

THEREDA

The German Database Concept for
Performance Assessment
Studies of Waste Disposal Sites



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THEREDA – Thermodynamic Reference Database

- Background and General Objectives
- Project Organization
- Quality Management System
- Quality Objectives
- Data Management

Background: Prediction of geochemical processes in German underground waste disposal sites

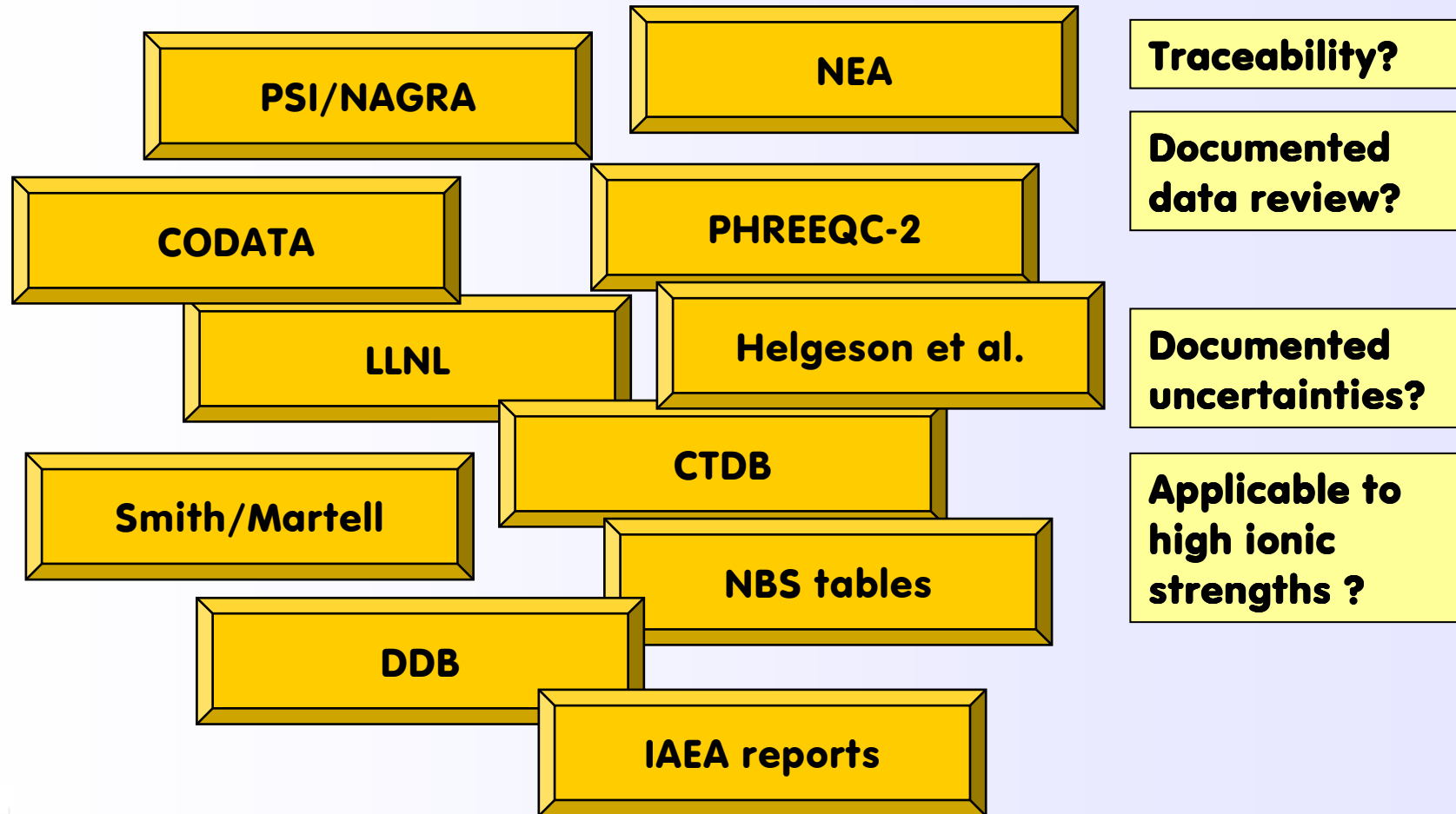
Host rock formations:

