Agenda for meeting 4-5 May 2023 in Udine

The 4 May the meeting will begin 13.00 (UTC+1, Tokyo 21.00; New York 07.00)

Maybe Italy has summertime, i.e. UTC+2, one hour earlier in Tokyo and New York.

1. 13.00 Welcome and a short presentation by each participant.
2. 13.30 An attempt to summarize the important tasks of a database manager: Participating in assessments, collecting published assessments, testing extrapolations, estimating missing parameters, updating old assessments, incorporate feedback from database users, information useful for future managers. What can be documented in the database or need additional files/figures? All are welcome to prepare a few slides!
3. 14.30 Coffee break
4. 14.50 Details of the XML format and how it can be adapted for TDB files to improve the documentation and consistency.
5. 15.10 Survey of old and new models used in the TDB file and how they can be handled in the XML file.
6. 15.30 A simple independent software to upload a TDB file to a rudimentary XMLTDB format.
7. 16.00 Discussion how we should organize the project with the limited funding. Tasks for each participant. Next meeting.
8. 17.00 End of the first day.

Second day 5 May the meeting will start 09.00 (bad time for TEAMS, probably only participants in Europe)

1. 09.00 Economy.
2. 09.30 New unary models and parameters.
3. 10.30 Coffee break
4. 10.50 How to handle particular models in the XMLTDB file.
5. 11.10 Structurng model parameter identifiers including non-thermodynamc properties.
6. 11.30 Free discussion
7. 12.00 End of meeting.

Some ideas of organizing the database management

I have (again) summarized some ideas here and feedback from all users and developers are important. You are all welcome to circulate your opinon of what to discuss prepare a short presentation of how to manage a thermodynamic database for the meeting 4-5 May.

A TDB file consists of data for elements, species and phases. All thermodynamic data is associated with the phases and the models for the phases. The current TDB format have a number of features that can be improved, in particular how to describe different model features. For example the **TYPE_DEFINITION** keyword should be replaced by an **AMEND** specifying for each phase some particular model feature.

I want again stress that the XMLTDB file will normally not be read directly by a thermodynamic software, nor by the database manager. There will be an "upload" and"download" software to convert an XMLTDB file to the software specific TDB file format and vice versa. That was the original idea with TDB the format.

Some points (several already stated):

1. An XMLTDB file will normally not be edited directly which means there must be efficient software to upload/download this format to the software specific TDB format. A main objective is that the database managers must be able to add critical information about the models and parameters used in a database. Such information is very important for the second and later generation of database managers.

   There must be efficient means for "comments" in the "master TDB" file edited by the database manager to be included in the XMLTDB file. These comments my be supressed on a TDB file provided to a user.

2. Different database managers have different ways of organize their "master TDB" file and it should be possible to upload and download the XMLTDB file in their preferred way including all their comments. For the general user the data are normally ordered by phase but for updating it may be better to have them ordered as unary, binary, ternary and higher order systems. But it would be interesting to know how each manager handles the database and if there are some useful ideas to share.

3. Some model features have different implementation in various software but the way to handle them in the XMLTDB file should be independent of a particular implementation. When downloading a TDB file from an XMLTDB file the downloading software should be able to handle such differences.

4. The "model parameter identifier" (MPI) in a parameter associates the parameter with some model for the phase. A parameter with the MPI **G** is associated with the fundamental Gibbs energy function, **TC** and **BMAG** are associated with different magnetic models.

   Several new MPI have also been added by the new unary models and by different software, also for handling data that are not associated with the thermodynamic data, for example

variants of **MQ** for mobility data. Some of these may be unique for different constituents or components. We should try to establish an agreed set and format for the MPI.

A parameter is a function of T and P and has a reference to the phase and the constituents, the fraction of which should be multiplied with the parameter. This makes it possible for a parameter to appear anywhere in a TDB file (or at least anywhere after the phase and its constituents have been entered). But each database manager may have his/her own preference.

5. It should be checked that particular MPI parameters for a phase have the appropriate model associated with the phase when uploading a TDB file. Also check that a phase with a model requiring a particular MPI have such parameters, unless the model will give zero contribution with no such parameters. I am not sure if the new magnetic model does that.

