

THERMOGAP

Thermodynamic Experimental Research and Methods for Overcoming Gaps in Analysing Performance

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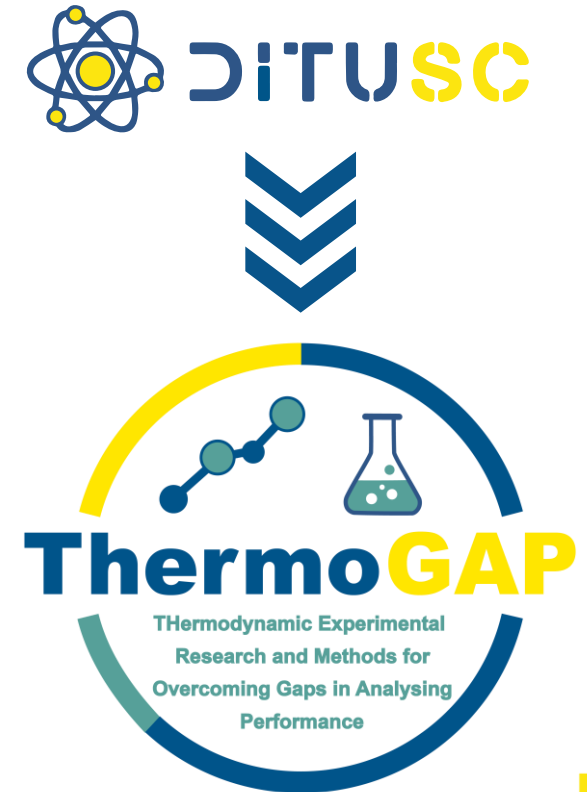


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Thermodynamic Experimental Research and Methods for Overcoming Gaps in Analysing Performance - ThermoGAP

“Advance thermodynamic understanding by closing key safety-relevant gaps and delivering reliable methods that reduce uncertainty and strengthen safety assessments and engaging civil society representatives”

- **Project built on the outcomes of EURAD-2 DITUSC Strategic Study (2024-2026)**
 - Transversal shared vision on possible future R&D needs to support the Safety Case
 - Short-term and longer-term calls to action as defined in DITUSC White Paper
- **3-Y R&D Work Package**
 - Focus on radionuclides, whereas non-radioactive CTs have been discarded
- **PME total = c.a. 256 PME (funded at 50% for eligible partners)**



eu[r]ad 2

THERMOGAP CONSORTIUM

28 organisations from 13 countries

- 17 eligible for EC funding
- 11 non-eligible for EC funding

Partners (P)

- 9 Research Entities
- (5+1) Technical Safety Organisations
- 2 Waste Management Organisations

Associated Partners (AP)

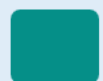
- 7 "Research Entities"
- 1 "Technical Safety Organisation"
- 3 "Waste Management Organisations"

	Countries	#
P	Belgium	2
	EU CS	1
	Finland	2
	France	2
	Germany	4
	Slovenia	1
	Spain	2
	Sweden	1
	Switzerland	2
AP	Japan	2
	Norway	1
	South Korea	3
	UK	1
	USA	4



Registration as an End User is now open !

Task	Subtask	(A) P involvement	Leader	Co-Leader
T1 Management and coordination of the Work Package	1.1 S/T coordination		S. BRASSINNES	X. GAONA
	1.2 Dissemination / outreach / impact			
	1.3 Quality control			
T2 Knowledge Management	2.1 Development of documentation materials (SotA)	To be defined	U. ALONSO	
	2.2 Training materials	To be defined		
	2.3 Harmonization & format of experimental and thermodynamic data tables			
T3 Improvement of scientific basis to feed thermodynamics databases (experimental work & estimation methods)	3.1 Cement systems, including new cement materials		P. REILLER	X. GAONA
	3.2 Fe/S/Se redox and solubility topics			
	3.3 Ternary/quaternary systems			
	3.4 High saline systems, including sulfate and mixed saline systems			
T4 Thermodynamic model development and refinement	4.1 Development of solid solutions models		G-D. MIRON	J. POONOOSAMY
	4.2 Verification approaches, sensitivity studies, uncertainty propagation, approaches for the decrease of conservatism			
T5 Development of methodologies/recommendations for applications in the Safety Case	5.1 Baseline – how current Safety Cases compensate for the lack of knowledge resulting from gaps in thermodynamic data		A-M. JAKOBSSON	E. VEILLY
	5.2 Evaluation – simplified cases, assessment, methodologies/practices, and communication			