- Iron ore
 - Potash rock
 - Salt rock
 - Clay
 - Crystalline rock
- Operating or licensed sites for hazardous and radioactive waste (LLW/MLW)
- Considered for high level radioactive waste

Thermodynamic data needed for:

- Stability of complexes and solid phases, activity coefficients
- Host rock components, radionuclides, other toxic metals
- Temperature about 20 to 90°C (-150°C)
- Ionic strengths up to 15 mol/kg

Another database - aren't there enough already?



→ Existing databases don't fulfil German requirements

Folie 4

h8

Modellierung des Gesamtprozesses nur so gut wie die Modellierungsqualität der Einzelprozesse

has; 14.04.2005

Objectives

Develop a thermodynamic database that

- **enables the prediction of the activity, speciation and solubility of relevant toxic elements in underground waste disposal sites**
- **is applicable from low to high ionic strengths**
- **fulfils specific German quality requirements**
- **will be the reference database for PA studies in Germany**

Project organization

**Consortium of major research institutions
(founded 2003)**



**Gesellschaft für Anlagen- und
Reaktorsicherheit (GRS)**



**Technical University TU Bergakademie
Institut für Anorganische Chemie**



**Forschungszentrum Rossendorf
Institut für Radiochemie (FZR-IRC)**



**Forschungszentrum Karlsruhe
Institut für Nukleare Entsorgung
(FZK-INE)**



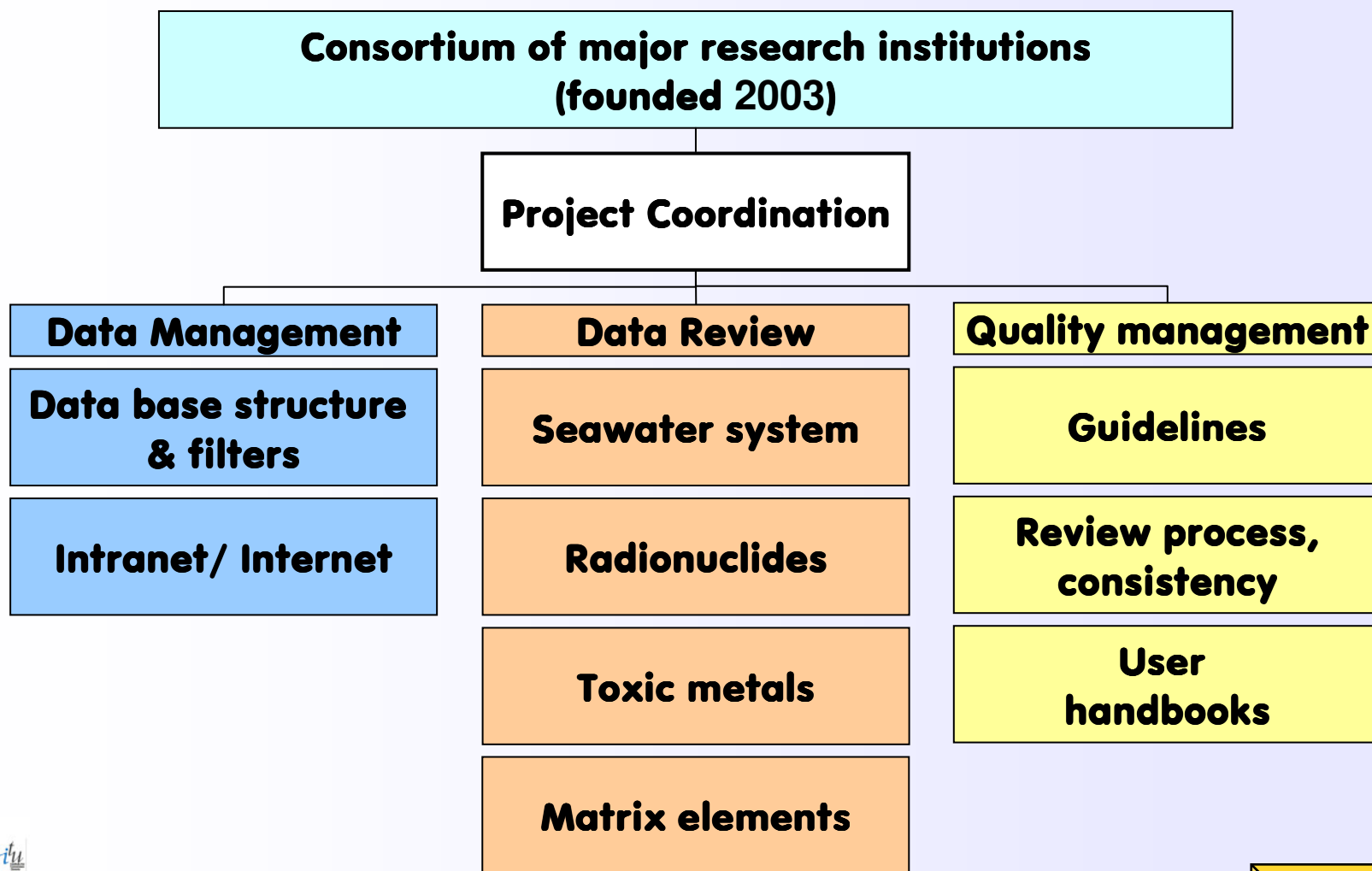
Colenco Power Engineering AG

Colenco Power Engineering AG (CH)



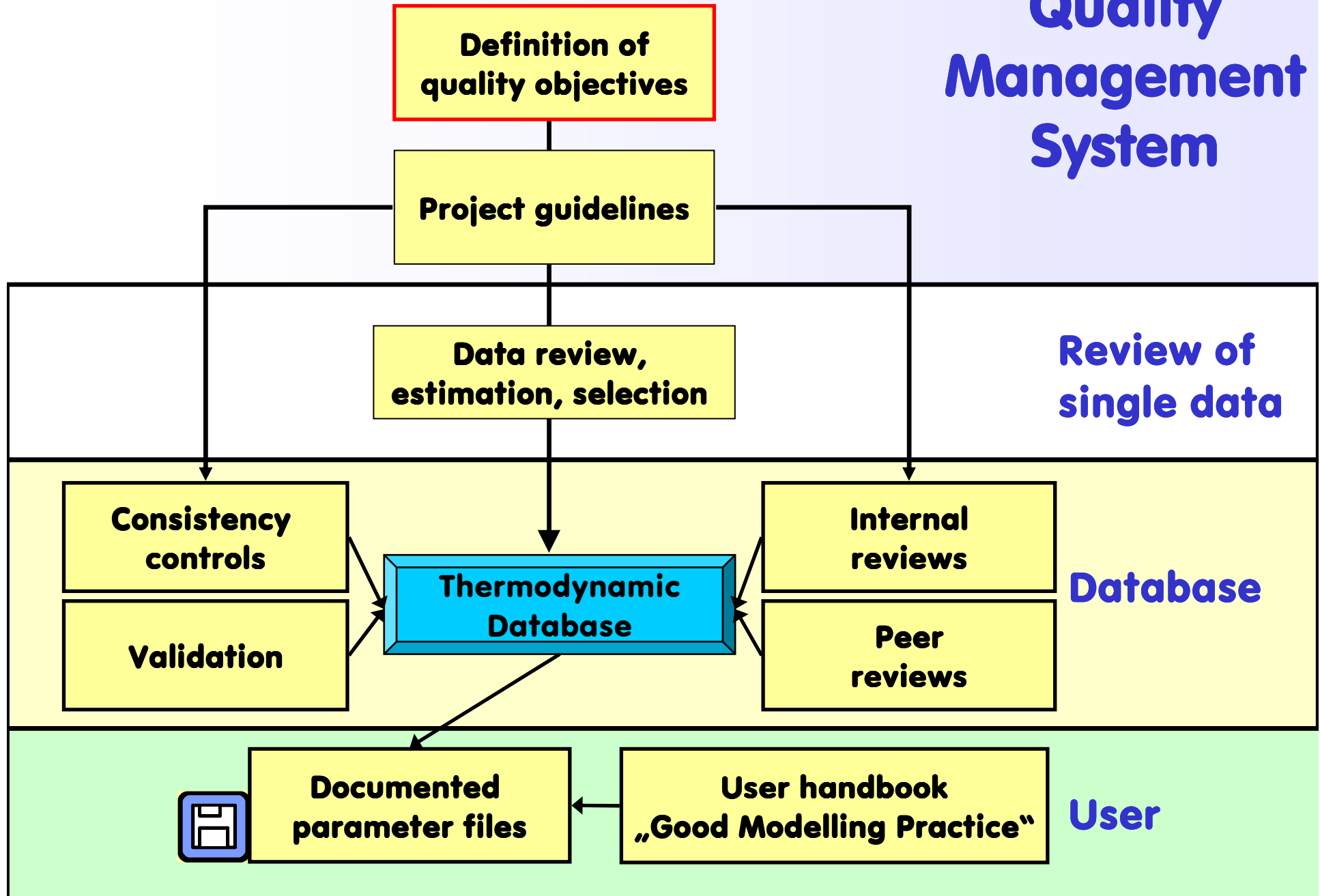
Institut für Transuranelemente (ITU)

