EURAD-2 WP description Template #2

Please see Instructions for Work Package Preparation Team, public document for guidance (available on EURAD and PREDIS websites)

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<table>
<tr><td>Short Acronym and full Title</td><td colspan="3">DITUSC: Development and Improvement of Quality Assured Thermodynamic Understanding for use in Nuclear Waste Disposal Safety Case</td></tr>
<tr><td>Type of activity</td><td>☐R&D</td><td>☒Strategic Study</td><td>Knowledge Management – covered by a separate committee and template</td></tr>
<tr><td>Budget estimation (total budget in M€, i.e ~ 1.5 M€)</td><td>0.5</td><td>Duration of the WP
(in months)</td><td>18</td></tr>
<tr><td>Links with EURAD SRA / Roadmap Themes
(if multiple choices, indicate the primary link in bold – maximum 3)</td><td colspan="3">☐Programme Management (Theme 1)
☐Pre-disposal (Theme 2)
☒Engineered Barrier Systems (Theme 3)
☒Geoscience (Theme 4)
☐Disposal facility design and optimisation (Theme 5)
☐Siting and Licensing (Theme 6)
☒Safety Case (Theme 7)</td></tr>
<tr><td>Links with EURAD SRA topics
(if multiple choices, indicate the primary link in bold – maximum 3)</td><td colspan="3">4.2.1 Perturbations
4.4.1 Geo-datasets and conceptual models
7.2.2 […] Further develop transparent and quality assured thermodynamic databases for use in performance assessments and supporting models.</td></tr>
<tr><td rowspan="2">SRA drivers (maximum 3)</td><td>☒Implementation Safety</td><td>☐Tailored Solutions</td><td>☒Scientific Insight</td></tr>
<tr><td>☐Innovation for Optimisation</td><td>☐Societal Engagement</td><td>☒Knowledge Management</td></tr>
<tr><td>Objective (What) – 1 sentence</td><td colspan="3">Quality assured thermodynamic understanding and data in support of the Nuclear Waste Disposal Safety Case, with special focus given to a transversal understanding, i.e. with all actors involved.</td></tr>
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Justification: impact / innovation / added-value (Why) – bullet points or short paragraph **(maximum quarter of a page)**	This WP targets the improvement and consolidation of the knowledge to predict processes over long timescales in key fields for geological disposal of radioactive waste. Beyond the need to identify, critically assess and eventually close existing data gaps and maintaining the know-how in the area of thermodynamics, this WP supports present and future capabilities to perform reliable use of thermodynamic model calculations for the performance evaluation of various disposal configurations, for Safety Analyses and the development of the Safety Case. Special focus is given to the thermodynamic description of perturbations, including temperature, high saline / pH conditions, organics and redox. Current reactive transport models often fail to describe the formation of zeolites at the cement clay interface (observed experimentally) due to lacking thermodynamic data. Special focus is given to the interplay of thermodynamics and kinetics, and the possible implications for the Safety Case. As a strategic study, this WP aims at developing a white paper on the thermodynamic understanding for use in Nuclear Waste Disposal Safety Case.
List of planned tasks / subtasks with % of effort per task (5% increments) **(Maximum 10 bullets)**	• Task 1 (10%): Management/coordination of the WP. • Task 2 (10%): Knowledge Management. • Task 3 (15%): Thermodynamic data gaps. Identification of data gaps within the NEA-TDB project and beyond, e.g., organics, zeolites, RN in relevant oxidation states / boundary conditions. Seek for synergies with on-going projects (NEA-TDB, ThermoChimie, THEREDA, etc.). A precise definition of the systems to be covered in the gap analysis will be completed in the next proposal step. • Task 4 (15%): Perturbed systems. Thermodynamics in high saline systems (e.g., nitrate, chloride) and elevated T conditions (< 150 °C), including estimation methods. • Task 5 (15%): Thermodynamics of solid-solutions, including clay or cement systems, zeolites, baryte, LDH, with emphasis on end-members incorporating anionic species / RN. • Task 6 (15%): Interplay of thermodynamics and kinetics, including solid phases (transformation (am) → (cr)), redox phenomena, spent fuel dissolution, etc. Seek for synergies with on-going projects. • Task 7 (20%): Thermodynamics and safety case. Integral assessment and documentation. [Note: task to be implemented if participation of WMOs is confirmed]
List of expected outcomes linked to the identified SRA drivers **(Maximum 6 bullets)**	• Summary of state of knowledge for thermodynamic understanding of identified SRA drivers, as prepared by teams of experts (2-3 per Task) • Involvement of the EURAD community, including: o Exchange meetings with WP leaders and target experts (national, international) with the aim of implementing lessons learnt from previous projects (t = 3 months). o Exchange meetings with other WPs in EURAD II (t = 3 + 12 months). Several of the proposed WPs have been identified as (potential) users of thermodynamic data, and close interaction with them will be specifically targeted (e.g. WP9 Spent fuel B, WP11 Containers / Canisters, WP12 Bentonite /

