

THEREDA 2020 Release Notes



The THEREDA management board proudly announces the 2020 release of THEREDA.

The present THEREDA data release differs from earlier ones. Formerly separated into small parameter files dedicated to only a few, well-tested systems each, all datasets are now combined into a single parameter file, one for each supported code. The reason for this step is that the effort of updating and testing many small parameterfiles turned out to be unsustainable

Due to this paradigm shift in the release strategy it is now in principle possible to model chemical systems for which THEREDA has never been tested, or for which experimental data are lacking. Therefore, a “positive list” has been created which presents examples of applications of THEREDA to specific systems. This list will be continuously extended. Registered users may access through the menu item “Tested Systems”.

The following updates and new data are included in the THEREDA 2020 release:

New data:

- System Np(+V)-CaCl₂-H₂O
- System U(+VI)-NaCl-KCl-MgCl₂-H₂O(l)
- Systems Tc(+IV)-Tc(+VII)-NaCl-MgCl₂-CaCl₂-H₂O(l)
- System MgCl₂-Mg(OH)₂-NaCl-H₂O(l) (“Sorel phases”)
- Se(+IV)/Se(+VI)-Na, K, Mg, Ca-Cl, SO₄, CO₃-H₂O(l)
- Solubility of O₂(g) in saline solutions

Updates:

- improvement of NaCl solubility data, now up to 200°C
- System Ca(OH)₂-CaCl₂-H₂O(l) (correction of ternary solid phase compositions)
- Update to CEMDATA18 (Lothenbach et al. 2019, *Cement and Concrete Research*, **115**, 472–506)

Supported codes / formats:

- Geochemist’s Workbench: formats jan19 (v. 14+) and jul17 (v. 12-13)
- PHREEQC
- CHEMAPP
- New: TOUGHREACT
- JSON

Specific notes regarding CEMDATA18:

- For the correct representation of the solubility of cementitious phases solid solutions are necessary in some cases. However, TOUGHREACT and Geochemist’s Workbench cannot handle solid solutions and endmembers are exported as regular, stoichiometric mineral phases. If the user wishes to work with solid solutions as described in CEMDATA18, it is advised to use PHREEQC or CHEMAPP.
- Regarding cementitious phases the users is urgently advised to consult publications relating to CEMDATA18: metastable equilibria are of utmost importance and can only be accounted for by selectively disabling certain solid phases in CHEMAPP or PHREEQC.

- In addition, CEMDATA18 supplies different solid solution models for CSH-gels, which are designed for specific applications. The user is advised to consult Lothenbach et al. (2019) for a correct selection: <https://doi.org/10.1016/j.cemconres.2018.04.018>.
- While THEREDA is focussed on equilibria in high-saline solutions using Pitzer coefficients, CEMDATA18 is qualified for low ionic strengths only. For the time being the user is therefore strongly discouraged to use THEREDA for the calculation of cementitious phase equilibria in high-saline solutions.

All released parameter files were subjected to more than 200 test calculations. The objectives of the test calculations were to ensure compatibility with the supported codes, the integrity of internal conversion calculations in THEREDA, the correctness of data capture, and the equality of results with different codes. As the database is continuously being developed, the test calculations also help to detect potentially adverse side effects of changes in the data.

With the present release being active, previous releases from THEREDA are no longer maintained. However, for the interested user they are still available in the “Data Downloads” section following the link “Earlier releases”.

The following persons are responsible for this release:

Name	Institution	Responsibilities
Tina Scharge	GRS	Cs, Sr, Phosphate
Helge Moog	GRS	Database management, O ₂ (g)
Daniela Freyer	TUBAF-IAC	Oceanic salt system, Sorel phases
Anke Richter	HZDR-IRE	U(+IV/+VI) data compilation, Web administration
Frank Bok	HZDR-IRE	Se(+VI/+IV) and O ₂ data compilation, Export parser testing, Tested systems
Tres Thoenen	PSI-LES	Update to CEMDATA18
Nese Cevirim-Papaioannou	KIT-INE	Np(+V) in CaCl ₂ systems. Contribution to U(+VI) in NaCl-KCl-MgCl ₂ systems
Xavier Gaona	KIT-INE	
Christian Marquardt	KIT-INE	Audit

GRS: Gesellschaft für Anlagen- und Reaktorsicherheit mbH, Department for Final Repository Research. TUBAF-IAC: TU Bergakademie Freiberg, Institute for Inorganic Chemistry, Department for Salt, Mineral and Construction Materials Chemistry. HZDR-IRE: Helmholtz-Zentrum Dresden-Rossendorf, Institute of Resource Ecology, Department of Surface Processes. KIT-INE: Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal, Department for Radiochemistry. PSI-LES: Paul-Scherrer Institute, Laboratory for Waste Management.

In behalf of the THEREDA management board,

Helge C. Moog

(October 2020)