Research Entities



Technical Safety Organisations

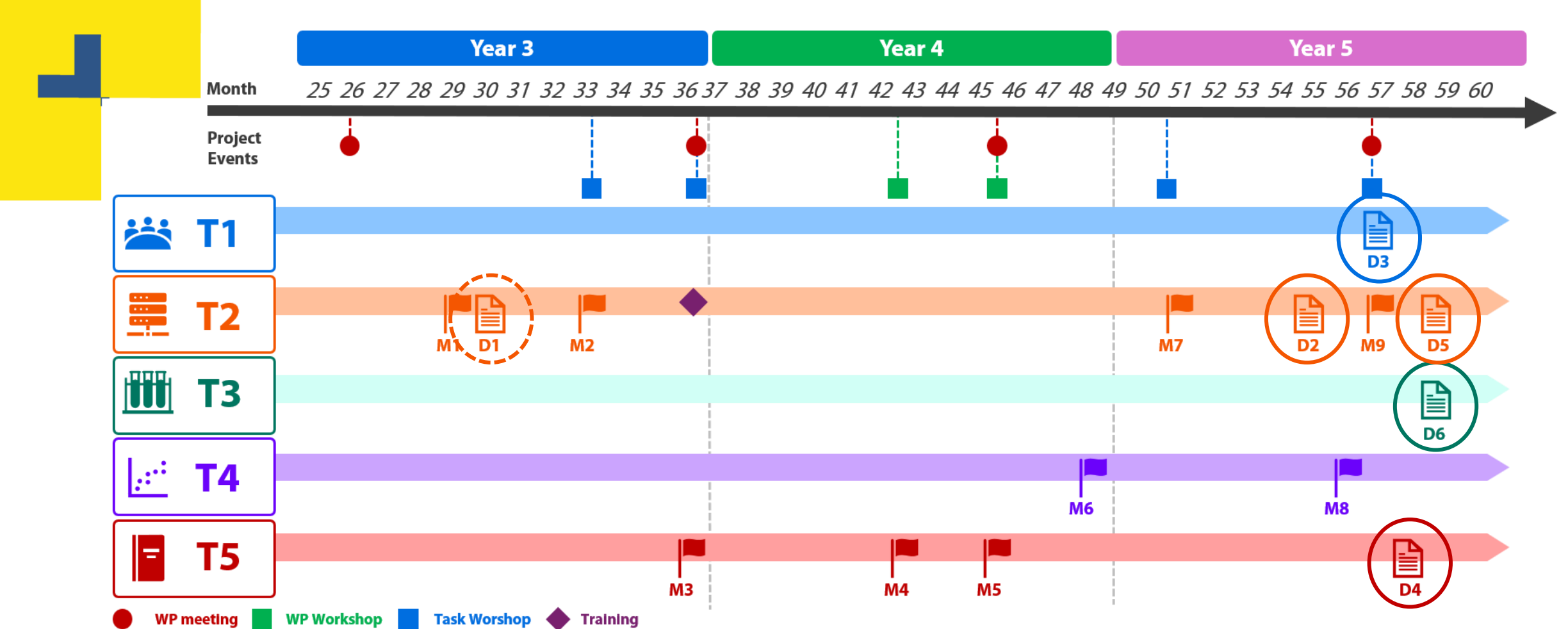


Radioactive Waste Management Organisations



Civil Society Organisations

eurad₂



- M1** Experimental work, estimation methods and model development: input to SotA
- M2** Harmonised Framework for Thermodynamic Data Management: exchange within ThermoGap and with ECOFRAME
- M3** T5 survey consolidation
- M4** Workshop on “Consolidation of practices and considerations (illustrated by examples for the selected simplified cases)”
- M5** Workshop with CS: structured dialogue on the role of thermodynamics in the SC
- M6** Report on sensitivity analysis and uncertainty propagation workflows, with demonstration on representative cases
- M7** Workshop on “Good practices for the use of thermodynamic databases in radioactive waste management applications”
- M8** Report on thermodynamic model development
- M9** Experimental work, estimation methods and model development: input to updated SotA

- D1** SotA – ThermoGAP
- D2** Harmonised framework for thermodynamic data management and interoperability
- D3** Outcome/impacts report to Member States and End Users - ThermoGAP
- D4** ThermoGAP: Development of methodologies/practices for applications in the Safety Case
- D5** Update SotA – ThermoGAP
- D6** New datasets generated within ThermoGAP

TASK 2 – KM INCLUDING HARMONISED FRAMEWORK FOR THERMODYNAMIC DATA MANAGEMENT

- **Scope**

- Knowledge capture and transfer
- Harmonised reporting requirements for generated experimental datasets
- Improve long-term traceability and findability of generated experimental datasets
- Define together common metadata structure for thermodynamic databases
- Initial interoperability between existing thermodynamic databases

- **Expected outcome**

- Harmonised framework for thermodynamic data management and interoperability.