Project organization



[Back to overview](#)

Quality Management System



Quality objectives

- **Data quality**
- **Applicability**
- **Transparency**
- **Usability**

Quality objectives: data quality

- Reviewed data only
- Review based on common guidelines
- Consistency
- Frequent updating

Quality objectives: data quality

- **Quality classification (no exclusion but documentation of “bad” data)**
- **Uncertainties**

- **Reviewed data only**
- **Review based on common guidelines**
- **Consistency**
- **Frequent updating**



Quality objectives: data quality

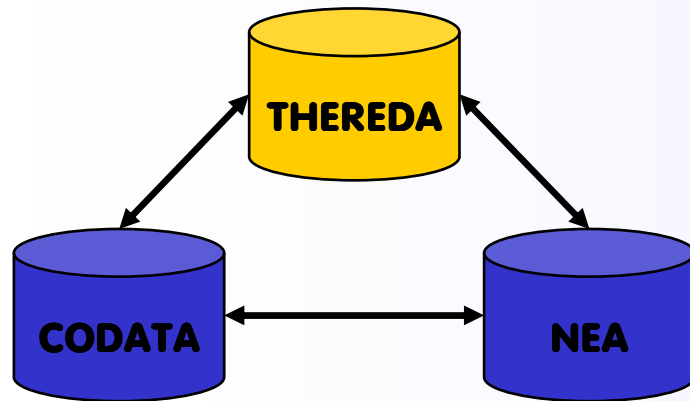
- Definition of:

- Objectives of THEREDA (+)
- Data review process
- Data estimation (+)
- Data uncertainties
- Ionic strength and temperature corrections

- Reviewed data only
- Review based on common guidelines
- Consistency
- Frequent updating

