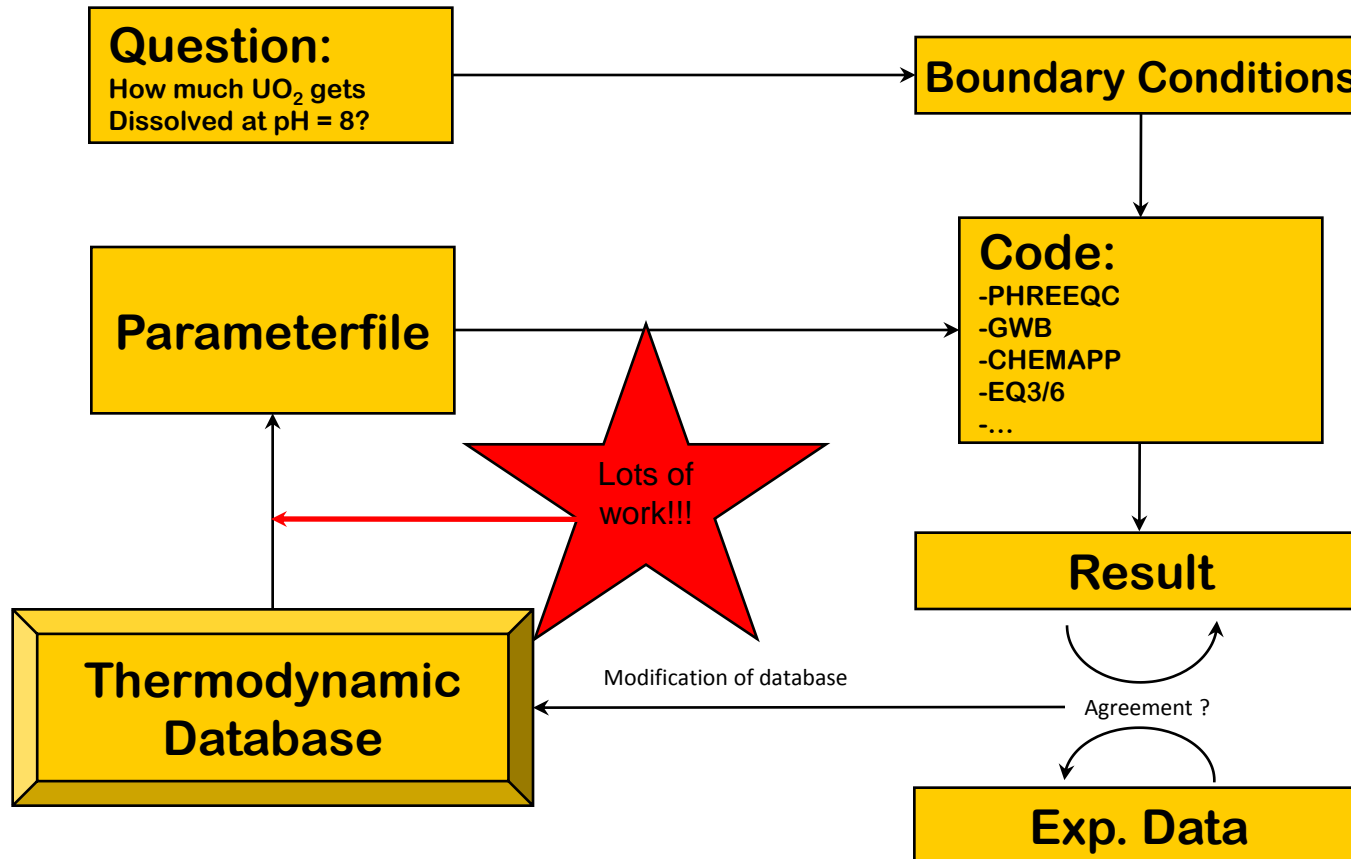




Thermodynamic **Re**ference **Da**tabase

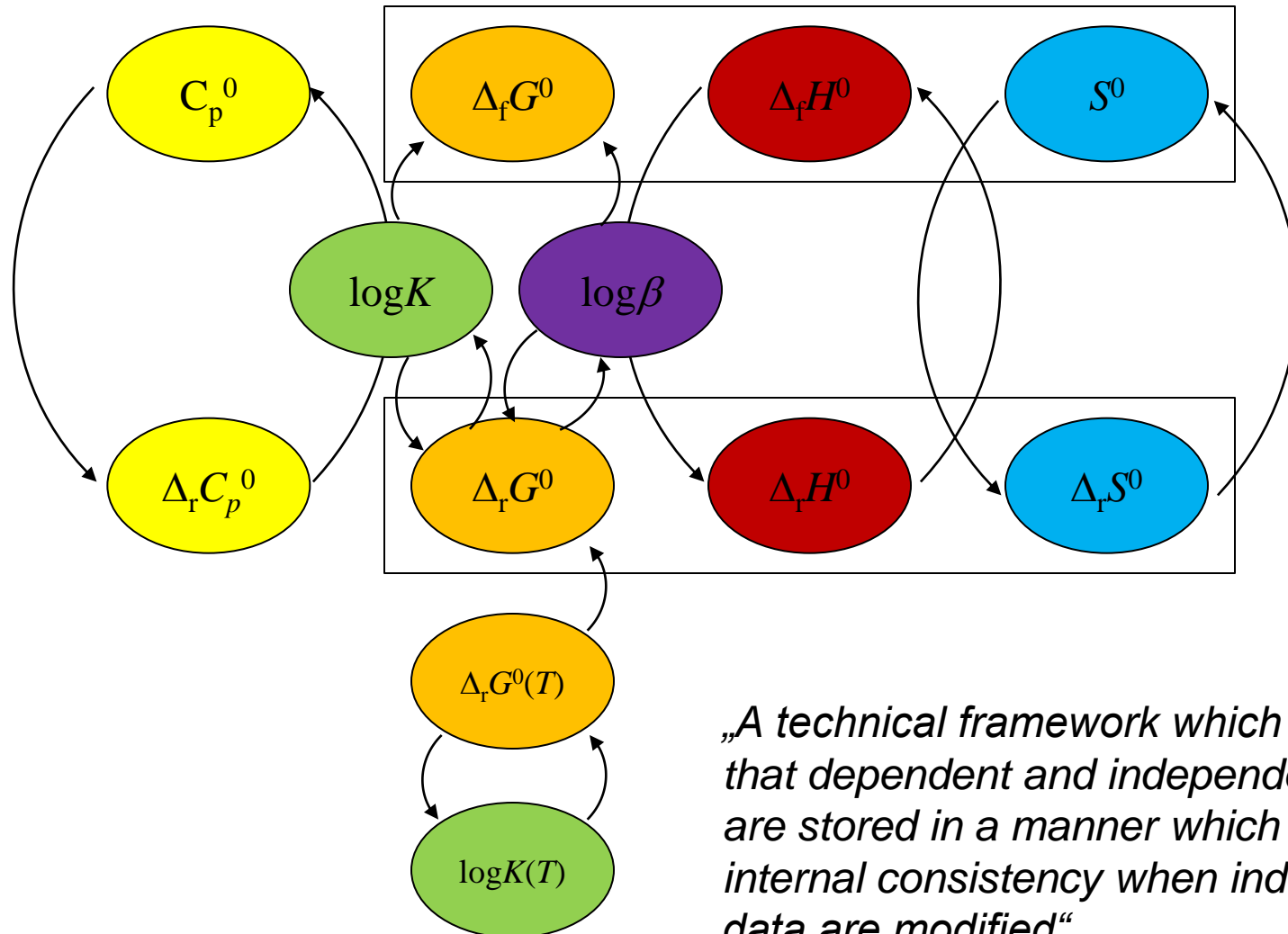
Helge C. Moog, W. Voigt, G. Wollmann

What do we need to perform a thermodynamic equilibrium calculation?



What do we mean by „thermodynamic database“?

Consistency of data



