WP 18 DITUSC: DEVELOPMENT AND IMPROVEMENT OF THERMODYNAMIC UNDERSTANDING FOR USE IN NUCLEAR WASTE DISPOSAL SAFETY CASE

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WP18 DITUSC - OBJECTIVE

Assessment of the current thermodynamic understanding in support of the Safety Case for radioactive waste disposal, with particular emphasis on a transversal understanding to allow identification of possible future improvements in knowledge and use.

- **Complementarity/synergies** with on-going TDB projects, e.g., NEA-TDB, ThermoChimie, THEREDA, PSI/Nagra TDB, JAEA-TDB, WIPP TDB, Thermoddem, Prodata etc;
- In close collaboration with the End-User Group, other EURAD-2 WPs and key actors of previous EC Projects, **identify, critically assess and prioritize data gaps of relevance to the Safety Case**;
- If possible, definition of **technical approaches** and possible scientific strategies to fill in the identified thermodynamic data gaps;
- **2 main deliverables:**
  - **Green Paper** framing the scope of interactions and take position on several topics relevant to use of thermodynamics (*September 2025*);
  - **White paper** summarizing the outcomes of the data gaps analysis and subsequent prioritization (*January 2026*).

DITUSC WP BREAKDOWN

Task	Task leaders
Task 1 - Management / Coordination of the WP	*ONDRAF/NIRAS & KIT*
Task 2 - Knowledge Management	*JFZ*
Task 3 - Thermodynamics: data gaps, solid-solutions, interplay with kinetics, and Safety Case	*A21 & PSI*

DITUSC TECHNICAL SCOPE

Thermodynamic data gaps

- Chemical elements (relevant elements, RNs, chemotoxics)
- Organic compounds
- Perturbed systems
  - High saline systems
  - High temperature

Thermodynamics of solid-solutions

- Cement phases
- Zeolites
- Carbonates/sulphates

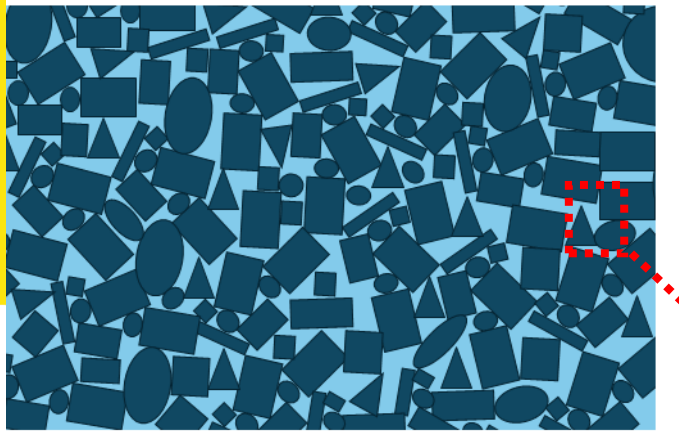
Interplay of thermodynamics and kinetics

- Solid transformations over time
- Redox disequilibrium for key inorganic reactions

Thermodynamics and Safety Case

- End-User needs relevant to the Safety Case

→ Extended to any other relevant topics based on feedback from TDB users and End Users (workshops, interaction meetings and DITUSC survey)