6. Originally the TDB file was read once sequentially but new models means that several rewind/read are often needed, in particular to pick up missing functions and "disordered parts" of phases. We should consider this when designing the download software.

7. The "disordered part" or "partitioned" model is an important simplification to handle parameters for phases with several sublattices. In the original TC implementation this was achieved by adding two separate phases, in OC there is a single phase with two sets of constituent set of fractions where the disordered fractions are calculated from the ordered set. This makes it easier for a manager to handle the model parameters.

   In some cases only the disordered part of an FCC phase is needed but it is better to keep the ordered and disordered parts together in the XMLTDB file. It can be an option when downloading to a TDB file to ignore the constituents and parameters for the ordered part.

   In other cases the disordered part is useful to reduce the number of parameters, for example in a 5 sublattice model of σ for a multicomponent system there many parameters G(sigma,A:B:C:D:E) which are not assessed and described by

   PARAMETER G(SIGMA,A:B:C:D:E) 298.15 2*GSIGMA_A+4*GSIGMA_B
   +8*GSIGMA_C+8*GSIGMA_D+8*GSIGMA_E; 6000 N!

   Such parameters can simply be ignored if there is a disordered fraction set for A, B, C, D, E with the pure element parameters. Only assessed ordered parameters are needed.

8. As proposed by Nathalie we should no longer use the model (for phases with order/disorder transformation) where the ordered part of a partitioned phase is subtracted using the disordered set of fractions in the ordered aublattices, i.e.

$$G_M \;=\; G_M^{\rm disord}(x) + (G_M^{\rm ord}(y) - G_M^{\rm ord}(y=x)) \qquad (1)$$

   where $G_M^{\rm disord}(x)$ is the Gibbs energy for the disordered part, $G_M^{\rm ord}(y)$ is that for the ordered part and $G_M{}^{\rm ord}(y=x)$ is the ordered part recalculated as disordered. The latter two cancel

in the disordered state. We should simply add the ordered and disordered parts:

$$G_M = G_M^{\text{disord}}(x) + G_M^{\text{ord}}(y) \quad (2)$$

The only advanatage of subtracting the ordered part "as disordred" is that the disordered part can be assessed independently of the ordered one but there are few systems where that is useful.

9. The "parameter permutation" feature is interesting for phases with order/disorder transformation. It can reduce significantly the number of parameters as all parameters
G(FCC_4SL,A:A:A:B)
with the B in different sublattices are the same. Preferably they occur only once in the XMLTDB file and are duplicated when downloaded to a TDB file for a software in which permutations are not implemented.

10. We have several models for the liquid and it might be interesting to have duplicate models of the same phase in the XMLTDB file because the other phases may be the same. At least a regular solution liquid phase in parallel with the I2SL model which in many cases is identical. It should be possible when downloading a TDB file to select the model for such a phase.

    As already mentioned an ordered or disordered version of FCC and BCC phases may be selected. But they would not require duplicate set of parameters in the XMLTDB file.

11. We must consider the models developed by the new unary project such as the low T vibrational entropy, new magnetic reference state, the two-state liquid model, the Equivalent Entropy Criteria (EEC). This has created new types of MPI.

    It has been decided not to use multiple composition dependent Einstein-T describing the heat capacity of a pure element down to 0 K. I am very much in favour of this but such a feature may be useful for oxides and some other kinds compounds. Multiple Einstein-T parameters for the unaries would create confusion for assessments.

12. The elements and species are simple to handle except that species has a problem handling the MQMQA and UNIQAC models. In these models the species have additional properties needed such as bonds and FNN/SNN ratios or volume and area needed to calculate the configurational entropy.

13. A favourite topic for me has been the names of phases. But I think we have reached a reasonable agreement using a "popular" name such as FCC augemnted with a "Structurbericht" notation, A1, for austenite. Although it is a complication that for example TiC is the same phase.

14. An important point is also to convince journals that all published assessments should provide the assessed parameters in an XMLTDB file as supplementary data.