→ KM, ECOFRAME, TOSCA, ...





TASK 3 – IMPROVEMENT OF SCIENTIFIC BASIS TO FEED THERMODYNAMIC DATABASES

- **Scope**

- Cement systems with and without RNs
 - Cement systems: CEM I, CEM III, alkali-activated materials, degradation stages (I, II, III)
 - RN: Ni, Cs, Sr, Eu, U, Ba, Cl, S, Se
- Redox and solubility phenomena
 - Ill-defined iron corrosion products (i.e., chukanovite - $(\text{Fe}_2\text{CO}_3(\text{OH})_2)$)
 - Se-redox chemistry (-II, +IV)
 - RN solubility controls (e.g., Ca-Nb(V)-OH(s), coprecipitation in Zr(IV)-An(IV)-Ln(III), Se-Fe and Sr-CaCO₃ systems)
- Ternary/Quaternary systems
 - U-Si-OH and M-U(VI)-CO₃ ternary complexes
 - RN (Nb, Zr, Th and Eu) complexation with organic ligands (e.g., ISA, citrate, phthalate and polycarboxylate ether)
- High saline systems, including sulphate and mixed saline systems
 - Solubility under saline conditions (e.g., Se(IV), Ni, Sn and Be)
 - Development of an extended SIT-based methodology and comparison with SIT and Pitzer

- **Expected outcomes**

- Generate consistent datasets to support thermodynamic database development
- Improve SIT-methodology for intermediate ionic strength (>3m)

→ **RAMPEC, SUDOKU, STREAM, SAREC, INCOMAND, ...**



TASK 4 – THERMODYNAMIC MODEL DEVELOPMENT AND REFINEMENT

- **Scope**

- Development/refinement of solid solutions models
 - LDH and carbonate solid solution models
 - Accounting for bulk cation solid solution and anion exchange processes in a consistent framework (solid solution and surface complexation)
 - Different formulations with increasing complexity, from discrete, ideal and to sublattice models
- Verification, sensitivity and uncertainty propagation in thermodynamic modelling
 - Conceptual uncertainty treatment
 - Sensitivity workflows and uncertainty propagation
 - Assessment and possible refinement of existing geochemical modelling tools

