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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Short Acronym and full Title	**HERMES**: High fidElity numeRical siMulations of strongly coupled processes for rEpository syStems and design optimisation with physical models and machine learning		
Type of activity	☒R&D	☐Strategic Study	Knowledge Management – covered by a separate committee and template
Budget estimation (total budget in M€, i.e ~ 1.5 M€)	4.0M€	48 Project Month(PM): 6 PM initialisation phase; 36 PM implementation; 6 PM finalisation/reporting;	
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**)	**5.2.2 Optimisation (of the facility components and design)** 7.3.1 Performance assessment and system models 7.3.3 Scenario development and FEP analysis		
SRA drivers **(maximum 3)**	☒Implementation Safety	☐Tailored Solutions	☒Scientific Insight
	☒Innovation for Optimisation	☐Societal Engagement	☐Knowledge Management
Objective (What) – **1 sentence**	This WP aims at the development of high fidelity numerical models for simulations of strongly coupled THMC processes in repository nearfield, repository design optimisation and interpretation of mock up experiments using a combination of physics based models and accelerated computing assisted with machine learning and artificial intelligence.		

Justification: impact / innovation / added-value (Why) – bullet points or short paragraph **(maximum quarter of a page)**	Process-based numerical simulations are the basis for in-depth system understanding, analysis of experimental observations and their upscaling to the natural systems. Despite the continuous growth of the computational resources, the realism of the models applied in the simulations of repository systems remains severely limited in terms of dimensions, time-space resolution and process couplings. Interpretation of experimental data, safety and cost driven design optimisation, model uncertainty analysis belong to the class of inverse problems. Numerical solution of inverse problems, imply iterative forward modelling until the solution converges to the optimal parameter set (e.g. satisfactory description experimental data, cost-safety design optimisation of repository optimisation, uncertainty analysis). For both forward and inverse problems, some **orders of magnitude improvement in the computational efficiency** can be obtained by replacing the **physical based solvers** or its components with **high fidelity surrogate models**. Particularly promising are the surrogate models based on **machine learning** for specific aspects of **THMC coupled models**, **data exchange between models at different scales**, **reduction of big data** and extraction of constitutive relations from big **numerical, experimental and monitoring datasets**. Recent developments in the field of data sciences and computational efficiency of surrogate models on modern computer infrastructure opens the way for realisation of efficient coupled numerical models (Digital Twins) for real time numerical analysis of laboratory and field experiments, repository design, components optimisation and comprehensive safety analysis. Such numerical tools are essential for repository conceptualisation and the repository design optimisation in both advanced- and early-stage waste disposal programs
List of planned tasks / subtasks with % of effort per task (5% increments) **(Maximum 10 bullets)**	**Work package is aimed at:** - Simulations of strongly coupled THMC FEPs (Feature Events Processes) in repository systems (nearfield and host rocks) - Use of advanced numerical tools and codes, development of methods, and benchmarking of innovative methods - Interpretation of laboratory and field experiments. Integration of experimental and modelling results including those gained in EURAD-I - Development of high fidelity process models to be coupled to BIM/Digital Twins of repository subsystem and experiments foreseen to be conceptualised in WP 17. - Building an EURAD model-hub for linking data and various codes within workflow applications **Possible project structure comprised 5 Tasks:** • Task 1 (10 %): *Management/coordination of the WP*: Annual meetings / reporting / coordination inter-task activities • Task 2 (15%): *Knowledge Management* SOTA report(s) & Knowledge gap analysis Implementation and professional maintenance of collaborative platform for code development and machine learning. Implementation of EURAD model-hub for linking data and models. Maintenance of open access platform with experimental data for model testing Joint workshops with WP17 (Digital twins) & WP12 (Bentonite) Summer schools on repository FEPs modelling

	• *Task 3 (30%): <u>Process couplings and computational performance</u>* Definition and development of unified interfaces for process coupling Development and coupling of tools for forward and inverse modelling as well as sensitivity analysis Development of models with dynamic integration of data Multiscale models couplings, parameters transfer and upscaling • *Task 4 (20%): <u>Surrogate modes of individual phenomena</u>* Processes addressed: Chemistry / Gas-Mass-Heat transport / Mechanics Application & implementation of machine learning methods and codes Benchmarking of surrogate models against physical models and experimental data • *Task 5 (25%) <u>Tailored models for SA/PA and field scale mock-ups</u>* Real time simulation of field scale experiments (link to DECOVALEX) Assessment of waste package integrity in extended storage High fidelity models for repository near-field simulations Dedicated models for optimisation and repository design Integration of the models into DT concepts to be formalised in WP17
List of expected outcomes linked to the identified SRA drivers **(Maximum 6 bullets)**	• Family of high fidelity/high computation throughput coupled models for multiscale simulations of THMC processes in repository nearfield and host rocks offered via an open access EURAD model-hub **(SRA-> Scientific Insight)** • Improved understanding of in situ repository evolution controlled by coupled phenomena **(SRA-> Scientific Insight)** • Surrogate models for inverse modelling and large scale simulations for sophisticated optimisation of repository design with respect to THMC FEPs **(SRA-> Innovation for Optimisation)** • Dedicated proxy (simplified) models for optimisation, PA/SA and repository design. Integration of the models into DT definition conducted in WP17. Adjustment of the modelling framework according to the output of WP17 on the DT formulations. **(SRA-> Innovation for Optimisation)** • Unified collaborative platform and protocols for surrogate model development. Open access database with experimental datasets (including numerical data) for model testing **(SRA-> Knowledge Management)**
Deliverables **(Maximum 6 – including the prescribed deliverables)**	• Impacts report for Member States and End Users • Initial and final SOTA reports • Report on surrogate model development methodologies and documentation of cross benchmarking of methods efficiency • Report on inverse modelling for THMC processes in repository system with surrogate models; Field scale models validation • Report on application of high fidelity/high computation throughput coupled models for bounding scenarios in repository nearfield

