TOPICAL SESSION 2: PREDICTIVE MODELLING OF RN BEHAVIOUR AND THERMODYNAMIC DATABASES (RAMPEC AND DITUSC)

Outcomes

- There is a clear need for improving thermodynamic databases in order to conduct accurate geochemical modelling.
- Conducting **accurate geochemical simulations** is essential for a number of modelling efforts in EURAD-2 and is a necessity for reliable safety assessment.
- There is a need for thermodynamic database development accounting for **speciation schemes** in order to derive correct sorption models.
- **Previous projects clearly identified the need** for thermodynamic data but there were no direct activities deriving new thermodynamic data for inclusion in the projects.
- In order to **avoid a duplication of sorption databases**, there needs to be an emphasis on international networking and knowledge exchange related to this issue.
- DITUSC is providing a state-of-the-art of the data gaps without prioritization at the moment. In the future, the aim of DITUSC is to **prioritize the data gaps** for future studies and for end users.
- The modelling work to be performed in RAMPEC helps to demonstrate the **constraints that occur due to data gaps**.

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Follow-up actions

- Maintain and further enhance the **international networking and knowledge exchange** related to sorption databases.
- **DITUSC workshop in Nantes** in November 2025 with discussions on prioritization and particular emphasis on end user input.

Key Takeaway

 There is a general consensus on the relevance of thermodynamic databases and that significant potential exists for their continued improvement.

