

## Thermo-Calc Newsletter - Number 24, May 2000

- New Thermo-Calc for Windows - TCW
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### **New Thermo-Calc for Windows - TCW**

Thermo-Calc for Windows is now available with a graphical user interface in order to make it easier to use. The classical Thermo-Calc, TCC, has an extremely high flexibility which gives it great functionality but also makes it quite hard to learn. To be able to remember all commands and get the most out of the program, one has to use it almost every day. This first version of TCW has a somewhat reduced functionality but, on the other hand, really easy to learn. With TCW you can make all calculations an ordinary user needs just by clicking on menus and buttons with the mouse, no commands to memorize!

Classical Thermo-Calc, TCC, is still recommended for very advanced users. Some of the functions not yet implemented in TCW are: Optimization, setting start values, adding composition sets and plotting functions. We are planning to improve the flexibility in the future without reducing the user friendliness and, in the end, we hope to have implemented all the functions of classical Thermo-Calc.

Some comments from one of our beta-testers:

"The new windows version of Thermo-Calc, TCW, simplifies thermodynamic calculations a lot. TCW is easy to use and it's no longer necessary to remember 20-30 commands in order to calculate a diagram.

Features such as easy export of figures to MS Word for reports and an alloy database where the materials you most frequently do calculations on can be stored makes life much easier for less experienced users."

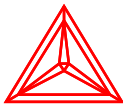
### **New release of DICTRA scheduled**

A new version of DICTRA is planned to be released later this year

### **New license manager**

Until now a signed license has been required to prevent from illegal copying of the Thermo-Calc and DICTRA software. From version N the well known Flexlm licensing software will be used. This means that new licenses do not require any signature but instead, the user must provide TCAB with information about the hardware where the software will be used.

Users with maintenance contracts must also install this license manager when they receive version N. In most cases, this is just a file that is tested by the Thermo-Calc/DICTRA programs. But if you have several installations on different computers, each of them must have a unique file. If you have an installation on a server you must, in addition, install the



Flexlm license manager.

The Flexlm license manager can handle all kinds of hardware, PC windows NT/95/98/2000, Linux, SUN, SGI, IBM etc, but a separate license is required for each hardware.

Upon receipt of the installation CD or tape, there is a program on it that you must run in order to find the unique identification code for your hardware. This identification code must be sent back to TCAB which will provide you with a proper Flexlm license key.

License Option Form. There are several license options available with the Flexlm license manager. An option form showing the different options has been sent out to all maintenance customers. It is essential that all customers complete this form and return to Thermo-Calc Software in order to receive their copy of version N of Thermo-Calc.

### **New databases**

TC-Ni database is a thermodynamic database for Ni-base superalloys. It contains 7 elements: Al, Co, Cr, Ni, Ti, W, Re. The thermodynamics of the  $g$  and  $g'$  phases are modelled with a single Gibbs energy function taking into account the crystallographic relation between these two phases after Ansara et al. All the assessed binary systems constituting this database can be calculated with the BINARY module. The assessed ternary systems included in the database are the following:

Al-Co-Ni, Al-Cr-Ni, Al-Ni-Ti, Al-Ni-W,  
Co-Ni-W, Cr-Ni-Re, Cr-Ni-Ti, Cr-Ni-W,  
Ni-Re-Ti, Ni-Re-W, Ni-Ti-W, Al-Cr-Ti,  
Al-Ti-W.

TC-ER databases are databases for environmental problems associated with metallurgical and chemical processes.

The TCER database for Recycling/Remelting

The database contains the elements

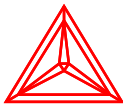
Al, Ar, B, Bi, C, Ca, Cd, Cl, Co, Cr,  
Cu, F, Fe, H, K, Mg, Mn, Mo, N, Na,  
Ni, O, P, Pb, S, Sb, Si, Sn, Ti, Zn

In scrap remelting operations in an electric arc furnace, the resulting gradual increase in the concentration of minority elements in the metal that is of particular importance. Apart from a knowledge of the possible losses of these elements to the gas phase, and/or their transfer to the slag phase, information on the solubilities of minority elements in liquid and solid Fe-rich alloys is needed, since their presence can have deleterious effects on the properties of the steels produced.