„A technical framework which ensures that dependent and independent data are stored in a manner which ensures internal consistency when independent data are modified“

Thermodynamic equilibrium modeling for nuclear and non-nuclear modeling in the future

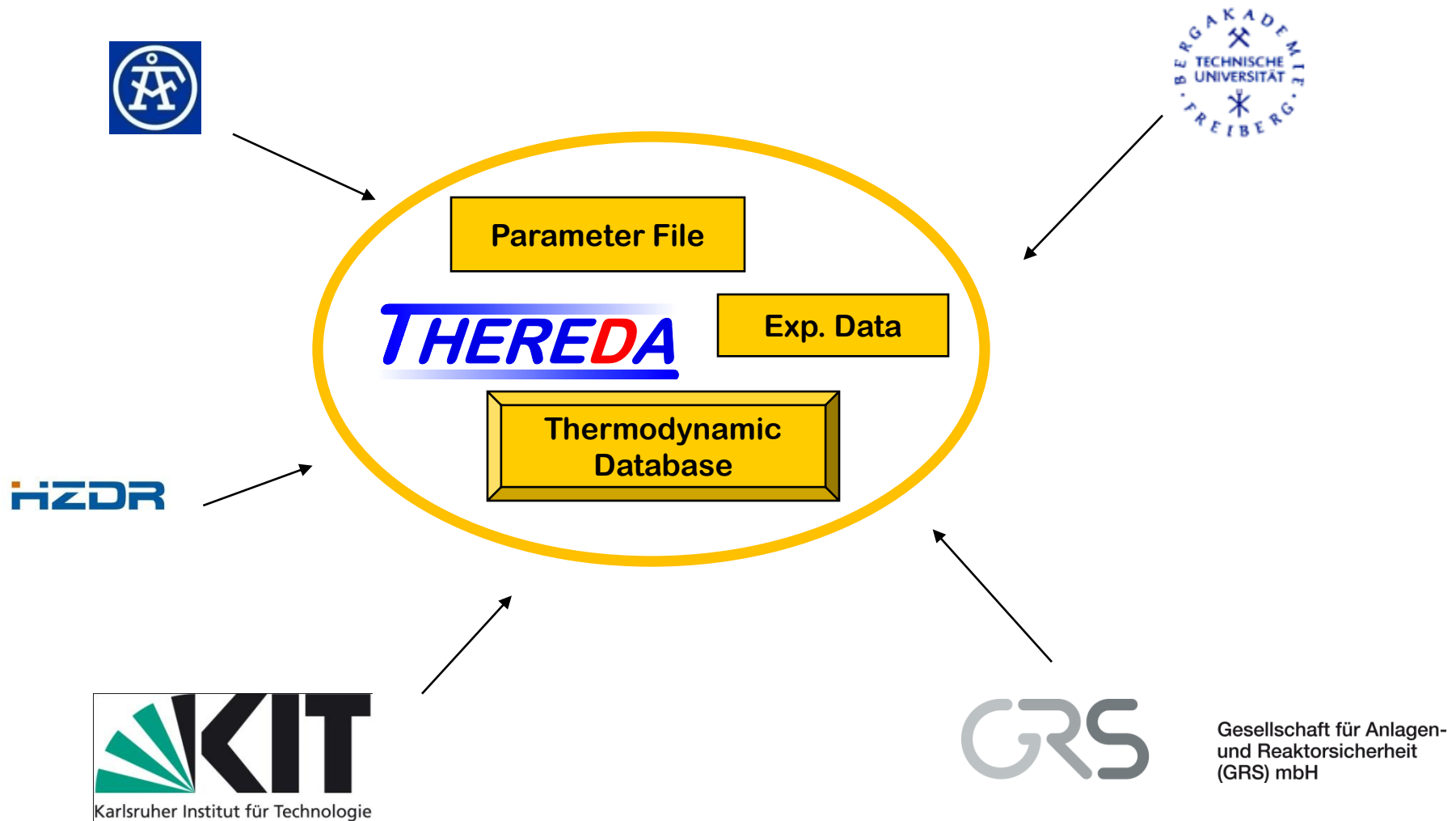
Creation of a consistent, mutually agreed and quality-assured reference database