	Buffers / Backfills, WP15 Radionuclides, WP17 Digital Twins, WP18 High-fidelity numerical simulations, WP21 Natural analogues). o Series of workshops focussing on the individual Tasks, feeding also into the state of knowledge document and identification of gaps and limitations. The workshops will be open to any interested parties. [Tool purposedly used to trigger the exchange with WMOs, in case they finally do not actively participate as partners in the WP] o Training actions, with focus on students and young post-doc / researchers, of course open to all interested colleagues / partners. • Identification and prioritisation of needs from the three colleges. • Complementarity / synergies with on-going thermodynamic projects, e.g., NEA-TDB, ThermoChimie, THEREDA, PSI/Nagra TDB, etc. Workshops with TDB-projects will be targeted to promote communication and avoid redundancies.
Deliverables **(Maximum 6 – including the prescribed deliverables)**	• Document summarizing individual Task-level workshops (t = 6 + 12 months). • White paper on the thermodynamic understanding for use in Nuclear Waste Disposal Safety Case (t = 18 months), including: o State-of-the-art summary of the systems considered within Tasks 3 to 6. o Definition of priorities and actions to fill-in limitations / gaps identified. • Outcome/impacts report to Member States and End Users (prescribed Deliverable for all WPs). A list of milestones will be included in the next step of the WP preparation. This will include a milestone defining the specific topics to be tackled in the scheduled workshops. The documents summarizing the main outcomes of the individual workshops will be also defined as milestones.
Critical input requirements & identified risks	• Limited feedback from EURAD community. (low risk, except for Task 7 if WMOs are finally not willing to join) • Tasks not working in a complementary way. (low risk)
Major achievements expected by end of Year 2 (Go/No Assessment)[1]	This strategic study is envisaged with a total length of 18 months. As major achievement, the study will provide to the RE, TSO and WMO colleges with detailed information on the current status and potential future needs for an improved thermodynamic understanding in the context of the SRA drivers Engineered Barrier Systems (Theme 3), Geoscience (Theme 4), Disposal facility design and optimisation (Theme 5) and ultimately for the Safety Case (Theme 7).

[1] EC budget being only allocated for the first 2 years, each work package progress will be reviewed at the end of Year 2, to assess its continuation based on the total budget that EURAD-2 will be granted.

(Maximum 5 bullets)	
(Optional - Explain what is out of the scope?)	Review of existing studies to derive thermodynamic data. Hydraulic and mechanical properties. Experimental studies. Modelling studies.
List of preliminary interested organisations as partners in the WP contributing effort; **% of effort (person months, by College)**	The list below corresponds to organizations that have expressed interest in this WP, but does not imply the participation in the WP. The WP is aiming at a joint evaluation of the different topics, ideally with equal share between colleges (33%). **REs:** KIT (DE), Subatech (FR), Amphos21 (ES), FZJ (DE), PSI (CH), SCK-CEN (BE), Uni Szeged (HU), Empa (CH), Uni Delft (NE), Uni Manchester (UK), BRGM (FR), CEA (FR), HZDR (DE), Uni Bern (CH), UJV (CZ), CTU (CZ) **TSOs:** CIEMAT (ES), GRS (DE), VTT (FIN), SURO(CZ). **WMOs?**: (To be identified after evaluation of Template #2 since this WP proposal has been rethought as a strategic study.)
If applicable - links with previous projects / work packages	CORI, FUTURE, CEBAMA, ReCoSy, MICADO. Several others where thermodynamic data are used or have been used to evaluate experimental studies or are key requirements in modeling studies.
WP Preparation Team (1 member per College) contact (**organisation + person**, email)	RE: Xavier Gaona (KIT, xavier.gaona@kit.edu) TSO: Tiziana Missana (CIEMAT, tiziana.missana@ciemat.es) WMO: Stéphane Brassinnes (ONDRAF-NIRAS, S.Brassinnes@nirond.be) CG observer: Lara Duro (Amphos21, lara.duro@amphos21.com)