→ Based on NEA-TDB guidelines

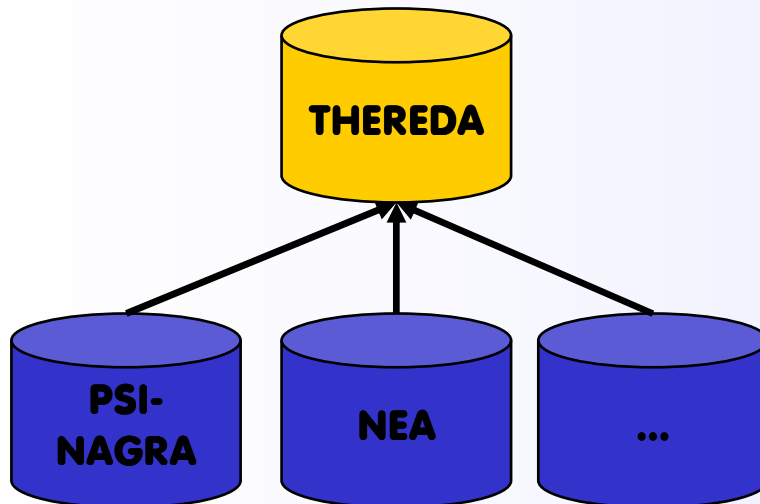
Quality objectives: data quality



- Retain consistency with CODATA and NEA TDB

- Reviewed data only
- Review based on common guidelines
- Consistency
- Frequent updating

- Implement data and updates from qualified TDB (NEA, PSI-NAGRA, ...)
- No reinvestigation if not strongly recommended



Quality objectives: applicability

- **Covers all relevant aqueous species and solid phases**
- **Applicable to high ionic strengths**
- **Validation**

Quality Objectives: applicability

Host Rock components
Seawater system:
H, Na, K, Mg, Ca, Cl, SO₄, CO₃,
OH, H₂O
Granite/ Clay
Al, Fe, Si

**Container, waste matrix
components**

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

- Covers **all relevant aqueous species and solid phases**

- **Applicable to high ionic strengths**

- **Validation**

- **Avoid phantom species and high temperature phases**
- **Include data on minerals**
- **Include reliable estimated data**

Quality objectives: applicability

- **SIT + Pitzer ion interaction parameters**

- **Covers all relevant aqueous species and solid phases**
- **Applicable to high ionic strengths**
- **Validation**

Quality objectives: transparency

- **Common DB for all participants of the PA process**
- **Documentation of data review**
- **Free public access/ Interactivity**
- **Traceability**

Quality objectives: transparency

- **Most important users are participants of the project**
- **Responsible governmental institutions (regulator) are involved in an early stage**

- **Common DB for all participants of the PA process**
- **Documented data evaluation**
- **Public access**

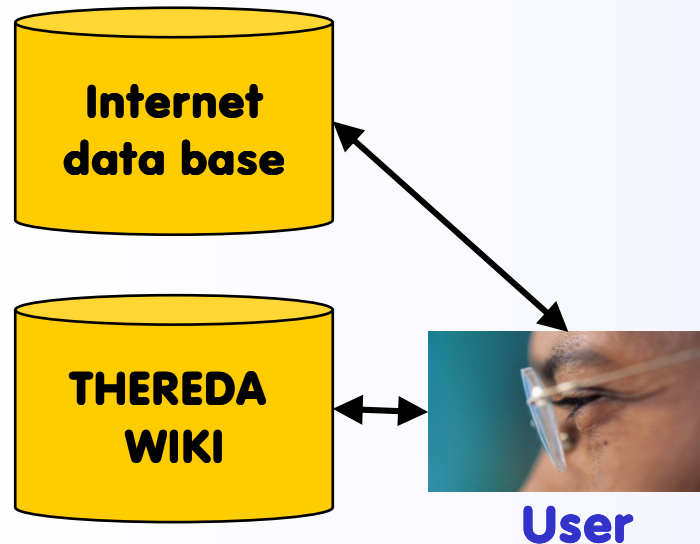
Quality objectives: transparency

- Part of the printed report
- Part of the database
- Live! in the THEREDA-WIKI



- Common DB for all participants of the PA process
- Documentation of data review
- Public access

Quality objectives: transparency



- **Common DB for all participants of the PA process**
- **Documented data evaluation**
- **Free public access/ interactivity**