The TCER database for Sintering/Incineration/Combustion

The data, which is a subset of the TCER database, contains the elements

Al, As, Br, C, Ca, Cd, Cl, Cr, Cu,  
F, Fe, H, Hg, I, K, Mg, Mn, N, Na,



Ni, O, P, Pb, S, Sb, Si, Sn, Te, Ti, Zn

Iron ore sintering is carried out prior to reduction processes and results in considerable, including toxic, emissions, which require comprehensive filtering operations to avoid transfer of hazardous species to the environment. In the sintering process, the ore is mixed with coke and sintered at temperatures up to 1200 °C.

## **New features in Thermo-Calc version N**

- Flexlm licensing software
- Nested MACRO files
- In Windows, TC and DICTRA can be started by clicking on a file
- In Windows, a Graphical User Interface is available
- TDB error messages and bug fixes in the database module
- Flexible references in the database
- Tetrahedron CVM module with regular solution excess terms
- Quasichemical liquid model implemented
- Flory-Huggins model implemented
- Phase code F saves memory and computation time for 4 sublattice ordering
- Phases which never disorder can have a disordered excess
- SET\_INTERACTIVE in GES
- Limits in POLY increased to 1000 species and 40 components
- COMPUTE\_TRANSITION simplifies calculations of solubility limits
- Shorter output for LIST\_STATUS
- Shorter output during STEP/MAP
- Some bug fixes in PARROT

## **General information**

**Flexlm** The software licensing system Flexlm is now used with Thermo-Calc and DICTRA. This is described above. Each computer that will use TC, DICTRA or the TQ interface must install the Flexlm software. This will prevent unauthorized copying and use.

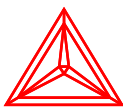
**Macro** Macro can be nested in 5 levels, i.e. a macro can call another macro. If a macro is terminated by a "set-interactive" command it will be resumed at the next command in the previous macro. If it is terminated by end-of-file Thermo-Calc or DICTRA will be aborted.

Macro files can have a pause "@&" but one may prevent stopping at any pause by typing any character (except Y) after the macro file name.

## **Particular for the Windows version**

**Registry** Thermo-Calc and DICTRA now modify the registry when installed. Thus all files with extensions that is recognized by TC and DICTRA, like \*.POLY, \*.TCM, \*.TDB etc can now start the appropriate program and read the file, just by clicking on the file. For \*.POLY files, the user will find himself in the POLY module with the file read, and with \*. TCM files, the macro will start executing etc.

**GUI** A Graphical User Interface (GUI) to Thermo-Calc will be released together with the new version. This provides all the basic functions of Thermo-Calc like single equilibrium



calculations, STEP for property diagrams and MAP for multicomponent phase diagrams.

### Database module, TDB

Error messages Databases created by Users are becoming larger and more complex. The error check in the TDB module is rather rudimentary and the error messages are difficult to understand. A line number has been added to the error messages indicating the line where the error occurred. This line number is valid only if the database is all in one file, also the error may actually have occurred a few lines earlier than indicated.

Some errors may still pass the check, typically if parameter is written on two lines like this

```
PARAMETER G(LIQUID,A,B) 298.15  
-100000; 6000 N!
```

The parameter read from the database will be +100000 rather than -100000. The reason for this is that the database module will concatenate all lines and remove extra spaces before trying to enter the parameter in GES. Thus the parameter will be

```
PARAMETER G(LIQUID,A,B) 298.15-100000; 6000 N!
```

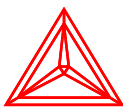
and the - sign will be taken as delimiter between 298.15 and 100000. This mistake can be avoided if one follows the simple rule that one should always have a space as first character of a line. The maximum length of a line in a TDB file is 78 characters, but a function that can be spread over several lines with a space starting each line.

The historical reason for why TDB does not treat the "newline" as a delimiter is that databases sent via E-mail frequently had extra newlines added by the mailers which often occurred with lines such as

```
FUNCTION GHSERLI 200.00 -10583.817+217.637482*T-38.940488*T*LOG  
(T)  
+35.466931E-3*T**2-19.869816E-6*T**3+159994*T**(-1); 453.60 Y  
-559579.123+10547.879893*T-1702.8886493*T*LOG(T)+2258.329444E-3*  
T**2  
-571.066077E-6*T**3+33885874*T**(-1); 500.00 Y  
-9062.994+179.278285*T-31.2283718*T*LOG(T)+2.633221E-3*T**2-0.43  
8058E-6*T**3  
-102387*T**(-1); 3000.00 N !
```

It was considered easier to require a space at the beginning of each line that was not artificially broken into two than to change all mailers or other editing devices around the world.