Joining competences for a common sake

Easy access via the world wide web

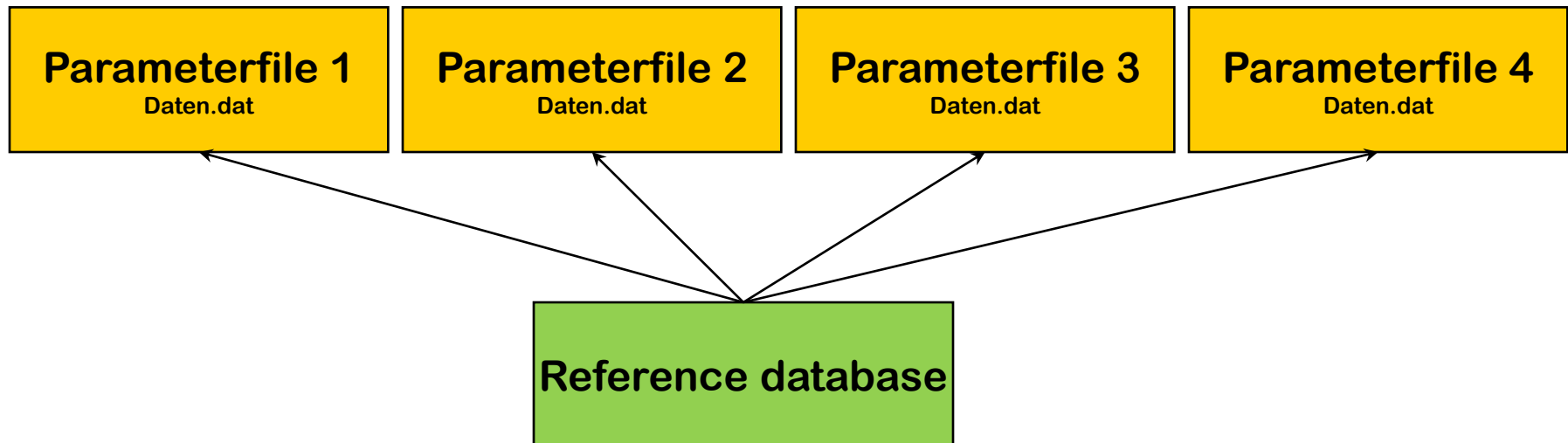
Making available ready-to-use parameter files

Thermodynamic equilibrium modeling for nuclear and non-nuclear modeling in the future



Basic idea

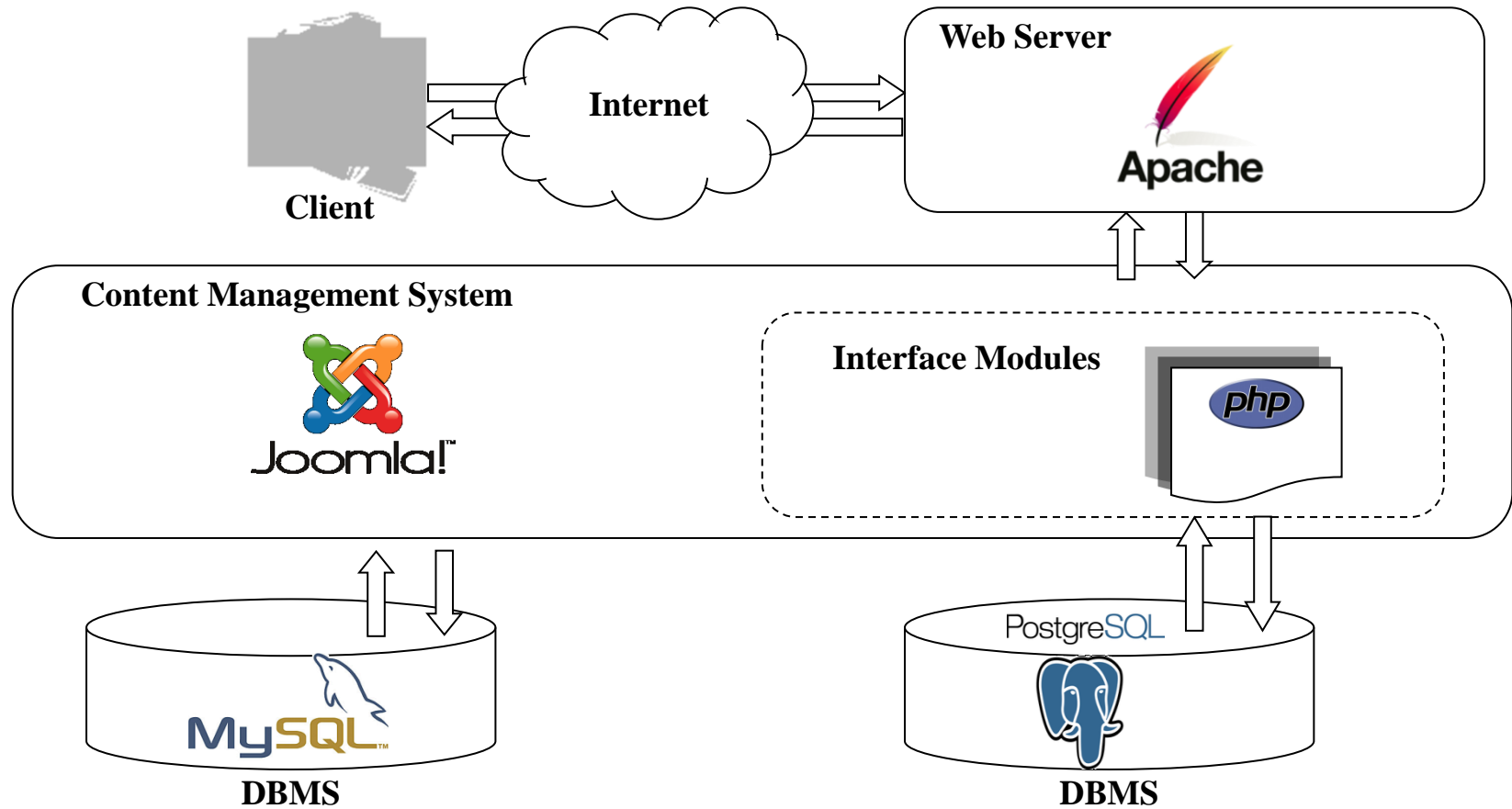
Thermodynamic calculations of various institutions become comparable, by creating parameter files from a common database.



