2011-06-30

RELEASE NOTES

The management board of THEREDA is proud to announce the first official release of data to the public. This release covers systems made up by the primary species Na<+>, K<+>, Mg<2+>, Ca<2+>, Cl<->, SO4<->, H<+>, and H2O(l). Valid temperatures for the released data range between 273.15 and 523.15 K, dependent on the specific system. The released data represent only a small part of all data stored in THEREDA. As documentation, assessment, amendment and testing of the data is an ongoing process, there will be further releases in the future covering more elements, reactions and interactions.

While THEREDA can store data for various models of non-ideal interactions in the aqueous phase, the present release is valid only for the well known Pitzer formalism, which allows for the calculation of solution-mineral equilibria at high ionic strengths.

To access the data you will need to log-in on the THEREDA homepage and select "THEREDA data query". The data are available in various forms:

- You may select "Single data Query", where you get access to individual data of various types.
- Upon selection of "Tailored databases" you will have the choice to download ready-to-use parameter files for either PHREEQC or CHEMAPP. Along with the parameter files you will get a document which describes benchmark calculations for the released data. Please use the results to put the downloaded parameter files to the test. Your own calculations should conform to the results in the document. With more releases to come, the number of benchmark documents will increase. Any release of data will be tested with this forthcoming line of benchmark calculations.
- A third option of "Tailored databases" is called "json". This file represents a generic data format. It is not intended for use with a geochemical code but aims to offer a convenient way to process the data with an own program, perhaps to create parameter files for other geochemical codes.

Much work was spent to provide the released data with as much documentation as possible. However, the documentation of data inside the databank is supplemented with a growing number of what we call "Technical Papers". Please refer to the Downloads section on our website.

For the time being we provide parameter files for PHREEQC and CHEMAPP only. However, we are working to provide parameter files for EQ3/6 and Geochemist's Workbench as well. Please stay in touch on this development and consult the News section on our web site regularly. Note, that parameter files for Geochemist's Workbench will be valid for 298.15 K only, as the code doesn't conform to temperature functions implemented in THEREDA.

Despite all efforts we are aware that the possibility of errors cannot be excluded altogether. We encourage you, the user, to join in for our long-term goal to create a comprehensive, internally consistent, well documented and quality assured thermodynamic database. If you encounter problems with our parameter files, if questions arise or important data gaps turn up which were not on our mind, please don't hesitate to contact us. To assist your feedback we created a forum (see the THEREDA navigation menu on the left side). It is inspected by members of the management board on a regular basis and we aspire to provide responses on short notice.

The forthcoming release will extend the present one by systems containing carbonate at 298.15 K. It is scheduled for autumn 2011.

On behalf of the THEREDA management board
Helge C. Moog