listing of state variables  
Table head: **list HM tc(bcc)**
  - \* Optional experimental data  
Table head: **experiment x(liquid,cr)=0.12:.01, x(bcc,cr)=0.28:.02**
  - \* Optional comment  
Table head: **comment experimental data from Kubaschewski 1955**
  - \* The table head is finished by an empty line or “table\_start”
  - \* For the rows in the table the user must first provide a unique name for each equilibrium (that is counted as column 0 (zero)) and values for all columns referred to in the table head.  
Table row:**EQ1 1573 BCC 0.3 0.05**
  - \* The table is finished by  
Table row:**table\_end**
- OPTIMIZE\_COEFF the coefficients for use in assessments are entered. They have the symbols A00 to A99. If the user wants fewer than 100 coefficients he can specify a number.
- PARAMETER the expression of a parameter of a phase. The phase, the constituent array and degree must be specified.
- PHASE a phase with sublattices, site ratios and constituents. The parameters are entered individually with ENTER PARAMETER.

- QUIT you did not want to enter anything.
  - SPECIES a species with name and stoichiometry. Its name must be unique but one can have several with the same stoichiometry.
  - SYMBOL (default) name and expression of a state variable function.
  - TPFUN\_SYMBOL The name and expression of a function of  $T$  and  $P$  that can be used in parameters.
- LIST of many things ...

Note the possibility to direct output to a file using /output=filename or /append=filename directly after the command, as mentioned in the beginning.

- AXIS lists current axis set by the user.
- BIBLIOGRAPHY lists bibliographic text for specific id or all.
- CONDITIONS lists all conditions in current equilibrium.
- DATA lists all parameters on different devices and ways:
  - \* SCREEN (default) Writes all parameters for all phases on the screen including the bibliographic information.
  - \* TDB Writes all parameters on file in TDB format.
  - \* MACRO Writes all parameters on file as a macro file (not implemented).
  - \* LATEX Writes all parameters on file as a LaTeX file (not implemented).
- EQUILIBRIA lists all entered equilibria with name and number (not the results).
- LINE\_EQUILIBRIA lists all equilibria stored during STEP or MAP. With the SET ADVANCED command one can copy one of these to the current equilibrium.
- MODEL\_PARAM\_ID lists all implemented model parameter identifiers like  $G$ ,  $TC$ ,  $BMAGN$ , elastic constants etc. that can depend on  $T$ ,  $P$  and constitution of a phase. The use of such parameters require implementation of the model in the software.
- OPTIMIZATION the result of an optimization is listed.
- PARAMETER lists the expression for a single parameter.
- PHASE asks for phase name and then lists for option
  - \* CONSTITUTION (DEFAULT) lists constitution for this phase.
  - \* DATA lists parameter for this phase (no bibliography).
  - \* MODEL lists some model information for this phase.
- QUIT You do not want to list anything.
- RESULTS (default) from an equilibrium calculation. the program asks for a number how to format the phase information.
  1. stable phases and composition in mole fractions in value order

2. stable phases and composition in mole fractions and constitution in value order
3. stable phases and composition in mole fractions and constitution in alphabetical order.
4. stable phases and composition in mass fractions in value order
5. stable phases and composition in mass fractions and alphabetical order.
6. stable phases and composition in mass fractions and constitution in value order
7. all phases and composition in mass fractions in value order
8. all phases and composition in mole fractions and constitutions in alphabetical order
9. means all phases and composition in mole fractions and constitution value order

The conditions are listed first, then some global properties, then some data for each component and then the stable phases with amount and composition.

– SHORT

- \* A writes one line for all elements, species and phases.
- \* P writes one line for all phases sorted with stable first, then max 10 entered phases in decreasing stability, finally the dormant in decreasing stability.

- STATE\_VARIABLES asks for state variable symbol and lists its value. Can also be used for the current value of model parameters as Curie temperature, TC(BCC), MQ&FE(FCC), etc.

**I will try to merge list state\_variables and compute symbol to a SHOW command**

- SYMBOLS lists all entered state variable symbols (same in all equilibria).
- TPFUN\_SYMBOLS lists one or all TP function symbols and expressions (same in all equilibria).