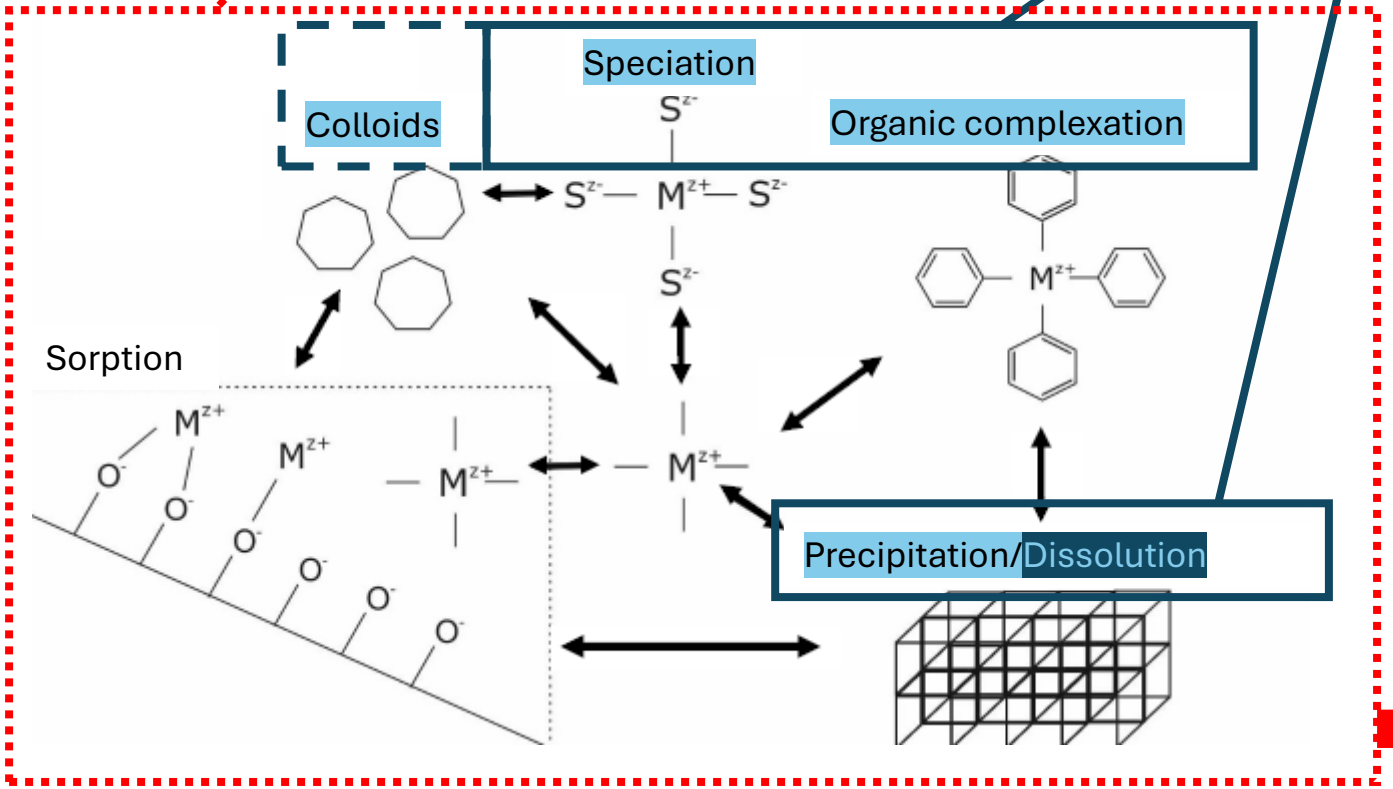


System compenents/conditions/properties

- ***Material-forming solid phases***
- ***Pore-water composition***
- ***Eh***
- ***pH***
- ***Temperature***
- ***(Pressure)***

Example: Porous medium

ELEMENTAL DISTRIBUTION



M=RN, CT, other element[PW/ barriers/waste/…]

λs for chemical species (aqueous/solid):

- **$Log_{10}K°$**
- **$\Delta_r G°_m$**
- **$\Delta_r H°_m$**
- **$\Delta_r S°_m$**
- **$\Delta_f G°_m$**
- **$\Delta_f H°_m$**
- **$S°_m$**
- **$V°_m$**
- **$C°_{p,m}$**

λs for ion interaction models:

- ***ε(j, k)***
- ***Pitzer parameters***

- **Geochemical modelling → Transport parameters**

TDBS – PARAMETERS (λs)

MAIN TYPE GAPS

(From technical discussions, DITUSC survey and direct interactions with the End-User Group and other EURAD-2 WPs)

- Stability constants of system components constitutive phases (e.g., new generation of cement-based materials)
- Data for inorganic speciation and related solubility of a large set of elements (e.g., coffinite solubility, Cu-Cl complexes)
- Stability constants of relevant organics and complexation constants with relevant elements (e.g., Nb-ISA complexes in alkaline environment)
- Existence of ternary complexes and related datasets (e.g., U(IV)-OH-SiO_4)
- Ion interaction model parameters for high saline systems (e.g., sulfate/nitrate perturbations)
- Solid-solutions parameters and possible uptake of RNs (e.g., anion uptake in cement phases)
- Solid phase transformation over time (e.g., time dependency of solubility products)
- Redox disequilibrium (e.g., inorganic redox reactions frequently modelled using kinetics that may influence the redox evolution of repositories)

2ND OPEN WORKSHOP

eurad 2
European Partnership
on Radioactive Waste Management

IMT Atlantique
Bretagne-Pays de la Loire
École Mines-Télécom

NANTES

DEVELOPMENT AND IMPROVEMENT OF THERMODYNAMIC UNDERSTANDING FOR USE IN NUCLEAR WASTE DISPOSAL SAFETY CASE

19-20 November 2025

https://indico.in2p3.fr/event/36375/

(i) Feedback survey
(ii) Prioritization of knowledge/data gaps in relation to the Safety Case

DITUSC

Thank you for your attention !

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