New features in the Open Calphad software version 2

Bo Sundman, October 7, 2014

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 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 requirements imposed by the 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 decrsibed 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 current OC software is available on [http://www.opencalphad.org]. For software collaborations there is also 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. In a few years it may be as stable as the commercial software and can be used also for teaching computational thermodynamics.

2 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.

  As this was the first package developed it makes use of a number of general untility packages needed also 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 and adopted to the new Fortran standard.

- The command line user interface with a VAX/VMS flavour.

- 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.

- 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 package for calculating and plotting diagrams. It uses HMS for calculating equilibria for conditions varying along the axis and the free software GNU-PLOT for plotting on various devices.

- The OC-TQ software interface to integrate OC in general application software for various simulations.

3   Features in version 1

The version 1 release of OC in 2013 could calculate multicomponent equilibra 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 has a grid minimizer to ensure finding the global minimum and detect miscibility gaps. There was also a limited application software interface called OC-TQ.

4   New features in version 2

The most important new facilities since version 1 are generating property and phase diagrams. However, these and many of the other features are still fragile and may not work properly for some calculations. 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 compiler for Fortan 95 like GNU gfortran 4.8 or later is required.

A new documentation of the code, a user guide and additional examples as macro files will also be provded.

1. 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.

2. 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 without destroying the previous results. As an emergency removing lines that are wrong it is possible to edit the input file to GNUPLOT.

3. GNUPLOT version 4.6 or later is used for 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.

GNUPLOT does not support triangular diagrams.

4. The ionic two-sublattice liquid model (I2SL) which can handle liquids with and without short range ordering is now implemented.

5. 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 derivatives. 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 finished but derivatives of several state variables with respect to T and P are available.

6. The user can select the reference state of the elements for the thermodynamic properties.

7. The partitioning of the Gibbs energy for phases with order/disorder transformations has been revised and made simpler to use.

8. The grid minimizer for global equilibria has been improved handling phases with ions.

9. An example calling the OC-TQ interface from C/C++ has been made. It is rather clusmy and a better way to transfer data should be found.

10. An UNFORMATTED output to a file of the data and results from a single equilibrium calculation is now possible and the file can be read back with all data. It is still not possible to save the result from a STEP or MAP calculation on a file.

11. The user can enter several equilibria for the same system and have different conditions in each and calculate them separately and transfer data between them. This facility is used for storing step/map results and is a preparation for the software to assess experimental data. Each equilibrium is independent and can be calculated in parallel.

12. 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 interactivly or by application software in the same way as thermodynamic state variables.

13. Reading TDB files is now less strict and it is possible to specify the elements to be selected from the database. With some minor editing it is also possible to read data for ordered phases modelled with the Thermo-Calc partitioned method.

    There is still no output of TDB files from OC. If you enter parameters interactivly and want to keep a copy of these on a text file use the "set log" command in advance.

14. Parallelization has been tested for the grid minimizer and it has been indicated in the code where it can be useful to speed up other parts of the calculations. In particular for the calculation and inverting of the phase matrices at each iteration it should have a significant influence as the calculations of the Gibbs energies and derivatives can be done in parallel for all the phases.

    Mapping of phase diagrams can also be done in parallel for all the lines. For assessments all equilibria representing experimental data can be calculated in parallel.

5 Known bugs and problems and not yet implemented features

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

- Ternary isothermal sections are difficult to calculate and cannot be plotted (even in a square diagram).

- Redefinition of the components to other species than the elements is still not possible.

- Conditions on state variables like V, H etc are not yet implemented.

- Conditions which are expressions are not implemented.

- The corrected quasichemical model for liquids is not implemented.

- There is no check on miscibility gaps during a step or map command.

- The Scheil-Gulliver solidification model is not implemented.

- Saving results from step and map of a file is not possible except graphically.

- The mapping is very fragile, lines are frequently missing or incomplete.

- Composition sets created automatically by the grid minimizer are not removed even if they are not needed.

- conditions not restored after finished step/map.

- one cannot plot tie-lines.

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

6   Long term goals

- A full Fortran/C++ application software interface.

- An assessment module with a lot of help for beginners.

- A teaching package for computational thermodynamics and phase diagrams.

References

[81Hil] M Hillert, Physica, **103B** (1981) 31

[01Hil] M Hillert, J of Alloys and Comp **320** (2001) 161

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

[http://www.opencalphad.org] http://www.opencalphad.org

[http://github.com] opencalphad at http://github.com.