- PLOT asks for state variables or symbols for x and y axis and after that the user can plot directly or change anything in the submenu below.

OC generates a command file for GNUPLOT and a data file with the values to plot and then executes this in a separate shell. The user can edit the command file to add options and execute it again inside gnuplot. But beware not to overwrite the files you want to edit. There are 10 colors for the lines to plot. If more than 10 lines to plot the colors are repeated cyclically.

OC keeps the previous values set of all options set (except the scaling of an axis with a new variable and the output file which is always reset to the default “ocgnu”) unless changed explicitly.

I have no idea how to overlay a calculated result with for example experimental data. Hopefully some GNUPLOT expert will tell me how to do that.

- RENDER (default) finally plot when all options set.
- X RANGE set plot range on x axis.
- Y RANGE set plot range on y axis.
- X TEXT set text on x axis.
- Y TEXT set text on y axis.
- TITLE set title of plot.
- POSITION\_OF\_KEYS select position of the labels (identification) of the lines in the plot. The labels can be placed inside/outside of the plot, to the left/center/right and top/bottom. See the explanation of “set key” in GNUPLOT.
- GRAPHICS\_FORMAT set type of terminal (P for postscript, G for gif). You will also be asked for output file.
- OUTPUT\_FILE set name of plot file (default is ocgnu.dat).
- GIBBS\_TRIANGLE set diagram to be a Gibbs triangle (not implemented).
- QUIT you do not want to plot.

**More options will be added when I understand GNUPLOT better**

- READ At present only TDB is implemented.
  - TDB (default) an unencrypted TDB file can be read. Many TYPE\_DEFS are not handled correctly and warning are given. For partitioned phases you may have to edit the parameters. The user can select which elements he wants to read.
  - UNFORMATTED an unformatted file with model parameters and results for a single equilibrium calculation. It was implemented in version 2 but due to changes in the data structure it does not work any longer.
  - QUIT you did not want to read anything.
  - DIRECT will save results from STEP and MAP on a random access file (not implemented).
- SAVE This is not yet implemented.
  - UNFORMATTED (default) A file is written with unformatted data for all thermodynamic data and conditions and results for a single equilibrium. There is no guarantee an unformatted file will be readable in a later version of OC.
  - DIRECT not implemented yet (intended for STEP and MAP results).
  - QUIT do not save anything.
- SELECT a few things.
  - EQUILIBRIUM (default) change the current equilibrium to the selected one (number or name or next or previous).



- MINIMIZER there is only one.
- OPTIMIZER there is only one.
- GRAPHICS there is only one.
- LANGUAGE there is only one (English).
- SET can be used for many things. The most important is conditions.
  - ADVANCED This is a command for very special things.
    - \* DENSE\_GRID\_ONOFF toggles the gridminimizer to use denser grid or normal. A dense grid is better to ensure the global equilibrium is found but will also take longer to calculate. About 10 times more gridpoints are calculated compared to the normal grid.
    - \* EQUILIB\_TRANSF transfer an equilibrium calculated along a line in STEP or MAP to the current equilibrium.  
*this is probably the most awkward command of all. But I do not want to have a TRANSFER or COPY command on the top level as that will certainly be misunderstood and misused*
    - \* QUIT you did not want to set anything advanced.
  - AS\_START\_EQUILIB use current equilibrium as start for step or map. Not necessary if there is only one start equilibrium.
  - AXIS axis “number” to an independent variable (must be a condition).
  - BIT some global bits can be toggled. Most of them are set or reset automatically by the software or by other commands.
    - \* 0 user is a beginner (set by default)
    - \* 1 user is experienced
    - \* 2 user is an expert
    - \* 3 gridminimizer must not be used
    - \* 4 gridminimizer must not merge comp.sets. (set by default)
    - \* 5 there are no data (cleread automatically)
    - \* 6 there are no phases (cleared automatically)
    - \* 7 comp.sets must not be created automatically
    - \* 8 comp.sets must not be deleted automatically
    - \* 9 data has changed since last save (set automatically)
    - \* 10 means verbose is on (not implemented)
    - \* 11 means verbose is permanently on (not implemented)
    - \* 12 means be silent (supress warnings)
    - \* 13 no cleanup after an equilibrium calculation
    - \* 14 use denser grid in grid minimizer (see also ADVANCED)

