
German activities towards a thermodynamic reference data base

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Abstract:

Leading research centres in the field of radioactive waste disposal in Germany have decided to combine their efforts in order to achieve a common goal, the development of a comprehensive and consistent thermodynamic reference database. All the thermodynamic data needed for the modelling of geochemical near- and far field processes in the geological media for high level waste repositories presently under discussion in Germany (salt, clay, granite) shall be collected and qualified in a single database. The partners participating in the project are a group of experts, who are generating, collecting and evaluating thermodynamic data of all relevant radionuclides and matrix elements according to uniform previously established and internationally accepted criteria. Special attention will be given to complete documentation and traceability of all data entries in the database. Existing data from international databases such as those of NEA, NAGRA, YMP will be integrated. Ion interaction coefficients (SIT, Pitzer) needed for modelling in a high saline environment will be included also.

1. INTRODUCTION

Thermodynamic databases belong to the most developed and most often used substance related databases. They are needed for chemical process design, material technology, geology as well as for environmental protection and monitoring. Most of the applications focus on the calculation of phase and reaction equilibria and in combination with transport the time evolution of concentration profiles is predicted. Particularly, in the treatment of geochemical and environmental problems the chemical systems become very complex involving many elements and species. Whereas modern numerical codes have no principal problems to solve the respective equations the reliability and quality of the results depend first of all on the availability and quality of thermodynamic standard data and coefficients for appropriate mixing models in the underlying database.

The past has seen many institutional, national and international initiatives to establish thermodynamic databases with varying purposes and sizes. The assessment of national concepts for radioactive and toxic waste disposal requires a database, which

- o allows the public to use it easily for this aim
- o is transparent concerning data quality
- o is updated continuously with minimum of manpower
- o is available at least for decades of years
- o considers specific national conditions or restrictions.

Within the last two years a group of scientists from different German and Swiss institutions and universities tried to draw conclusions from earlier experience and started to build up a

thermodynamic database concept suited for performance studies in waste disposal considering the features mentioned above. This German initiative was started in August 2006 and is known under project name of THEREDA (Thermodynamic Reference Data Base). One of the most difficult problems consists in the assurance of data quality in conjunction with maintenance and updating a database with limited resources. Many scientists of the "solubility community" are faced with these problems too and are also active in database projects. Therefore a workshop was organized and held in parallel to the 12thISSP, July 23-28th, 2006 in Freiberg/Germany for discussion of questions of quality and maintenance of thermodynamic databases. The purpose was not to achieve a complete survey on thermodynamic databases but to stress essential developments and experiences. At the same time, the German concept was introduced and brought into relation to others. Thus, presentations of specific databases were quite comprehensive and much room was given for discussion. With this paper we would like to bring the German database project to the attention of a wider international community and hope to contribute to a better understanding of general and specific aspects of databases. We also hope for an improved international collaboration in this field.

2 OBJECTIVES OF THEREDA

The main objective of THEREDA is the creation of a comprehensive and internally consistent thermodynamic reference database for the geochemical modelling of the near-field and far-field processes occurring in repositories for radioactive wastes in the different rock formations currently under discussion in Germany. These rock formations are salt rock, clay and crystalline rocks. Special emphasis will be laid upon a complete documentation and traceability of the registered data. It is planned to integrate data from existing qualified thermodynamic databases like the NEA or the PSI-NAGRA database. These data will be completed by the project partners, especially with data for the modelling in saline environments. The databank will serve as a central and common technical-scientific basis which will lead stepwise to a consistent database for all relevant thermodynamic information. At the same time the database will become a useful tool for the identification of knowledge gaps and for strategies to close these gaps. A strategy shall be developed which enables the user to trace back each single data in the parameter files to the primary literature. A group of experts will maintain and update the database far beyond the time span of its generation.