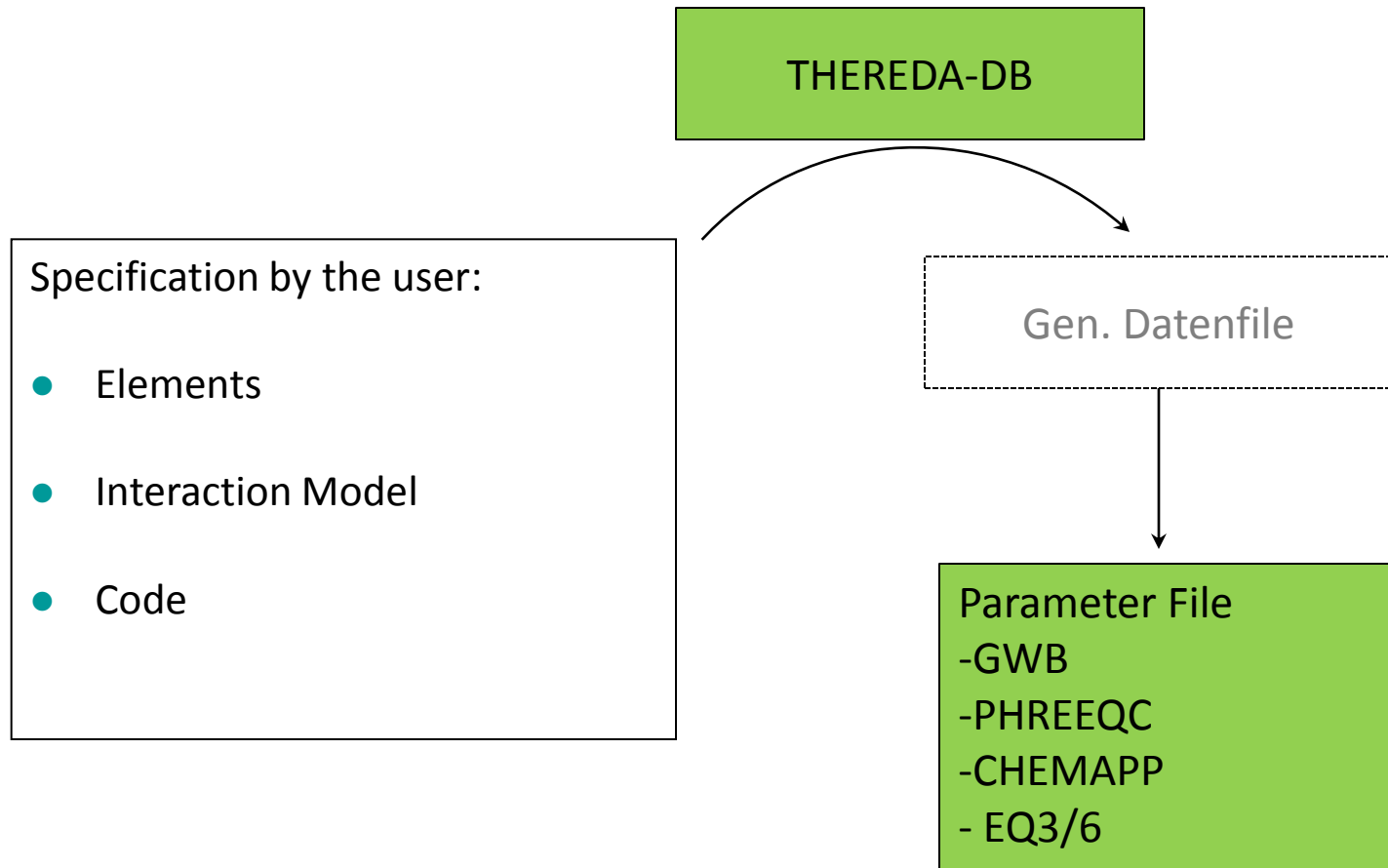
Further project data

- Phase I: 2006-07 bis 2010-03
- Phase II: 2009-10 bis 2013-03
- Funded by two Ministries: BMWi und BMBF, Funding approved by BfS (Federal Office for Radiation Protection) at 3.5. (Letter of Intent)