- \* 15 calculations in parallel is not allowed
- CONDITION (default) the state variable and value of a condition. Only single values are allowed, expressions not yet implemented.
- ECHO echo of the input from macro files on the screen. There is no way to turn off echo.
- FIXED\_COEFF to set an optimizing coefficient to a fixed value.
- GRAPHICS\_OUTPUT Not implemented (see PLOT command).
- INPUT\_AMOUNTS amount of species. These will be added together and used for conditions of the components.
- INTERACTIVE at the end of macro files.
- LEVEL I am not sure what this was intended for.
- LOG\_FILE the name of a file with a copy of all input and defaults. Useful for documenting errors!
- NUMERIC\_OPTIONS maximum number of iterations (default 500) and convergence limit (default  $10^{-6}$ ).
- OPTIMIZING\_COND depending on the optimizer used for assessment some conditions can be set.
- PHASE the user must specify a phase name and can then ...
  - \* STATUS (default) the status of a single phase, or all using an asterisk “\*”, can be set. See also SET STATUS PHASE with a more flexible way to specify phases.
  - \* DEFAULT\_CONSTITU the default constitution of the phase can be set. Same as AMEND PHASE name DEFAULT\_CONSTITU.
  - \* AMOUNT the amount of the phase (redundant).
  - \* QUIT nothing is set for the phase.
  - \* BITS some special bits for a phase can be set. At present there is no way to “UNSET” these bits ... so be careful. Most of these are set automatically by the software.
    - QUIT (default) no bit is changed.
    - FCC\_PERMUTATIONS to indicate 4 sublattice fcc or hcp permutations. Only one parameter stored for each unique permutation. Must be set before any parameters are entered.
    - BCC\_PERMUTATIONS to indicate 4 sublattice bcc permutations. Must be set before any parameters are entered (when implemented).
    - IONIC\_LIQUID\_MDL to indicate ionic liquid model. A phase with the ionic liquid model that is entered interactively must currently have the name ionic\_liquid and this bit is automatically set. If read from a TDB file the :Y after the phase name assigns this model. Setting this bit interactively has no function at present.

- AQUEOUS\_MODEL to indicate aqueous model (not implemented).
- QUASICHEMICAL to indicate quasichemical model (not implemented).
- FCC\_CVM\_TETRADRN to indicate CVM fcc tetrahedon model (not implemented).
- FACT\_QUASICHEMCL to indicate FACT quasichemical model (not implemented).
- NO\_AUTO\_COMP\_SET to prevent automatic creations of composition sets for this phase. One can forbid creating automatic composition sets (by the grid minimizer) for all phases with the AMEND GENERAL command.
- \* QUIT nothing is set.
- \* RANGE\_EXP\_EQUIL the first and last equilibrium included in an assessment or a CALCULATE ALL command must be specified.
- \* REFERENCE\_STATE the reference state of a component. The phase,  $T$  and  $P$  must be specified. The phase must exist with the component as its only component. When the phase can exist with the component in different ways, like O in a gas can be O, O<sub>2</sub> or O<sub>3</sub> the most molecule at current  $T$  is selected.
- \* SCALED\_COEFF can be used to set a coefficient to be optimized with a specified scaling factor and possibly a min and max value.
- \* STATUS
  - PHASE (default) one or more phases can be set as suspended, dormant, entered or fixed. You can use \* to mean all phases, \*S for all suspended, \*D for all dormant and \*E for all entered and \*U for all entered and unstable. The list of phases is terminated by an equal sign “=” or an empty line.  
If the new status is not already given after the equal sign it is asked for.  
If the new status is entered or fixed the amount is asked for.
  - ELEMENT an element can be entered or suspended.
  - SPECIES a species can be entered or suspended.
  - CONSTITUENT not implemented.
- UNITS like energy Joule/cal or mass kg/lb ... but not implemented yet.
- VARIABLE\_COEFF an optimizing parameter is specified.
- VERBOSE the software will write extra output. Not implemented
- WEIGHT to be used for assessments.
- STEP is used to calculate along a single independent axis variable.
  - NORMAL follow the axis variable from low to high limit.
  - SEPARATE calculate each phase separately.
  - QUIT do nothing.