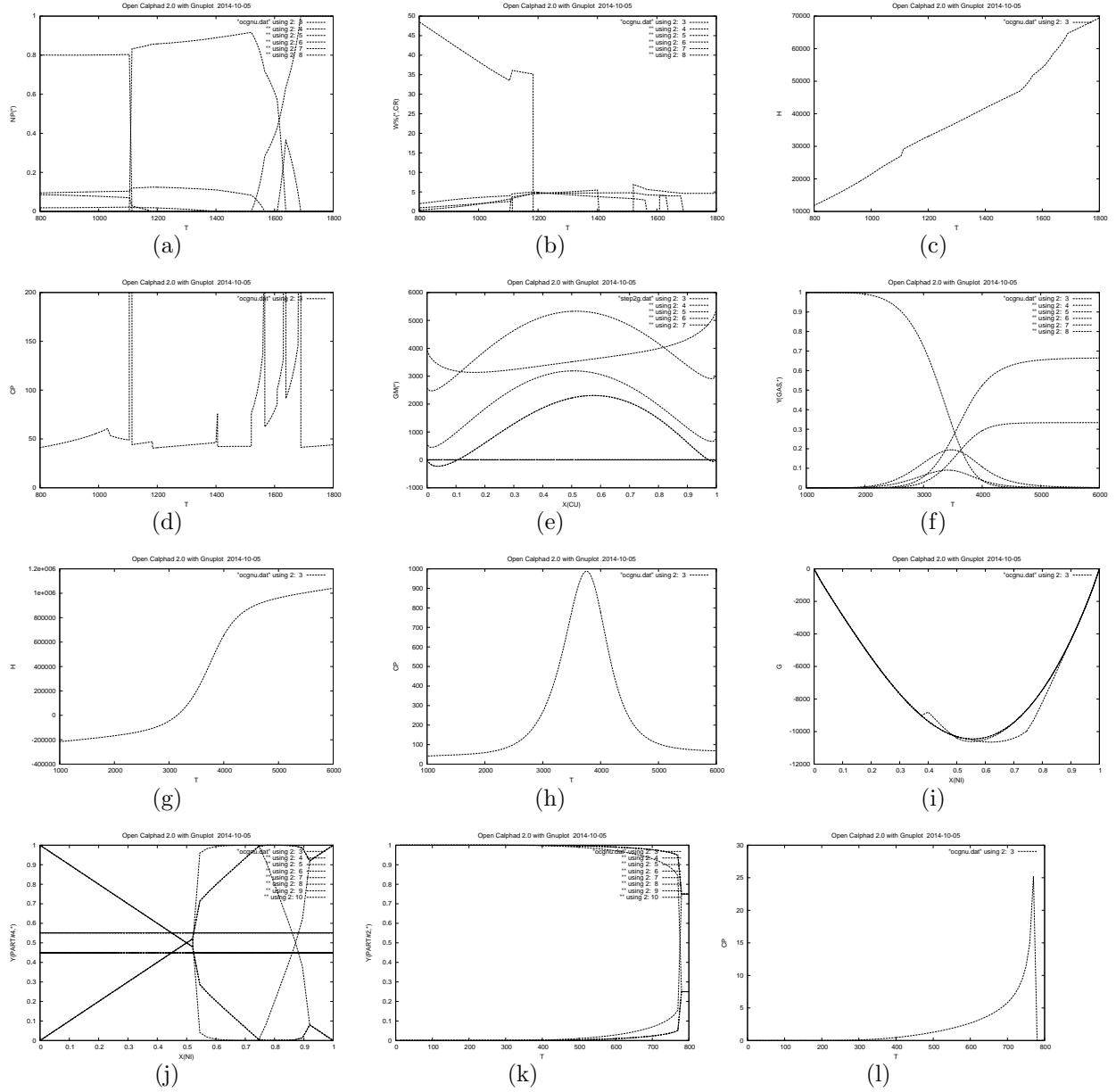# 7 Some diagrams generated with OCv2 macro files