THEREDA will:

- enable the prediction of the activity, speciation and solubility of radionuclides, heavy metals and other toxic elements in underground disposal sites
- be applicable from low to high ionic strength
- fulfil quality requirements established by the project partners
- be the reference database for performance assessment studies in Germany

3 PROJECT PARTNERS AND ORGANIZATION

The project THEREDA was planned and will be supported by major research institutions working in the field of radioactive waste disposal in Germany. The project partners listed below formed in 2003 a working group which convenes in regular time intervals and takes all necessary decisions unanimously:



Figure. 1 Partners in the THEREDA project and Logo of the project

GRS is responsible for the general project coordination. Necessary decisions concerning the data management and the quality management are taken unanimously by the project partners. For the data which will be incorporated into the database the responsibility lies with the institution which generates these data. The Technical University of Freiberg is responsible for the elements composing the sea water system, FZK-INE for the radionuclides, GRS for the heavy metals and matrix elements and Colenco takes care of the data concerning the cement system.

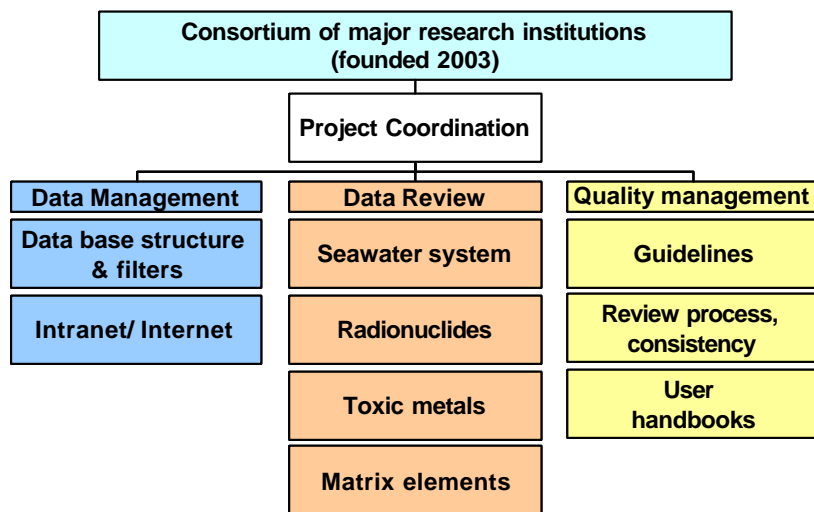


Figure. 2 Project organization

4 CONTENTS AND APPLICABILITY

The data to be incorporated in THEREDA will cover all relevant aqueous species and solid phases necessary to describe the interactions of groundwaters with the waste, the waste matrix, the containers, the host rocks and the materials of the technical barriers. For the host rock salt the components of the sea-water system H-Na-K-Mg-Ca-Cl-SO₄-CO₃-OH-H₂O will be included. For the description of the argillaceous and crystalline host rocks, the waste matrix and the containers in addition to the above mentioned components also Al, Si and Fe

must be incorporated. In a first step the following radionuclides and heavy metals will be included:

- Actinides: Th, U, Np, Pu, Am, Cm, Pa
- Fission products: I, Se, Cs, Rb, Sr, Sm, Tc, Ra
- Heavy metals: Zn, Cr, Co, Ni, Cu, As, Cd, Hg, Pb

As the database must be applicable for low as well as for high ionic strength solutions SIT and Pitzer ion interaction parameters shall be included.

5 DATA MANAGEMENT

In the course of the project tools will be developed which will automatically generate ready-to-use parameter files for important geochemical codes like EQ3/6, PHREEQC and Geochemist's Workbench. The parameter files will be available for free download at the project's web site. Such it is intended to obtain a useful feedback from the users from around the world. Figure 3 illustrates the data management in THEREDA.