- **Database freely accessible via Internet**
- **Open for response/ critic/ discussion on THEREDA-WIKI**

Quality objectives: transparency

- **Obligatory for all participants of the PA process**
- **Documented data evaluation**
- **Free public access/ interactivity**
- **Traceability**

- **Back to the primary source**
- **Information on secondary data**



Quality objectives: usability

- **Equilibrium constants**
log K
- **Thermochemical data**
 ΔG , ΔH , S , C_p

- **Code-independent data types**
- **Ready to use parameter files**
- **Long-term availability**



Quality objectives: usability

- Code-independent data types
- Ready to use parameter files
- Long-term availability



User



Free download on
www.thereda.de

Code specific
parameter files

PHREEQC, EQ3/6,
ChemApp, GWB

Quality objectives: usability

- **Continuous updating and maintenance**
- **Long-term support granted by governmental institutions, e.g. regulator**

- **Code-independent data types**
- **Ready to use parameter files**
- **Long-term availability**



Formulation of guidelines: Data classification

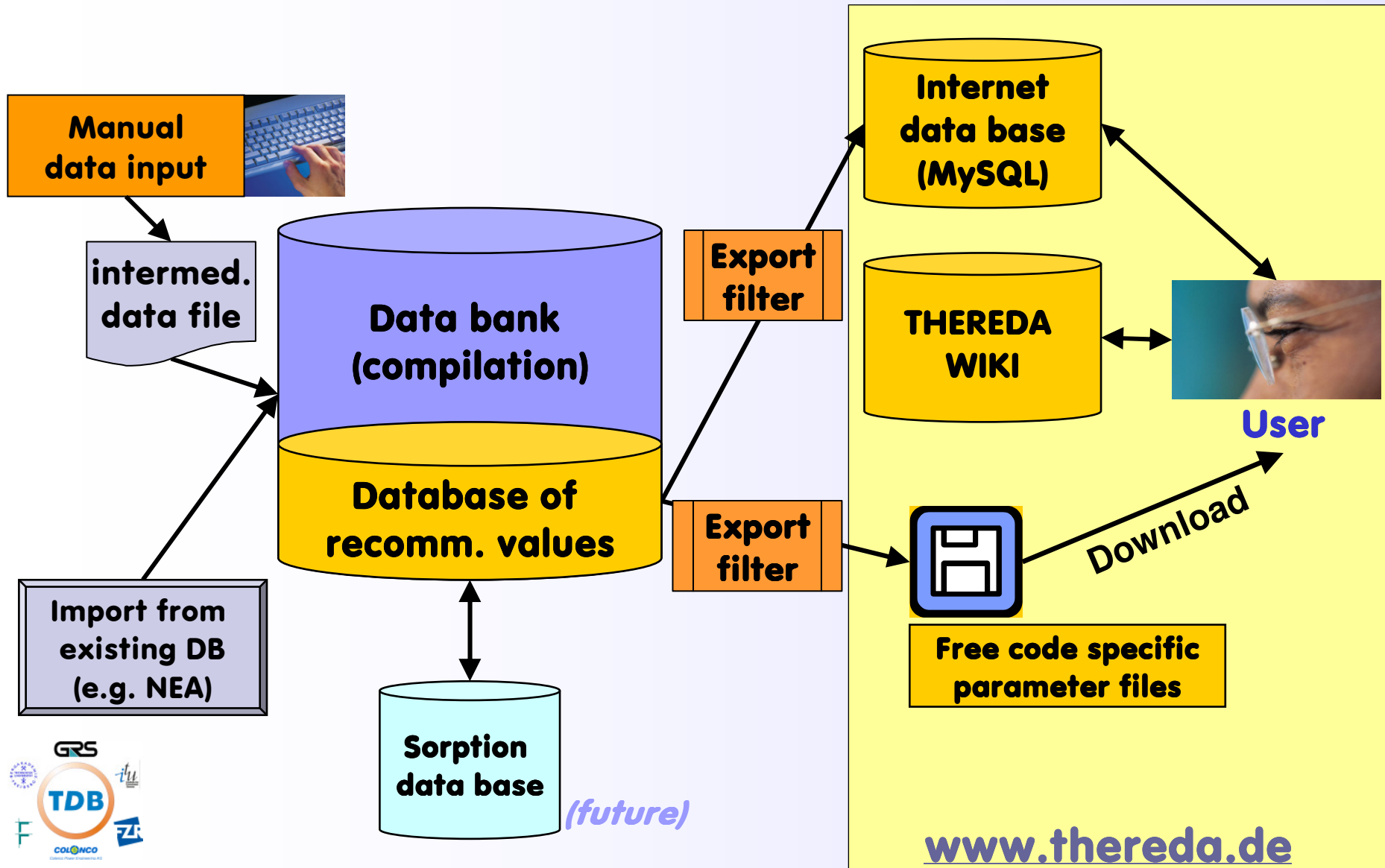
- **Type of experiment (aq. equil./ thermochem./ estim.)**
 - **Data qualification (reviewed?/ several sources?)**
 - **Data quality level (reliable/questionable/unsuitable)**
- **additional information for developers and users of THEREDA**