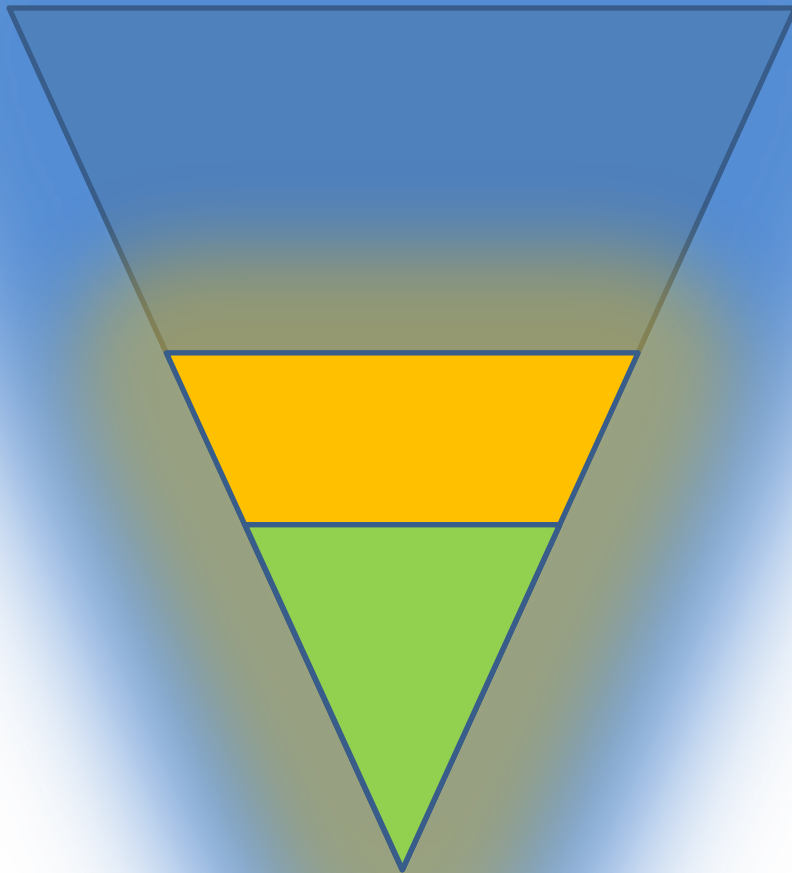
Technical Basics



How it is used



„Released Data“ \leftrightarrow „Non-released Data“



Not released

Actinides, Fission- and activation products

- Pa, Th, U, Np, Pu, Am, Cm
- Rb, Sr, Tc, Cs, Sm, Ra, Nd

Hydrated cement phases

- Including Si, Al

R2

System of oceanic salts +

- $\text{CO}_2(\text{g})$, CO_3^{2-}

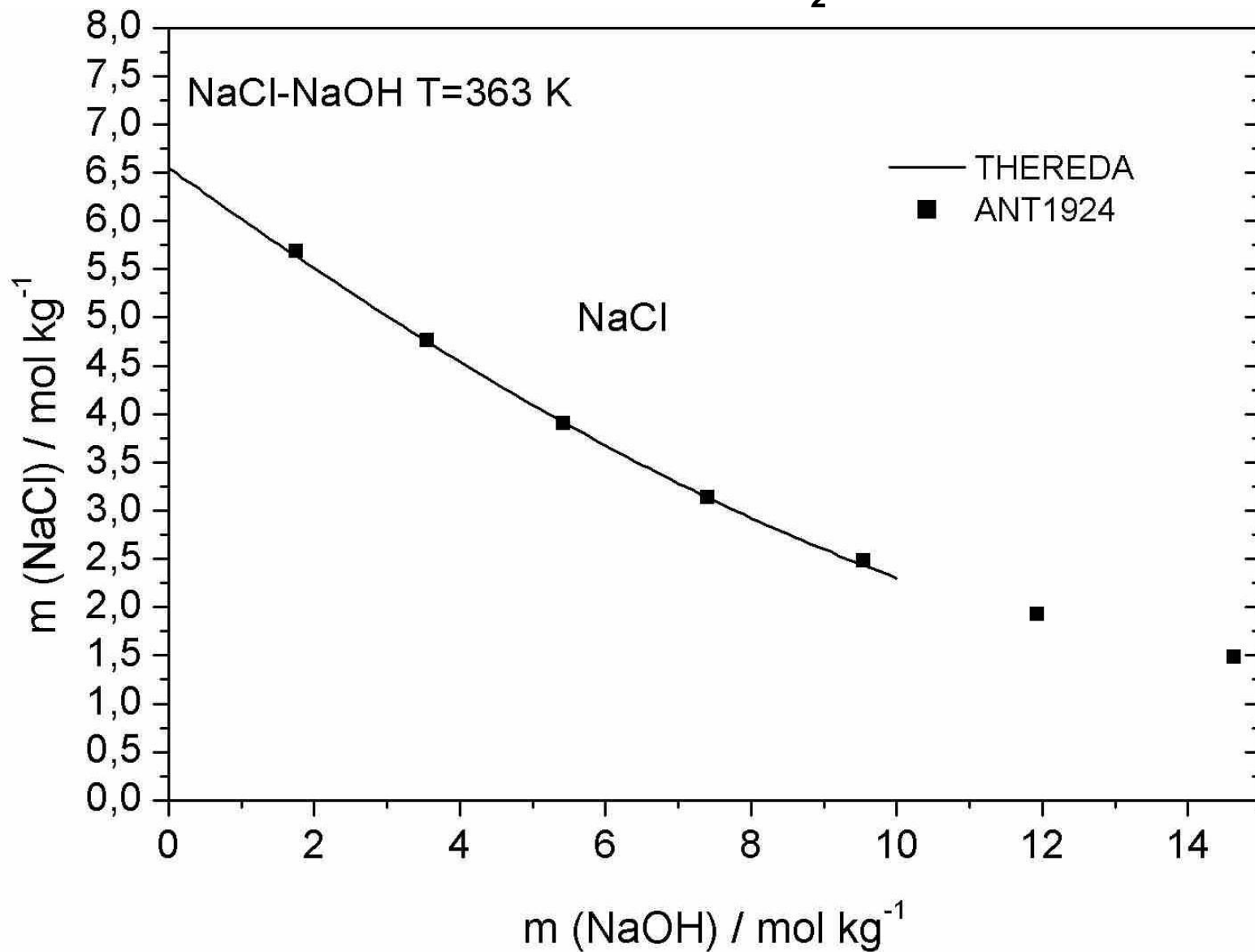
R1 (2001-06)

System of oceanic salts

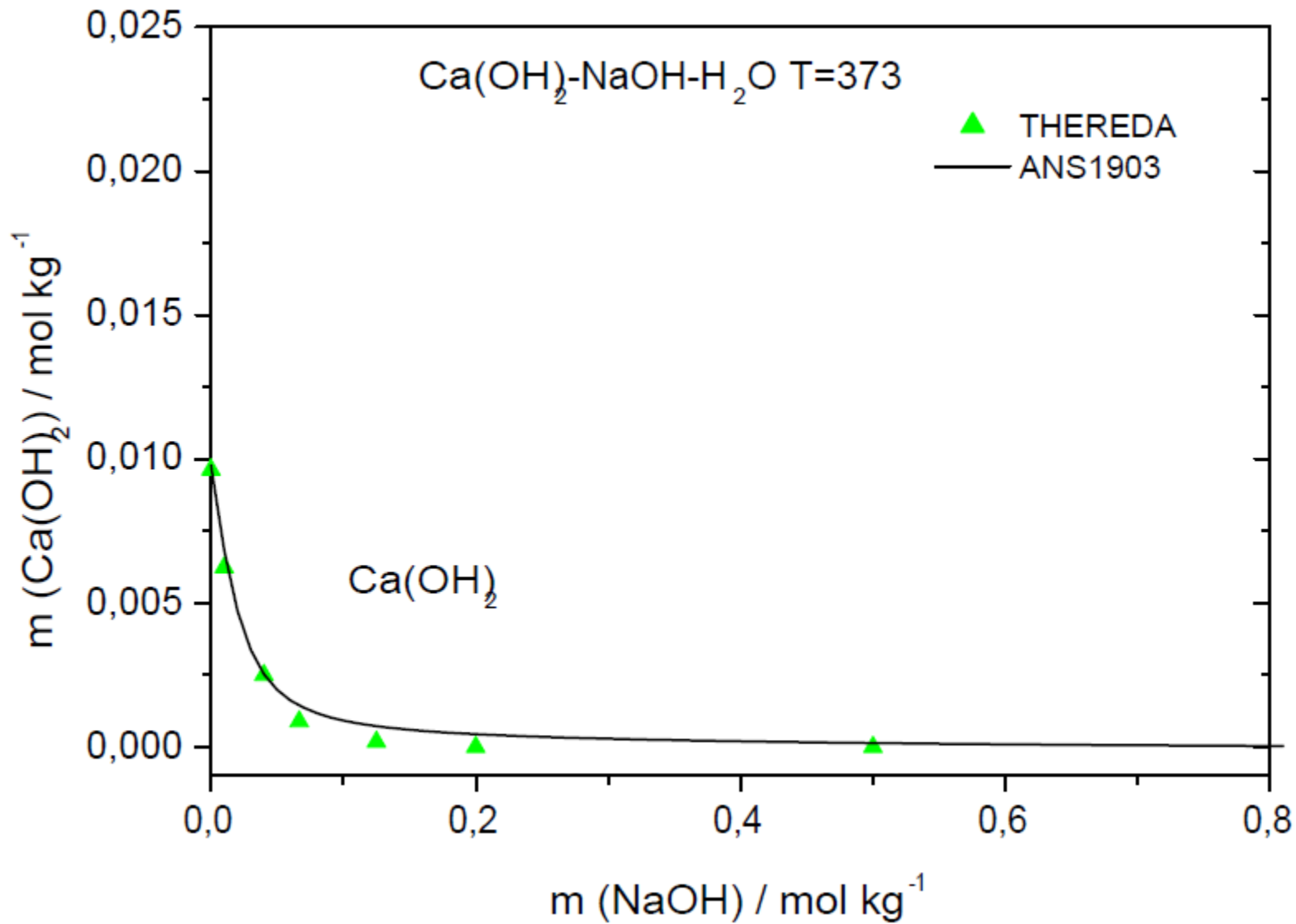
- Na^+ , K^+ , Mg^{2+} , Ca^{2+} , Cl^- , SO_4^{2-} , H^+ , $\text{H}_2\text{O}(\text{l})$