Critical input requirements & identified risks	• **Novelty, budget and project duration:** The estimation of the project budget (4.0 MEUR) and the project duration (4Y) is carefully thought through based on the previous experience in the EURAD-I and necessary engagement of the experts. The development of fully coupled THMC models and the use of surrogate modes in this project goes beyond traditional desktop studies based on application of standard simulation codes. This project requires both support of experts in repository near field evolution and strong engagement of computer science experts. The maintenance of the open-source coupled codes must be conducted with the support of IT experts and data scientists. The developments in the field of data sciences is very dynamic. A critical mass of experts is needed to achieve focused impact in the field in a timely manner. • The advancement in the THMC coupled code and the surrogate modelling will be a game changer in repository design and optimisation as well as PA/SA ant the stage of conceptualizations. This project will play a central role in facilitating collaboration between WPs focused on experimental studies and application of the results to SA/PA. The details of these interactions should be defined in the next stage of WPs preparation. • Detailed process understanding and system description based on physical models and experimental data from on-going experiments will be essential for models validation. Clear collaboration could be foreseen with WPs 7, 9, 12, 13, 15, 16 and 17 in the current WP pool. Exact definition of collaborations will be provided in the next phase, once the family of WP selected for next phase is defined.
Major achievements expected by end of Year 2 (Go/No Assessment)[1] **(Maximum 5 bullets)**	• Road map for model development and process coupling including definition of interfaces between models and codes • Demonstration of an order of magnitude of speed up of surrogate model for specific processes versus reference vs. conventional simulations • Joint definition of interface for the process coupling according to the output of WP17 on the DT formulations.
(Optional - Explain what is out of the scope?)	Project is focused on the modelling of strongly coupled THMC processes in repository nearfield including the repository effects on host rocks. To avoid the overlap with WP12, the bentonite and sand-bentonite-mix modelling are excluded. We see, however, a high benefit of collaboration between both WPs. Project builds upon experience in EURAD-I but does not repeat the activities of DONUT, MODATS or other related WPs. These projects were limited to very specific process couplings. HERMES embarks on these developments and strives for a truly coupled THMC-model's implementation. Project does not foresee dedicated experimental program but instead rely on the input from existing or ongoing experimental studies (e.g. experiments in DECOVALEX consortium) and the experimental data acquired within EURAD-I projects(e.g. ACED, CORI, FUTURE, GAS, HITEC, MODATS), and PREDIS.

[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.

	Out of scope are pure mathematical studies or theoretical numerical exercises: e.g. development of new machine learning techniques (existing packages should be used) or development of equation solvers for physical models
List of preliminary interested organisations as partners in the WP contributing effort; **% of effort (person months, by College)**	This is just a preliminary list of the organisation who have expressed their interest in the topic. It is neither complete nor closed. The list should be further refined/extended on the basis of specific input from partners to be detailed in the next phase. RE 50%: [Amphos21,UDC, UCLM] (ESP), [BGS, Egis, Galson] (UK), [CEA, BRGM, ULorraine, ULilie, EDF] (FR), [FZJ, UFZ, GFZ, HZDR](DE), IFE(NO), MITTA(FI) PSI(CH), SCK CEN(BE), [TUL,CTU](CZ), TUDelft(NL) TSO 25%: TSENERCON(HU), VTT(FI), CIEMAT(ESP), NTW, GRS(DE) WMO 25%: Andra(FR), Enresa(ESP), Nagra(CH), SURAO(CZ)
If applicable - links with previous projects / work packages	A proof of concept for the successful use of machine learning and surrogate modelling for the isolated coupling and repository components has been demonstrated, including benchmarking exercises, in the ongoing WPs in EURAD-I (e.g. DONUT, ACED, MODATS) and PREDIS. There are very clear differences however: HERMES is aiming at the development of fully coupled THMC-models, whereas DONUT and MODATS are only dealing with a subset of the processes and process couplings. Further, WP-HERMES is focused on a heavy use of the surrogate models supported by artificial intelligence concepts (machine learning, physics informed methods, data driven models, etc.) for the process description, coupling and upscaling. Such approaches have only been considered as prototypes of for a proof of concept in the previous studies.
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