EURAD-2 2nd wave Template #2

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Short Acronym and full Title	THermodynamic Experimental Research and Methods for Overcoming Gaps in Analysing Performance (ThermoGAP)		
Type of activity	☒R&D	☐Strategic Study	
Budget estimation (total budget in M€, i.e ~ 1.5 M€)	3 M€	Duration of the WP (in months)	36
Links with EURAD SRA / Roadmap Themes (if multiple choices, indicate the primary link **in bold – maximum 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)**		
Links with EURAD SRA topics (if multiple choices, indicate the primary link **in bold – maximum 3)**	- **7.3.1 Performance assessment and system models** - 3.4.1 EBS system - 4.4.1 Geo-datasets and conceptual models		
SRA drivers **(maximum 3)**	☒Implementation Safety	☐Tailored Solutions	☒Scientific Insight
	☒Innovation for Optimisation	☐Societal Engagement	☐Knowledge Management
Objective (What) – **1 sentence**	Based on the outcomes of EURAD-2 DITUSC Strategic Study, to advance thermodynamic understanding for safety-critical issues—such as low-sorbing radionuclides, complex chemical interactions (ternary-quaternary complexes), and overlooked beneficial processes like anion uptake in solids—by integrating experiments with model development to fill gaps and provide reliable methods and actionable recommendations that reduce uncertainty and support robust safety assessments		

Justification: impact / innovation / added-value (Why) – bullet points or short paragraph **(maximum quarter of a page)**	- Provide scientific evidence on previously overlooked processes –both beneficial and detrimental processes to safety - by addressing data and knowledge gaps with the goal of increase safety margins. - Assess the adequacy of thermodynamic databases (TDBs) for modelling chemical evolution of disposal system components, including novel materials and poorly defined degradation products. - Standardize and harmonize the format of experimental data to improve consistency, usability, and integration with existing TDB programs. - Develop best practices and recommendations to facilitate the integration of safety-relevant new thermodynamic data and models into Performance Assessment and Safety Analysis processes. - Engage with civil society on specific topics to demonstrate the complete thermodynamic workflow - from data collection to application in performance and safety assessment - and highlight its value while building trust with Civil Society.

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.
	  o 2.3. Harmonization and format of generated experimental and thermodynamic data tables
	- **Task 3** (50%): Improvement of scientific basis to feed thermodynamics databases (experimental work & estimation methods, based on joint (WMO, TSO, RE) prioritization exercise conducted within WP18 DITUSC StSt):
	  o 3.1 Cement systems, including new cement materials
	  o 3.2 Fe/S/Se redox and solubility topics
	  o 3.3 Ternary/quaternary systems
	  o 3.4 High saline systems, including sulfate and mixed saline systems
	  College: RE, TSO, WMO
	- **Task 4** (10%): Thermodynamic model development and refinement
	  o 4.1 Development of solid solutions models
	  o 4.2 Verification approaches, sensitivity studies, uncertainty propagation, approaches for the decrease of conservatism
	  College: RE, TSO, WMO
	- **Task 5** (15%): Development of methodologies/recommendations for applications in the Safety Case
	  College: WMO, TSO, RE
	- **Task 6** (5%): Communication and interactions with Civil Society to build trust around reference cases
	  College: TSO, WMO, RE

List of expected outcomes linked to the identified SRA drivers **(Maximum 6 bullets)**	- **Implementation for safety:** To increase confidence in current safety assessment approaches and, where possible, develop methodologies to enhance safety margins for critical system, including poorly retarded radionuclides and -complexation processes that can enhance radionuclide mobility - **Scientific Insight:** To extend knowledge of key safety-relevant processes, standardize experimental and thermodynamic data format and develop usable thermodynamic models. - **Innovation for Optimisation:** Evaluate the ability to model the chemical evolution of novel materials and enable informed decisions on optimisation routes, such as material selection, refinement of waste acceptance criteria to maximise the safe disposal of inventories.
Deliverables **(Maximum 6 – including the prescribed deliverables)**	• D1 – SOTA report – state-of-the-art report on relevant systems/processes • D2 – Update SOTA report • D3 – Methodologies and recommendations for Performance Assessment and Safety Analysis • D4 – Documentation of interactions with Civil Society • D5 – Outcome to Member States A list of milestones will be included in the next step of the WP preparation.
Critical input requirements & identified risks	• Tasks not working in a complementary way (low risk) • Poor engagement of WMOs for part on SA/PA
(Optional - Explain what is out of the scope?)	Modelling beyond the development of the thermodynamic models themselves BUT we do foresee synergies with modelling initiatives in relevant R&D WP.
List of preliminary interested organisations as partners in the WP contributing effort; **% of effort (person months, by College)**	**WMO (25%): 3 + 6 end users** <u>As partners:</u> SKB (Sweden), NIRAS-ONDRAF (Belgium), KORAD (South Korea) <u>As end users:</u> Andra (France), Nagra (Switzerland), BGE (Germany), NWS (United Kingdom), US Department of Energy (Office of Nuclear Energy, Office of Spent Fuel and High-Level Waste Disposition, USA), NWMO (Canada) **TSO (30%): 6** EU MS: ASNR (France), CIEMAT (Spain), GRS (Germany), NMBU (Norway), VTT (Finland), NTW (France) **RE (45%): 7 + 8 non-EU**

	KIT (Germany), SCK (Belgium), Amphos21 (Spain), FZJ (Germany), BRGM (France), CEA (France), UFZ (Germany), PSI (Switzerland), EMPA (Switzerland), LLNL (USA), Sandia NL (USA), PNNL (USA), Kyoto University (Japan), JAEA (Japan), GSL (United Kingdom)
If applicable - links with previous projects / work packages	Ongoing projects (EURAD II): WP12 RAMPEC, WP8 SAREC, WP9 INCOMAND, WP16 HERMES, WP6 STREAM, WP14 SUDOKU, WP18 DITUSC Previous EC projects: FUTURE, CORI, SKIN, RECOSY, (CATCLAY), CEBAMA
WP Preparation Team (1 member per College) contact (**organisation + person**, email)	WMO: NIRAS-ONDRAF – Stéphane BRASSINNES – s.brassinnes@nirond.be TSO: CIEMAT – Tiziana MISSANA - tiziana.missana@ciemat.es RE: KIT INE – Xavier GAONA - xavier.gaona@kit.edu