Figure 1: In 1(a) to 1(d) diagrams for a high speed steel generated with macro file step2-agcu. In 1(e) Gibbs energy curves in Ag-Cu generated with macro file step2-agcu. In 1(f) to 1(h) the speciation of a gas with H and O as function of T and its effect on enthalpy and heat capacity generated with macro file step3-hogas. In 1(i) and 1(j) the Gibbs energy curves at 400 K in the Fe-Ni system for the fcc ordering generated with macro file step4-feni. In 1(k) the variation of ordering in FeNi$_3$ as function of T. The constituent fractions and heat capacity variation. Generated with macro file step5-feni.
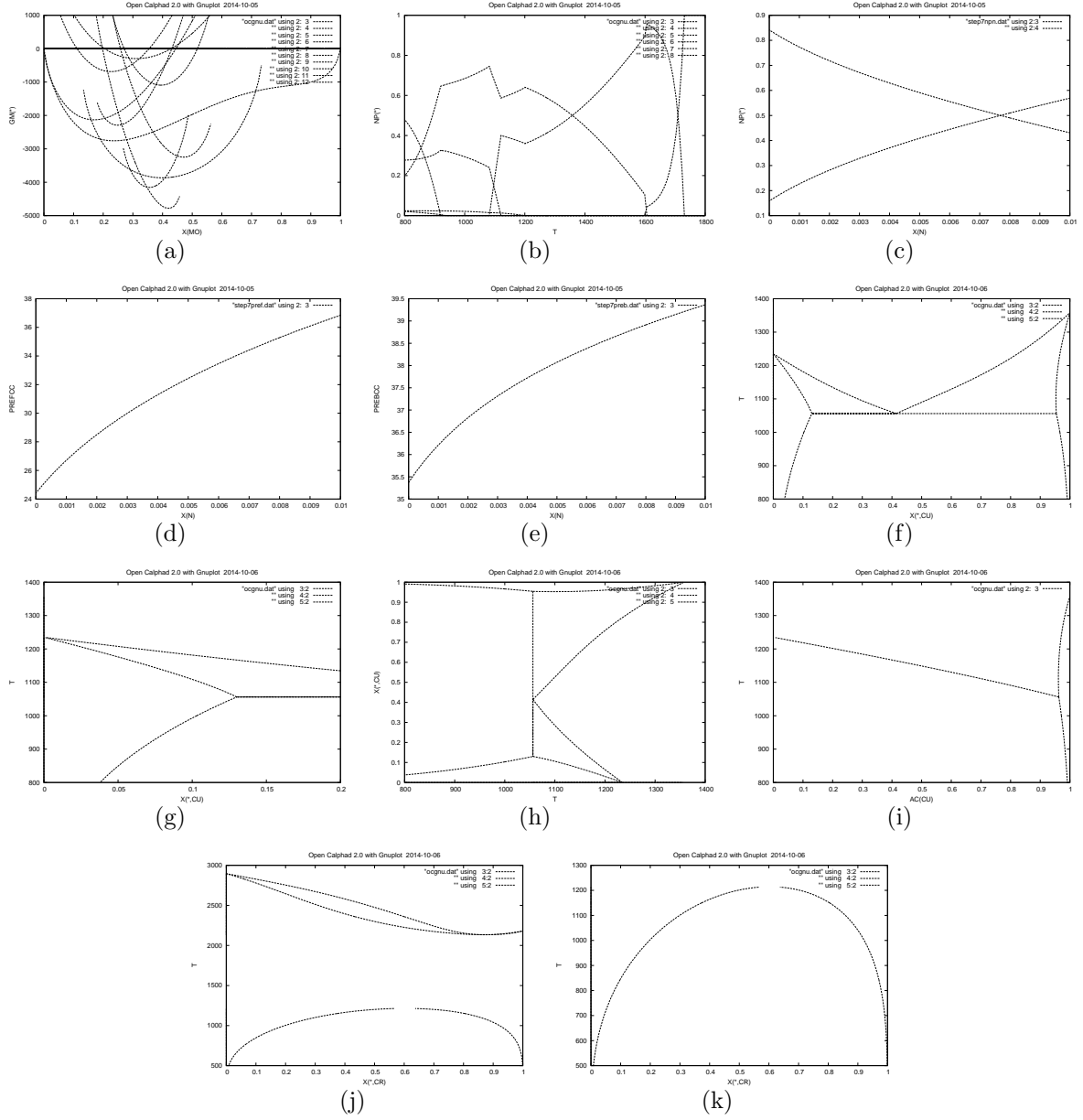
Figure 2: In 2(a) the Gibbs energy curves for the different phases in Fe-Mo at 1400 K, generated with macro file step6-femo. In 2(b) to 2(e) calculated phase amounts as function of T or mass fraction of N and "pitting corrosion equivalents", generated