References The references generated by LIST\_DATA <file> N are now in a form that can be read by the TDB module. The previous way, with references on a separate file, requires that the references are numeric. The references on the same file MUST start with a letter, it is recommended to use references like REF017 etc.



### **The GES module**

**CVM** The tetrahedron CVM model for binary systems can be connected to a substitutional phase with excess parameters. The Gibbs energy of the phases will be simply added, no subtraction as for the standard two-phase split of ordered CEF.

**Quasichemical liquid A** quasichemical model for ionic liquids implemented, including vacancies and neutral constituents.

**Polymer model** The Flory-Huggins model for polymers has been implemented.

**Phase code A** new phase code F means ordered fcc with 4 identical sublattices. Identical parameters will be stored only once which will reduce calculation time and storage requirements.

**Phase partitioning** Any ordered sublattice phase (OP) can have a substitutional phase (SP) appended with the command `AMEND_PHASE <OP> DISORDERED_PART <SP>`. Previously only ordered phases that could become completely disordered could have such a "two-phase" partitioning. The following requirements must be fulfilled:

The last sublattice in both phases can be an "interstitial" sublattice, however, it must have identical constituents and site ratios in both phases and these constituents may or may not occur on other sublattices. All constituents of the SP must dissolve in the OP.

The mole fractions of the SP will be calculated from the site fractions in the OP.

It is not necessary that all sublattices in OP have the same constituents.

The Gibbs energy will be the sum of the Gibbs energy of the two partitions, no subtraction is made from the Gibbs energy of the OP as disordered.

**New command** The `SET_INTERACTIVE` command is allowed in GES now.

### **The POLY module**

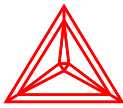
**Larger systems** The maximum number of species has increased from 200 to 1000 and the maximum number of components from 20 to 40.

**New command** A new command `COMPUTE_TRANSITION` calculates the equilibrium when a new phase appears. The user must select the phase and the variable parameter. After the calculation, the parameter is set to the value where the phase becomes stable.

This command is convenient to find melting temperatures or solubility limits for example. Previously such calculations required a clever combination of the `CHANGE_STATUS` and `SET-CONDITION` commands.

**Modified command** The `LIST_STATUS "phase"` command has been modified to avoid long outputs. Only 10 metastable phases will be listed, all others will be merged on one line like the suspended phases.

**Modified command** The `SPECIAL_OPTION SET_MISCIBILITY_GAP` command will now



also ask for major constituents in the first composition set.

STEP/MAP output Lengthy output of calculated equilibria during MAP and STEP has been removed. A new option in SPECIAL\_OPTION can set the listing back again.

#### **The PARROT module**

Alternate mode A number of bugs connected with the "Alternate mode" introduced in the previous version are now fixed.

Bugfix The bug in EDIT\_EXP with equilibrium labels shorter than 4 characters has been fixed.

Output The output for LIST\_RESULT is formatted in more organized columns.

#### **New pricelist**

New prices apply from version N of Thermo-Calc, May 2000. Pricelist can be obtained from Thermo-Calc Software upon request.

#### **New Newsletter format**

For the first time the Thermo-Calc Newsletter is now also available, not only as paper document,

but also in different on-line formats. Most of you will receive both the paper document and the e-mail News this time. If you have not received the e-mail copy and wish to add your name to the mailing list, send an e-mail to [request-newsletter@thermocalc.se](mailto:request-newsletter@thermocalc.se). If you wish to remove yourself from the e-mail list also use the above e-mail-address.

#### **Training courses**

A Thermo-Calc training course was arranged in Stockholm during May jointly arranged by Thermo-Calc Software and KTH.

A training course for DICTRA is scheduled for

- June 13-15, 2000 (3 days) at KTH

Detailed information about the course, schedules and course information, is to be found on the Thermo-Calc homepage at [www.thermocalc.se](http://www.thermocalc.se). For application to the DICTRA course please email [info@thermocalc.se](mailto:info@thermocalc.se) or submit an on-line application from the web page.