- **Expected outcomes**

- Improved representation of solid solutions in geochemical models
- Standard workflows for sensitivity and uncertainty propagation in thermodynamic geochemical modelling

→ **RAMPEC, SUDOKU, HERMES, STREAM, MOGARE, ...**



TASK 5 – DEVELOPMENT OF METHODOLOGIES/RECOMMENDATIONS FOR APPLICATIONS IN SAFETY CASES

- **Scope**

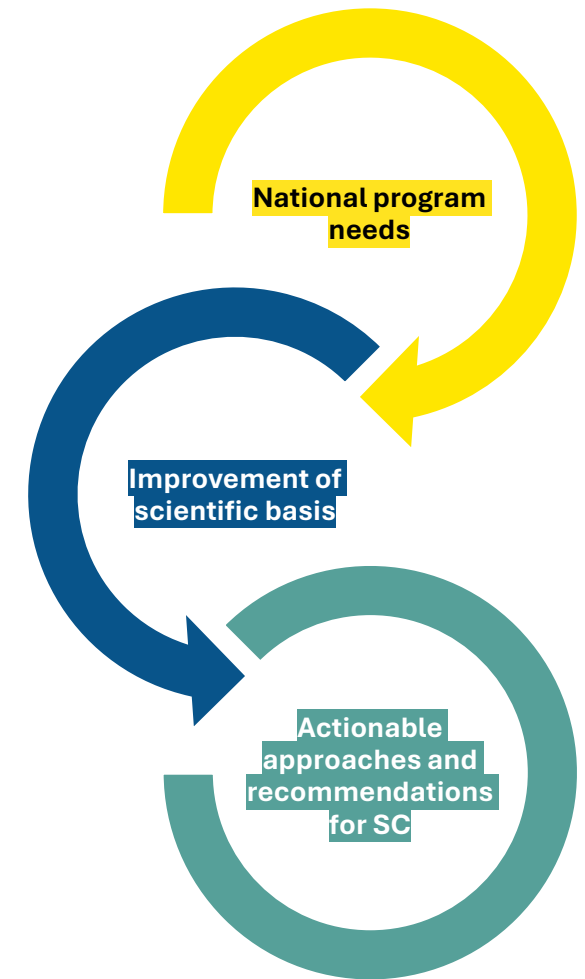
- Capture current thermodynamic practices in Safety Cases
 - Identification specific End-User needs related to ThermoGAP programme of work
 - Review of current PA/SA implementation approaches
- Assess the scientific outcomes resulting from the implementation of ThermoGAP
 - Selection of a set of representative systems and processes based on specific end-user needs
 - Assessment of impacts on disposal components performance (before/after ThermoGAP)
- Engage with Civil Society representatives
 - One dedicated workshop around “simplified” cases to exemplify thermodynamic approach (from data acquisition to implementation in the Safety Case)

- **Expected outcomes**

- Establish a common understanding of how ThermoGAP relevant thermodynamic knowledge is currently implemented in Safety Cases
- Illustrate the benefits of ThermoGAP research for the Safety Case
- Whenever possible, translate scientific advances into practical and actionable approaches for Performance Assessment and Safety Analysis.

FROM KNOWLEDGE GAPS TO SAFETY CASE IMPACT

- ThermoGAP is built on the outcomes of EURAD-2 DITUSC Strategic Study
- Continuous chain from experimental/modeling research to practical Safety Case implementation:
 - Harmonised and interoperable thermodynamic data management framework
 - New thermodynamic data addressing priority repository-relevant gaps (cement, redox, complexation, salinity)
 - Improved solid solution process representation through advanced thermodynamic models
 - Robust workflows for sensitivity analysis and uncertainty propagation in thermodynamic geochemical modelling
 - Reduced uncertainty and unnecessary conservatism in Safety Case assessments
 - Practical recommendations, methodologies and best practices for end users
- An integrated cycle from national program needs, thermodynamic research to Safety Case implementation





Thank you for your attention !

Questions ?