with macro file step7-saf. In 2(f) to 2(i) the phase diagram for the Ag-Cu system generated with macro file map1-agcu. In 2(j) to 2(k) the phase diagram for the Cr-Mo system generated with macro file map2-crmo.
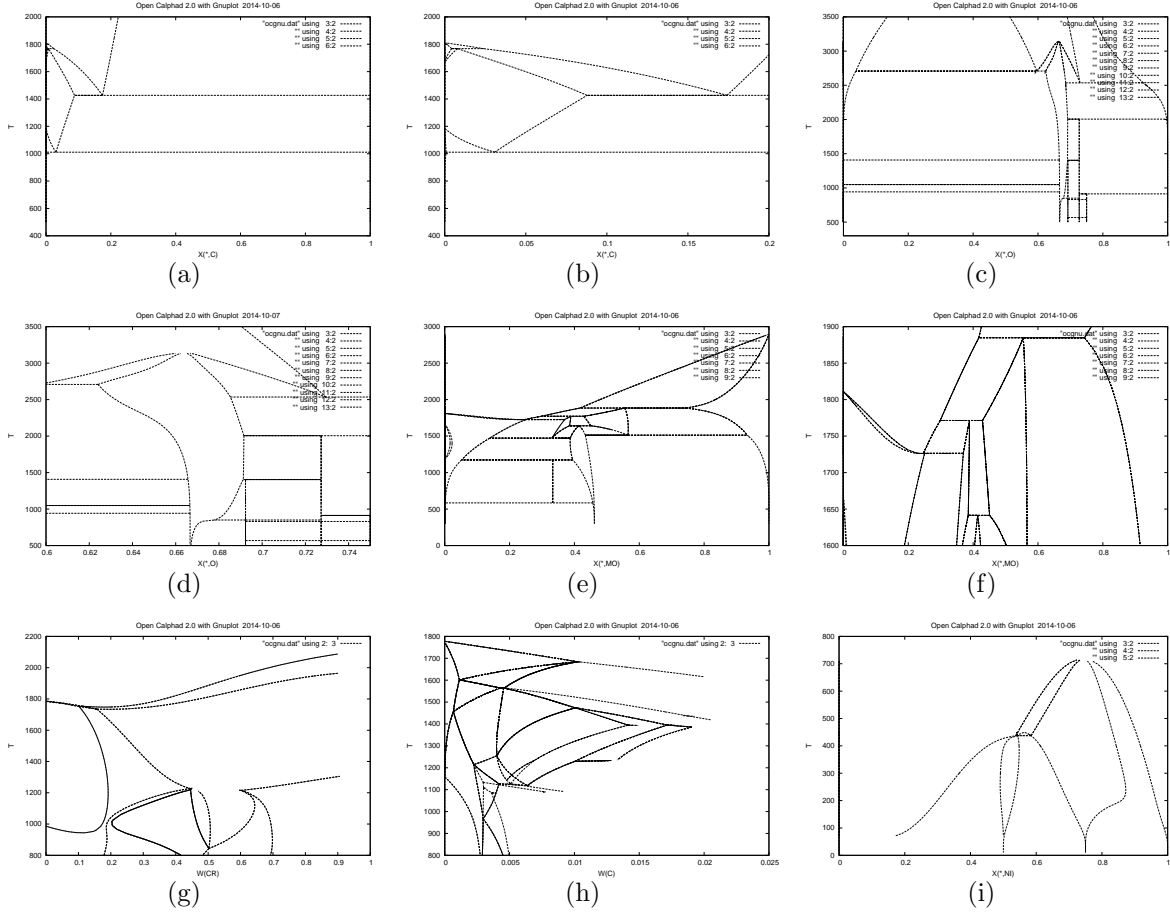
Figure 3: In 3(a) to 3(b) the phase diagram for the C-Fe system generated with macro file map3-cfe. In 3(c) to 3(d) the phase diagram for the O-U system generated with macro file map4-ou. In 3(e) to 3(f) the phase diagram for the Fe-Mo system generated with macro file map5-femo. In 3(g) the isopleth diagram for the Cr-Fe-Ni system at 8 mass%Ni generated with macro file map6-ss. In 3(h) an isopleth calclation for a high speed steel generated with macro file map7-hss. As can be seen there are still problems with mapping. In 3(i) a metastable phase diagram for the ordered fcc phase in Fe-Ni generated with macro file map8-feni.