Guidelines: Data estimation

It's better to estimate thermodynamic data than to omit them

- **Only for important species/solids with insufficient data**
- **Detailed description of estimation algorithms and secondary data used herein**
 - systematic correlations between thermodynamic and physical properties**
 - actinides, lanthanides, transition metals**
 - incl. estimation of uncertainties**

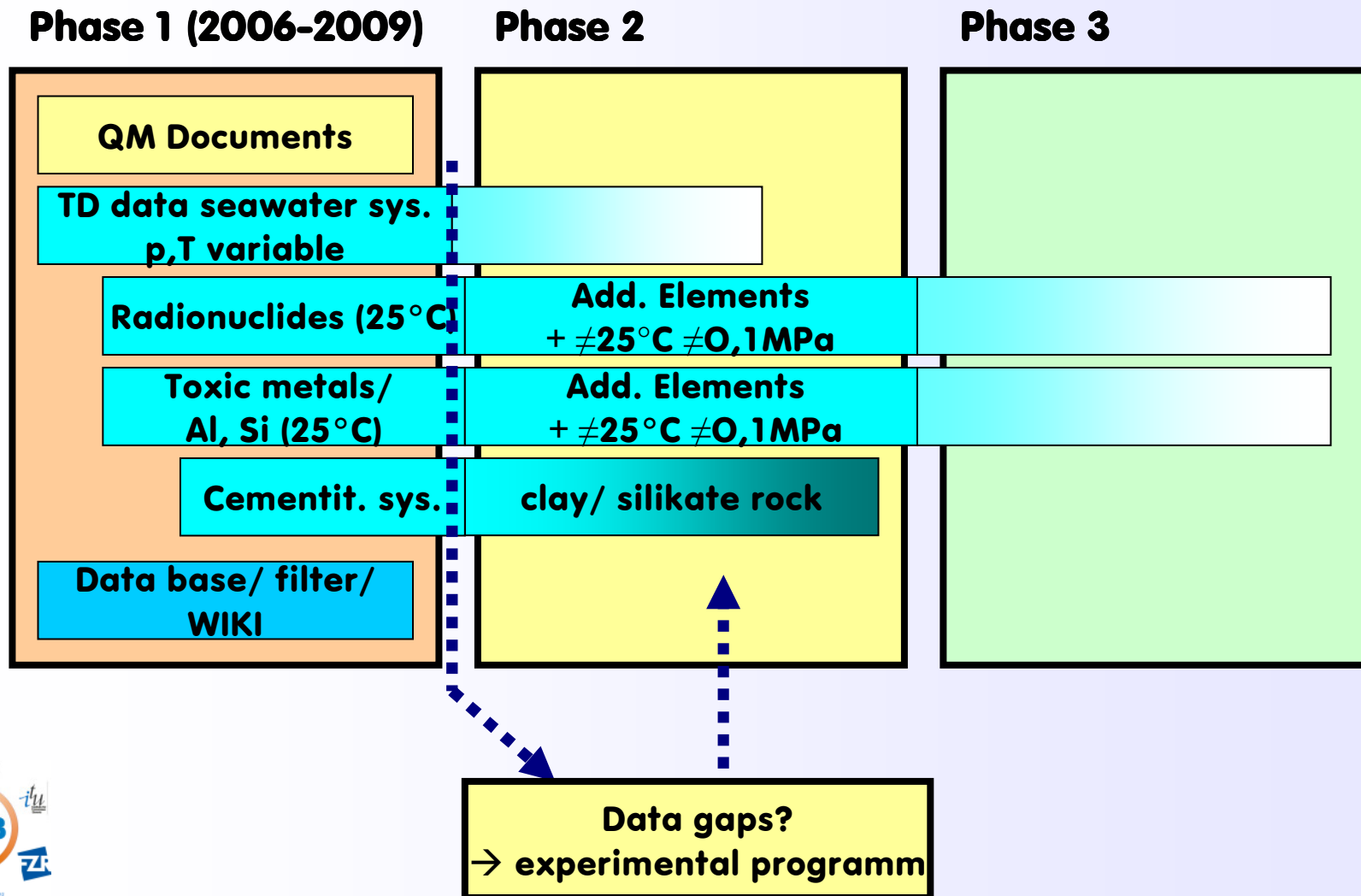
Data management



More than 50% of the work has already been done ...

Data	~1/2 from NEA/CODATA/PSI-NAGRA
Quality management system	Based on NEA-TDB system
Standards and conventions	Orientated to international standards (e.g. IUPAC-ThermoML)
More data?	Open for international cooperation

Time Schedule



THEREDA: Scientific and Technical Benefits

- **Applicable to all relevant geochemical conditions**
- **Consistent with existing quality assured data bases**
- **Data classification and uncertainties help identifying/quantifying modelling risks**
- **Identification of data gaps leads to better focussing of experimental programs**
- **Introduction of estimated values fills data gaps**
- **Free ready-to-use code-specific parameter files**
- **Public access improves review processes and public confidence**
- **First data base version planned for 2009**



Acknowledgements

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Bundesministerium für Wirtschaft und Technologie

Bundesministerium für Umwelt und Reaktorsicherheit/

Bundesamt für Strahlenschutz