< Demonstration >

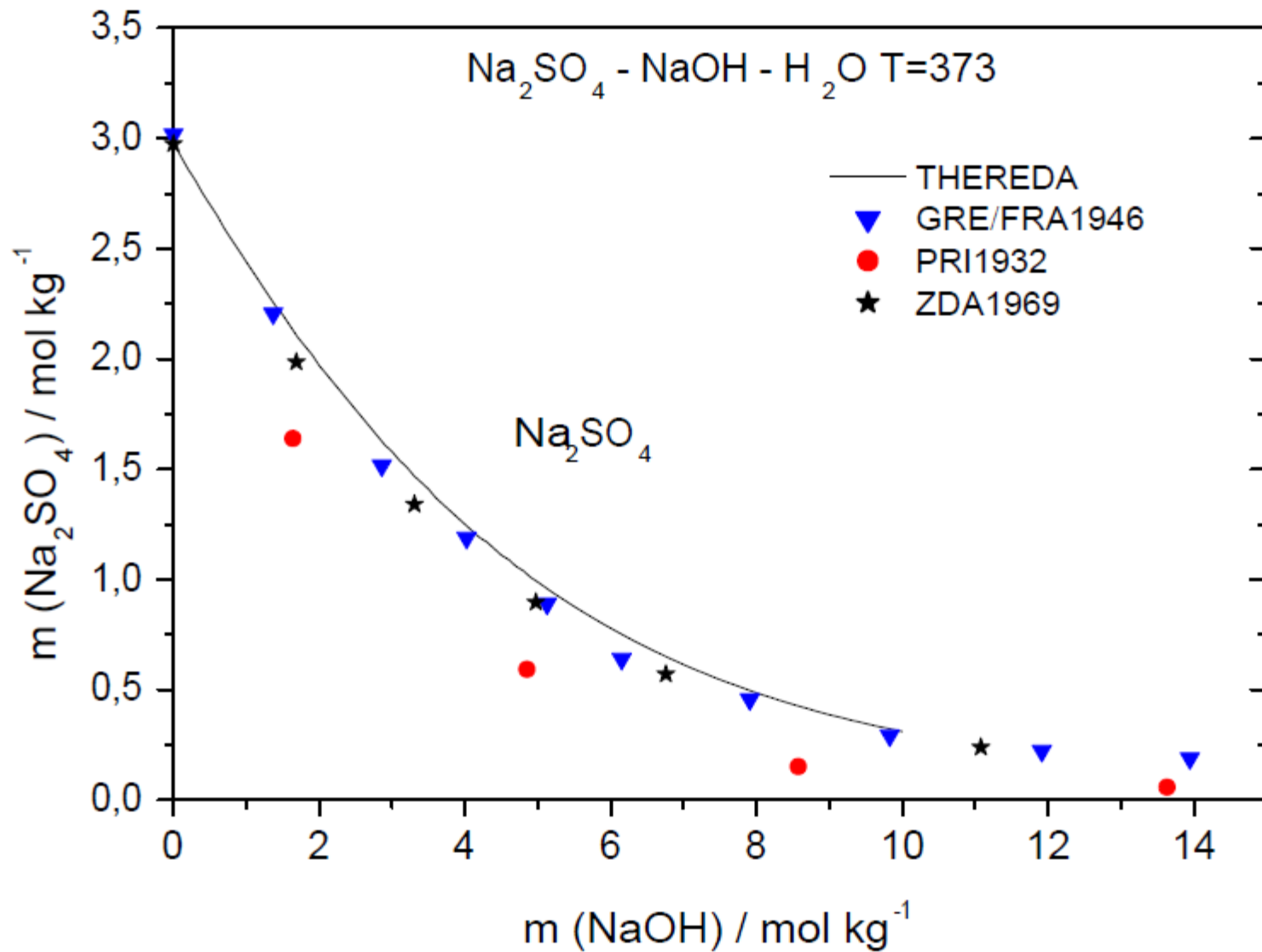
NaCl-NaOH-H₂O



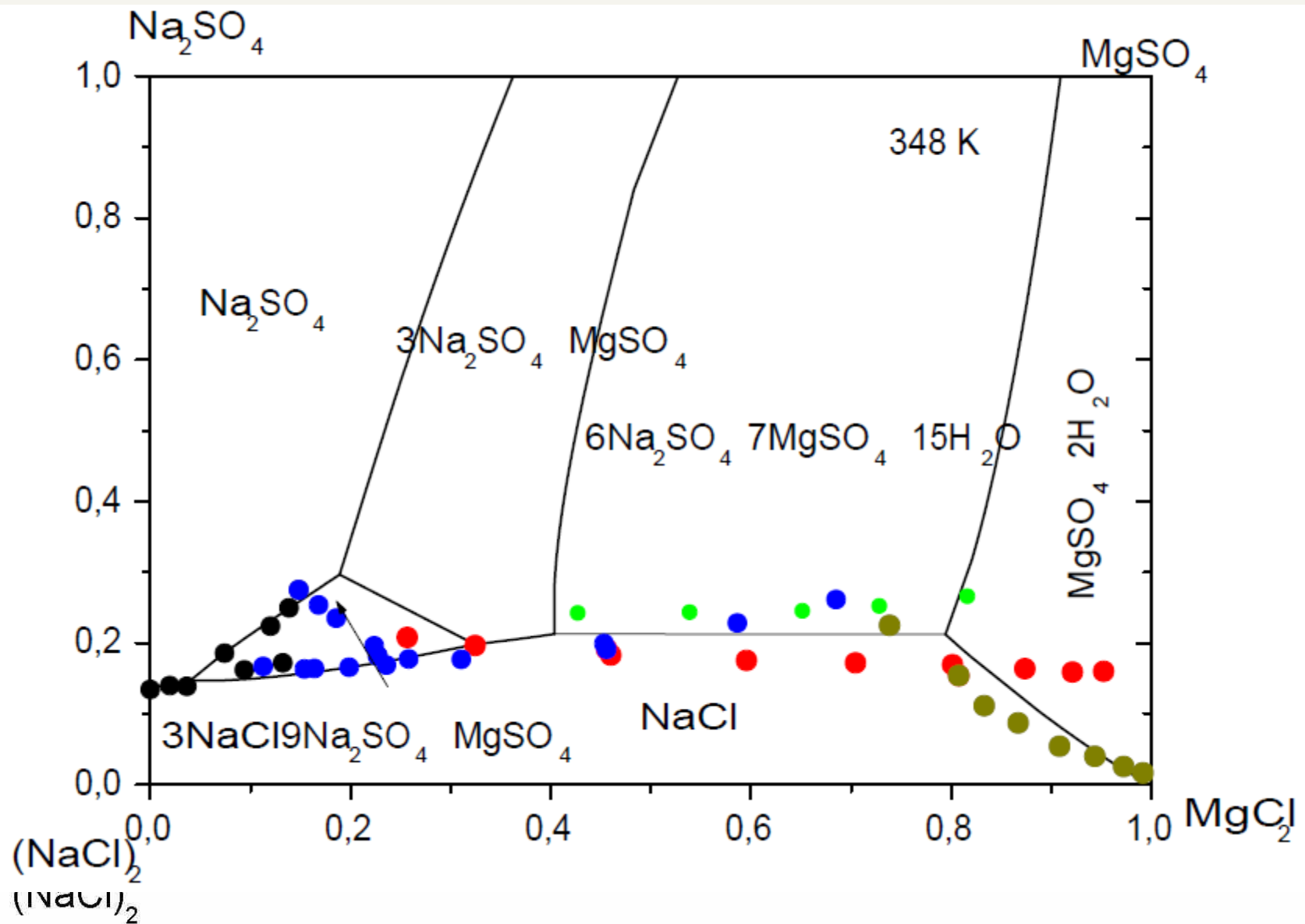