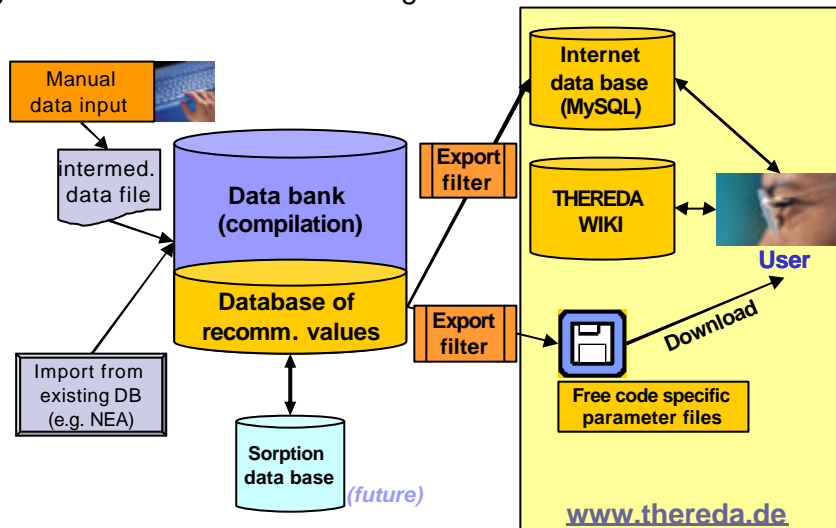


Figure. 3 Data management in THEREDA

6 QUALITY MANAGEMENT

The data review process is the core of the project's quality system. It will be based on quality guidelines the project partners have previously agreed upon. They describe, for example, procedures for the extrapolation of data to the reference temperature and to zero ionic strength. In many cases data for certain species, solids or aqueous equilibria are not available. These missing data may be of great importance nevertheless. In contrary to other databases THEREDA will not only contain data that are based on experimental investigations but also carefully estimated data, if they are needed for performance assessment calculations. The project partners aim to limit the database for real system constituents. If no spectroscopic proof or strong evidence exists, a species will be regarded as a "phantom species" and excluded from the database. In order to achieve the highest possible quality all data that find their way into the final parameter files must be reviewed. Data of a low quality level will not be excluded but their quality will be carefully documented and uncertainties will be assessed. The consistency of THEREDA with CODATA and NEA databases will be observed.

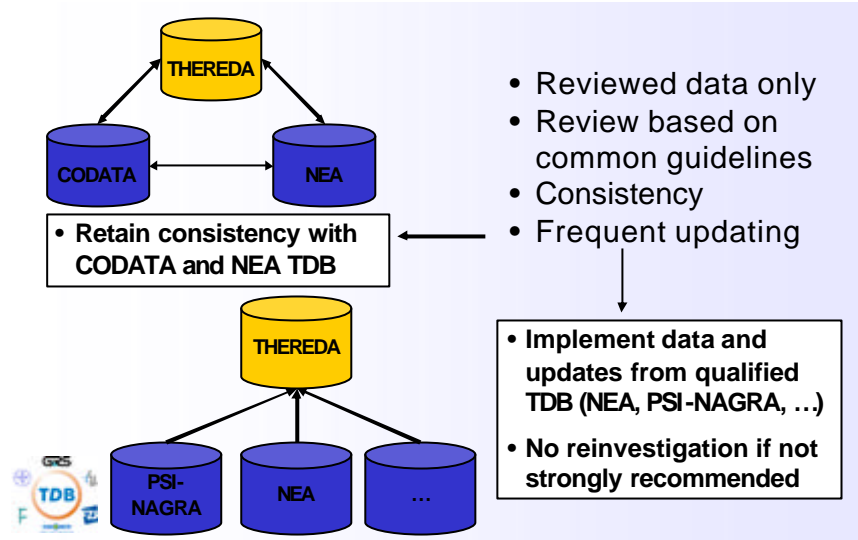


Figure. 4 Procedures for the generation of THEREDA and assurance of data quality and internal and external consistency

