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Work Package 18 - DITUSC



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Executive Summary

The EURAD-2 Work Package (WP) "Development and Improvement of Thermodynamic Understanding for Use in Nuclear Waste Disposal Safety Case (DITUSC)" is a Strategic Study aiming to assess the current state of thermodynamic knowledge supporting the radioactive waste disposal Safety Case. DITUSC intends to identify knowledge gaps and evaluate strategies for improving the completeness of thermodynamic databases (TDB). It is foreseen to establish a common vision across the three EURAD-2 colleges for promoting future research and development initiatives to improve the application of thermodynamics in the Safety Case. The WP emphasises stakeholder engagement to understand their perspectives and needs regarding thermodynamic data and their use in relevant scenarios through various communication channels. To this end, DITUSC organized a series of virtual bilateral exchanges with key R&D Work Packages to identify, discuss, and align on critical thermodynamic knowledge gaps. This document presents both a high-level overview of cross-Work Package interactions and the resulting prioritized list of thermodynamic data gaps, forming part of the basis for the data gap prioritization evaluation conducted at the DITUSC Open Workshop in Nantes (19 to 20 November 2025).

Keywords

DITUSC, Thermodynamics, data gaps

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1. Introduction

The EURAD-2 Work Package (WP) "Development and Improvement of Thermodynamic Understanding for Use in Nuclear Waste Disposal Safety Case (DITUSC)" is a Strategic Study focused on assessing the current state of thermodynamic knowledge supporting the radioactive waste disposal Safety Case. DITUSC aims to identify knowledge gaps, evaluate strategies to improve thermodynamic databases (TDBs), and establish a common vision across the three EURAD-2 colleges to guide future research on relevant key aspects of the Safety Case. The WP also engages stakeholders to understand their perspectives, possible needs and priorities regarding thermodynamic data and its application in relevant scenarios.

Virtual Bilateral Exchanges: To achieve these objectives, DITUSC conducted a series of virtual bilateral meetings with technical Work Packages: WP8 SAREC, WP9 InCoManD, WP12 RAMPEC, WP13 OPTI, WP14 SUDOKU, and WP16 HERMES. Each WP presented its challenges and highlighted missing thermodynamic data, identifying areas where updated datasets, new experiments, or improved database consistency are needed to enable relevant and reliable modelling to be conducted. Recurring themes included uncertainties in cementitious systems under perturbed conditions, high ionic strength and temperature, gaps in radionuclide/organic interactions, stability of corrosion products and secondary phases, and challenges in solid solutions, redox processes, and kinetics.

RAMPEC & DITUSC Topical Session in Bologna: Following the bilateral meetings, a joint RAMPEC & DITUSC session was held at the EURAD-2 Annual Meeting in Bologna. The session focused on Predictive Modelling of Radionuclide Behaviour and Thermodynamic Databases, identifying improvements in geochemical modelling and opportunities to update thermodynamic databases.

Key points included:

- i. The need for better thermodynamic data to enable accurate geochemical simulations;
- ii. Ensuring consistent speciation and reliable sorption models;
- iii. Strengthening international knowledge exchange to avoid duplication of sorption databases;
- iv. Highlighting limitations caused by current data gaps through RAMPEC modelling.

Compilation and Prioritisation of Knowledge Gaps: All knowledge gaps identified through the virtual meetings and the Bologna session were compiled by the DITUSC team. This compilation formed the part of the basis for the data gap prioritisation conducted at the DITUSC Open Workshop in Nantes (19 to 20 November 2025), where each gap was evaluated for its significance and relevance to the safety of radioactive waste repositories by each represented organisation.

2. Summary of the exchanges

To provide a clear overview of the interactions between DITUSC and other EURAD-2 Work Packages, the key knowledge gaps identified during bilateral exchanges and the RAMPEC/DITUSC workshop in Bologna have been summarized below. The table highlights the main areas of scientific interest, recurring themes across WPs, and cross WP synergies that informed the prioritization of data gaps at the DITUSC Open Workshop in Nantes.

WP	Interaction Type	Data Gaps identified	Cross-WP Synergies	Actions undertaken
SAREC	Virtual	U(IV)-silicate interactions; secondary phases of doped fuels; epoxy degradation products; solid solution formation; U(VI)-peroxo complexes	Aligns with DITUSC Subtasks 3.1, 3.2 & 3.4	Share progress of DITUSC subtasks; updated SAREC-related data gaps for Open Workshop
InCoManD	Virtual	Thermodynamic data for traditional and innovative container materials; corrosion products in bentonite; Cu-Cl complexes	Overlaps with DITUSC focus on cement and clay interactions	Provide data gaps; participate in topical meetings
RAMPEC	Virtual + Bologna workshop	Radionuclide-organics; cement alteration under perturbed conditions; SIT/Pitzer thermodynamic modelling; zeolites	Strong overlap with DITUSC Subtasks 3.1 & 3.4	Update data gaps by Task; participate in 2nd DITUSC Open Workshop
OPTI	Virtual	Optimization of HLW repository structures; interface between concrete and clay; zeolite formation	Links to DITUSC Subtask 3.3 on cement phases and secondary minerals	Share case studies; review DITUSC Subtask 3.3
SUDOKU	Virtual	Degradation of cement barriers; radionuclide mobility; high ionic strength systems	Supports DITUSC evaluation of cement degradation and high-salinity conditions	Provide feedback via shared partners; participation in modeling workshop
HERMES	Virtual bilateral		Links to DITUSC technical evaluation on high-T, high-salinity systems	Share evaluation results of DITUSC for high T / high ionic strength systems