$\text{Ca(OH)}_2\text{-NaOH-H}_2\text{O}$



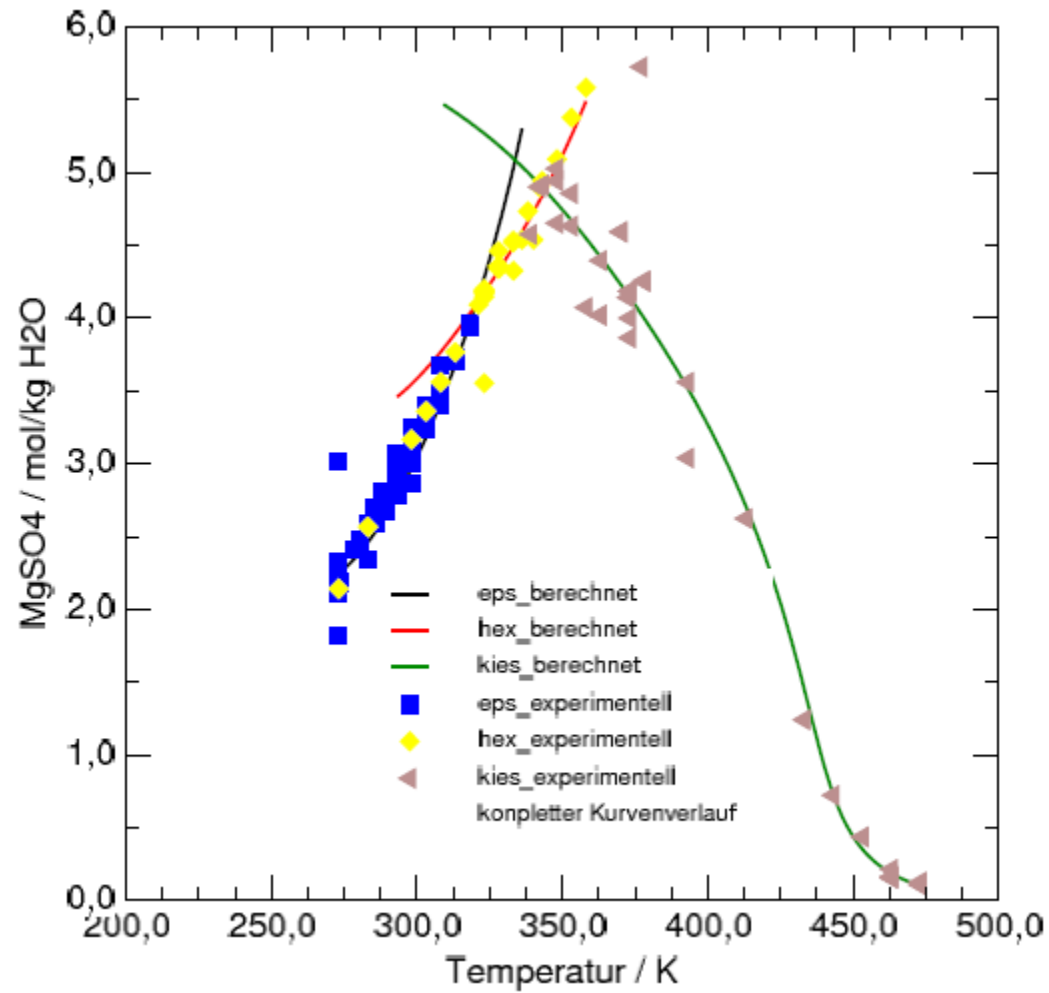
$\text{Na}_2\text{SO}_4\text{-NaOH-H}_2\text{O}$