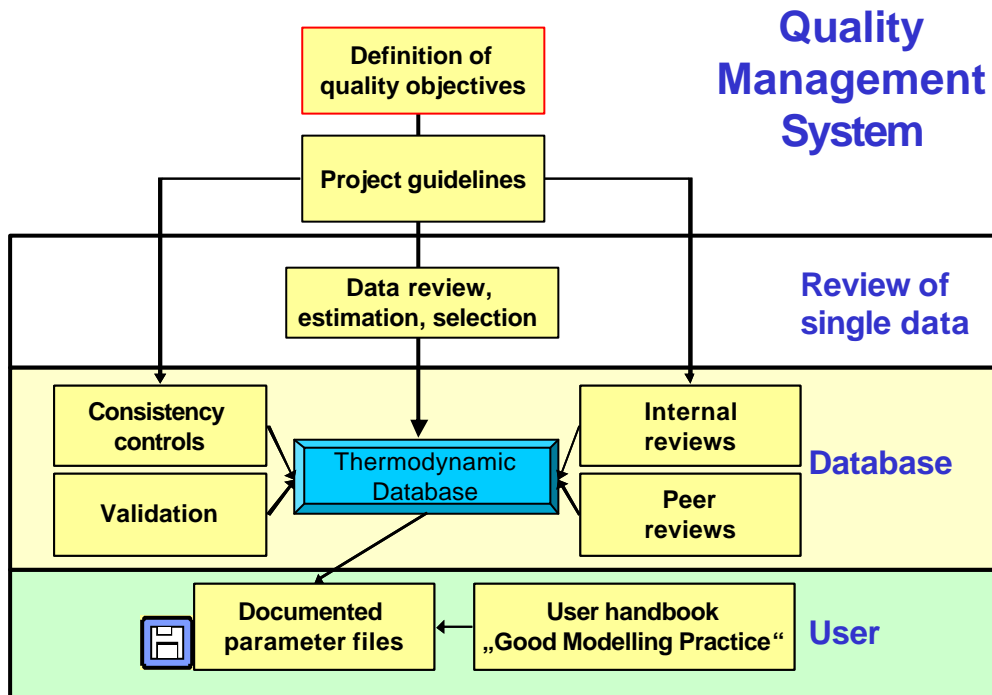


Figure. 5 Quality management system in THEREDA

7 TRANSPARENCY

The most important users of THEREDA will be the participants in the project as they work in the major German institutions involved in radioactive waste management. But THEREDA will be a common and freely accessible data base for all parties involved in the process of repository licensing. Public access is guaranteed. The responsible German governmental institutions, the Federal Ministry of Labour, the Federal Ministry of Education and Research and the Federal Ministry of Environmental Protection and Reactor Safety have been involved in the preparation of the project in an early stage. They are financing the project.

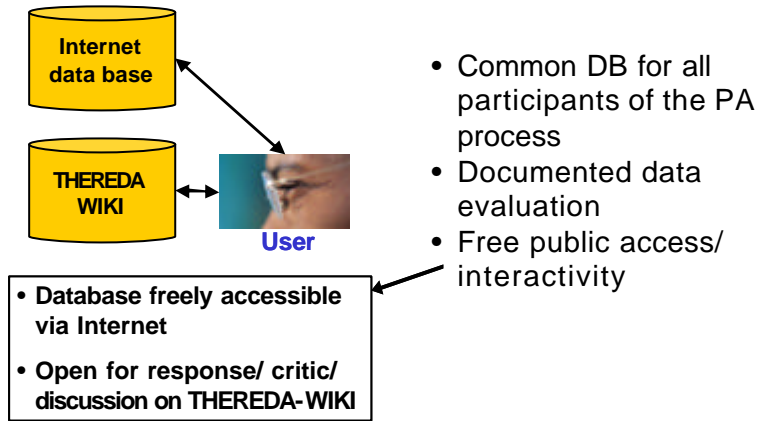


Figure. 6 Highest possible transparency is the philosophy of THEREDA

8 THEREDA ON THE INTERNET

Although the project has just been started an internet side was already set up (www.thereda.de). It will provide the interested user not only with the newest information about the progress of the project but will give direct access to the database and ready-to-use parameter files.