http://www.thereda.de/ - Microsoft Internet Explorer

GRS
TDB
F
COL@MCO
TU

THEREDA

Thermodynamische Referenzdatenbasis

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Welcome to THEREDA

THEREDA means Thermodynamic Reference Database. It's a scientific project with the objective of developing of a thermodynamic database that applicable for performance assessment studies for existing or potential underground waste disposal sites.

Why a new database?

There seem to be enough thermodynamic databases in the world already. But on a closer look all of them fail to fulfil the specific requirements that must be considered when dealing with existing or potential underground waste disposal sites in Germany. The most prominent knock-out criterion is the applicability to solutions of high ionic strength

The partners of THEREDA

THEREDA is a cooperative project of several institutes researching on the field of radioactive waste disposal in Germany:

- [Gesellschaft für Anlagen- und Reaktorsicherheit \(GRS\) mbH, Braunschweig \(Germany\)](#)
- [Forschungszentrum Karlsruhe, Institut für Nukleare Entsorgung \(FZK-INE, Germany\)](#)
- [Forschungszentrum Rossendorf, Institut für Radiochemie \(FZK-IRC, Germany\)](#)
- [Technische Universität Bergakademie Freiberg, Institut für Anorganische Chemie \(Germany\)](#)
- [Colenco Power Engineering, Baden \(Switzerland\)](#)
- [Institute for Transuranium Elements \(ITU\), Karlsruhe \(Germany\)](#)

Internet



See you on www.thereda.de !

Thanks!