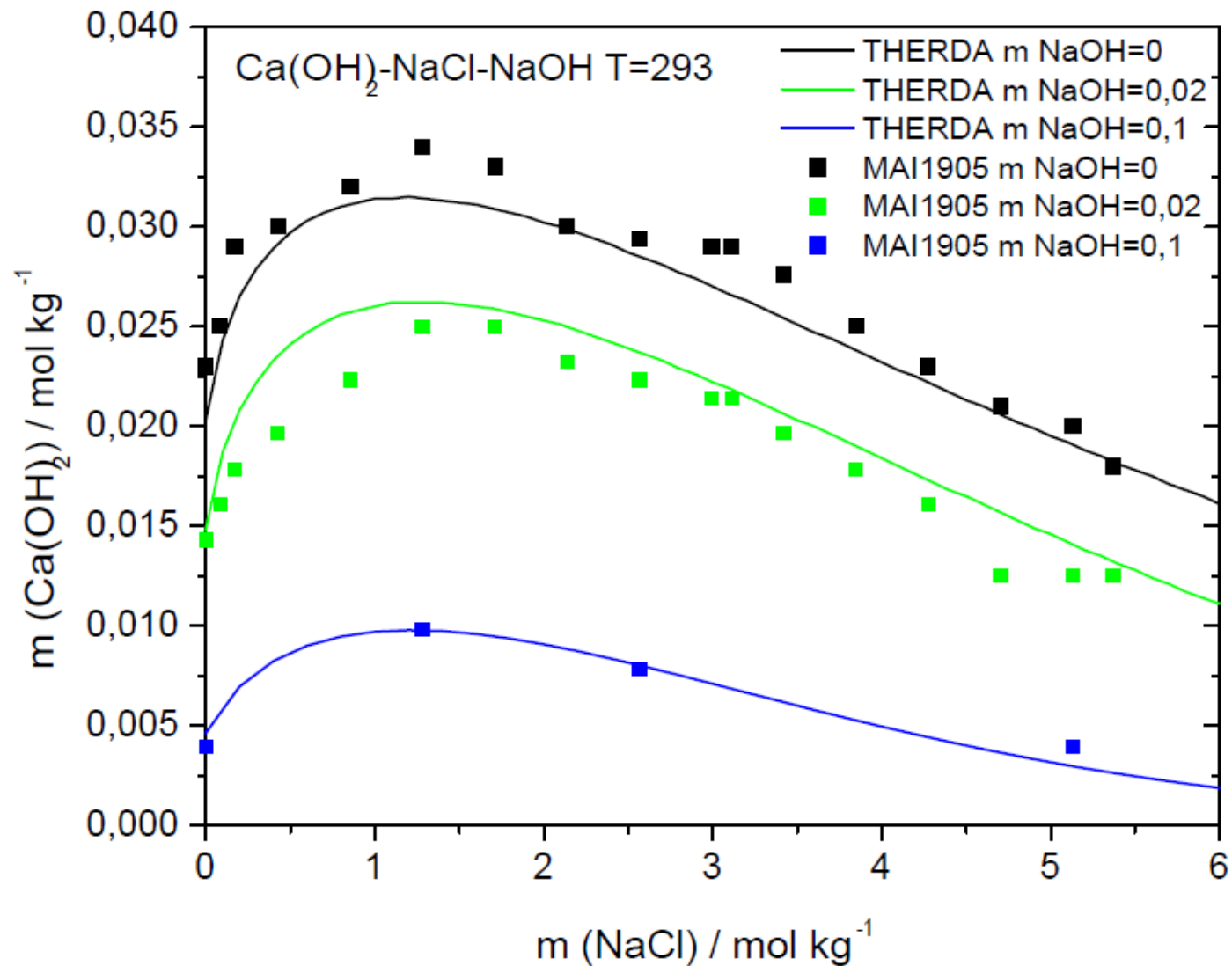
NaCl-MgSO₄-H₂O



MgSO₄-H₂O polytherm



NaCl-Ca(OH)₂-H₂O polytherm



Comprehensiveness (in part)

Umfang

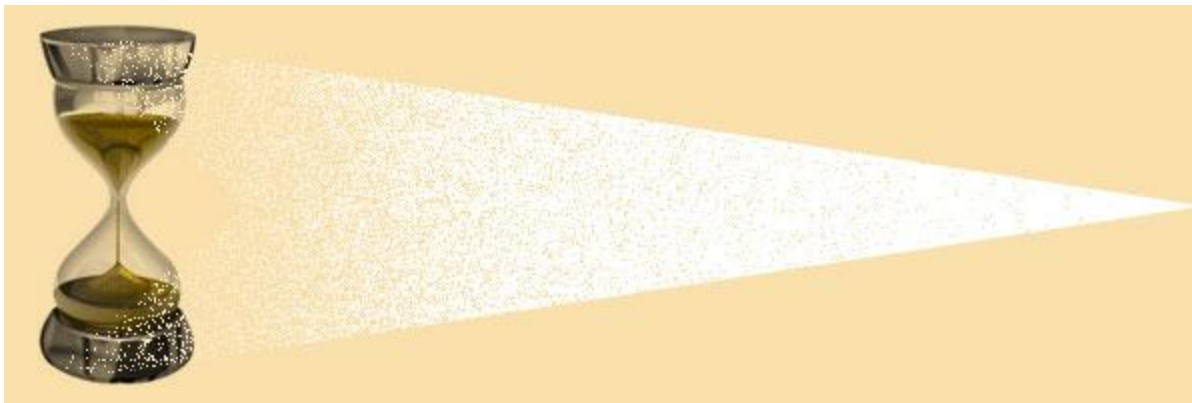
- 196 Phases
- 312 aq. Species (incl. 34 Primary Master)
- 336 formation reactions
- 789 Standard data sets (Pitzer)
- 717 interactions (Pitzer and SIT)

Current activities

- Preparation of second release of data for
 - Carbonate / CO₂
- Completion (and test!) of export programs for
 - Geochemist's Workbench (GWB)
 - EQ3/6
- Execution and documentation of benchmark calculations
- Completion of graphical user interface (web-application, editors only)

Long-term useability

- Useage of open-source programs
- Low degree of abstraction of the data model
- Documention of databank structure
- Flexible databank structure
- Joint project of five research institutions



Conclusion

- THEREDA offers a web-based, state-of-the-art thermodynamic reference database for aqueous systems in equilibrium with nuclear or non-nuclear waste forms in Germany
- Joint-project of five research institutions
- Comprehensive range of data
- Access to code-specific parameter files
- Means of directing future research and of quality assurance for government agencies, service provider, and research institutions
- Future extensions of the thermodynamic database for nuclear and non-nuclear waste forms in Germany in conjunction with THEREDA

Vielen Dank für Ihre Aufmerksamkeit!