- `CONDITIONAL` follow the axis variable and update `s` symbol after each step (to be used for Scheil-Gulliver simulations, not yet implemented).

## 9 The assessments procedure in OC

The normal procedure for an assessment would roughly be performed in the following steps.

1. On a macro file file you have the commands to:
  - `ENTER` elements, species, phases etc. from a macro file.
  - `ENTER OPT` to enter the coefficients to be optimized, A00 to A99.
  - `ENTER PARAMETERS` with coefficients to be optimized using the symbols A00 to A99.
2. on the same or on another macro file you have the experimental data.
  - The data is entered by `ENTER EQUILIBRIUM` or `ENTER MANY EQUILIBRIA` command with each experiment as an equilibrium. In addition to the necessary conditions you use `ENTER EXPERIMENT` to specify the experimental data.
  - With the command `SET RANGE_EXP_EQUIL` you specify the range of equilibria with experimental data.
3. The rest of the assessment is done interactively and the set of commands are used as needed. These must normally be reiterated many many times using different weights of the equilibria and optimizing variables.
  - You `SET VARIABLE_COEFF` to specify a coefficient to be optimized.
  - You `OPTIMIZE` to make a least square fit.
  - You `LIST OPTIMIZATION` to list the current result.
  - You may `SET WEIGHT` on the different equilibria.
  - You may `AMEND ALL_OPTIM_COEFF` to rescale or recover parameters and use many other commands.
4. When you finished you can use `SAVE TDB` or `LIST DATA TDB` to create a TDB file with the results (it will need editing).

### 9.1 Special commands for an assessment

The special commands for performing an assessment is described a little more in detail here. Many of the other commands in OC are also needed.

**ENTER OPTIMIZE\_COEFF** enters up to 100 coefficients to be optimized. They are called A00 to Aij (default A99). This must be done before any assessment. The symbols Aij can be used when entering TP functions or parameters.

**ENTER EQUILIBRIUM “name”** experimental data are related to an equilibrium. This commands enters the necessary data structure to set to conditions for an experiment and to add experimental data.

**ENTER MANY\_EQUILIB** to enter tables of experimental data See this command description above.

**ENTER EXPERIMENT** for each equilibria the experimental state variable, value and uncertainty is added with this command.

**AMEND ALL\_OPTIM\_COEFF** to rescale or recover their values.

**LIST OPTIMIZATION** lists results of the optimization in various ways. Only the SHORT option implemented.

**OPTIMIZE** calls the optimizer to obtain a least square fit of the values calculated from the model parameters to the experimental data.

**SET RANGE\_EXP\_EQUIL “first” “last”** must be given to specify the equilibria with experimental data. They must have been entered sequentially. An AMEND RANGE will be added.

**SET OPTIMIZING\_COND** to set some parameters for the optimizer.

**SET VARIABLE\_COEFF “index” “start value”** set a start value of a coefficient ij to be optimized.

**SET SCALED\_COEFF “index” “start value”** additionally asks for scaling factor, a min and max value for a coefficient. Not yet implemented.

**SET FIXED\_COEFF “index “value”** to set an optimizing coefficient ij to a fixed value (usually its current value)

**SET WEIGHT “value” “range”** assigns a value to the weight (default unity) to equilibria with names fitting the “range”. If the weight is set to zero the experiments from these equilibria will be ignored.

**SELECT EQUILIBRIUM “name/number”** to select an equilibrium to perform some changes.

There is no special “edit” module as in Thermo-Calc for modifying the equilibria with experiments, this can be done using the **select\_equilibrium** command. The first equilibrium (DEFAULT) cannot be used for experimental data. Using **step** and **map** will also create

new equilibria for node points, they may interfere with the experimental equilibria, this has to be tested. I have to implement some nice way to get rid of redundant equilibria, the **delete equilibria** is a bit dangerous. There is no way yet to save results like on a PAR file in Thermo-Calc.

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