TOWARDS HIGH FIDELITY NUMERICAL SIMULATIONS OF STRONGLY COUPLED PROCESSES FOR REPOSITORY SYSTEMS

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Safe geological disposal of radioactive waste employs a combination of engineered and natural barriers representing a so-called passive multiple barrier concept. Due to the complexity of the repository systems and the extremely long time-periods involved, the assessment of the repository safety relies, among other criteria, on model-based descriptions and simulations of possible repository evolution scenarios. Thermo-hydro-mechanical-chemical (THMC) process-based numerical simulations are, thus, the basis for in-depth system understanding, analysis of experimental observations. Despite the continuous growth of computational resources, the realism of the models applied in the simulations of repository systems remains severely limited in terms of dimensions, space-time resolution and process couplings [1]. Recent developments in the field of data sciences and computational efficiency of surrogate models on modern computer infrastructure open the way for developing efficient coupled numerical models (Digital Twins) for real-time numerical analysis of laboratory and field experiments, repository design, components optimisation and comprehensive safety analysis [2]. Such numerical tools are essential for repository conceptualisation and design optimisation in both advanced- and early-stage waste disposal programs. Interpretation of experimental data, safety or cost-driven design optimisation and model uncertainty analysis belong to the class of inverse problems. Numerical solution of inverse problems implies iterative forward modelling until the solution converges to the optimal parameter set. For both forward and inverse problems, some orders of magnitude improvement in the computational efficiency can be obtained by replacing the physics-based solvers or some of their components with high-fidelity surrogate models. Particularly promising are the surrogate models based on machine learning tools (e.g., surrogate models for geochemical solvers and parametrisation of material datasets), extraction of constitutive relations from big numerical, experimental and monitoring datasets. The HERMES work package implemented within the EURAD-II project aims at the development of open-access tools for simulation of strongly coupled THMC Feature Events Processes in repository systems (near-field and host rocks). In terms of model benchmarking, HERMES works closely with other national and international projects such as the new DECOVALEX 2027 project. The developed modelling tools, benchmarks and validation datasets will be made available through Model-Hub to support collaboration between modelling teams, provide an interface with experimenters and make the knowledge from the HERMES work package available to the broader scientific community.

[1] Churakov S.V., et al., (2024) Env. Earth Sci., 83, 521.
[2] Kolditz O, et al., (2023) Env. Earth Sci., 82:42.

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