Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.35493

Benchmarks for AI/ML-accelerated reactive transport models in the context of radioactive waste management – Activities in EURAD2 HERMES

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Coupled reactive transport models (RTMs) are indispensable to assess the long-term safety of underground radioactive waste disposal facilities. Given the large temporal and spatial scales to be considered, RTM often face prohibiting computational costs, with the simulation of geochemical processes usually being the bottleneck in speed. Therefore, replacing computationally expensive geochemical solvers with surrogates based on machine learning (ML) and artificial intelligence (AI), such as neural networks, look-up tables, boosted trees or gaussian processes, represents a promising approach to speedup this class of simulations. A first step in this direction was taken within the DONUT work package of EURAD project (European Partnership on Radioactive Waste Management) by benchmarking different machine learning algorithms for geochemical calculations of cement systems and uranium sorption in clays [1]. This work is continued in the HERMES work package of EURAD2, where the accuracy and computational gain of different surrogate models for use in coupled RTMs is evaluated. In this contribution, we present (i) a summary of the main outcomes of the first benchmarking activity from the DONUT project, and (ii) the benchmarks as well as the ML/AI approaches investigated in the ongoing HERMES project. We introduce the consortium and discuss the general approach and the specifications of different benchmarks, pertaining to (i) cement chemistry, (ii) diffusive uranium migration in clay subject to sorption, (iii) bentonite-iron corrosion and (iv) cement-clay interface interactions.

Acknowledgements: This research was funded by WP HERMES of EURAD-2 (Grant Agreement nº 101166718). The work was partly funded also by Spanish Ministry of Science and Innovation (PID2023-153202OB-I00) and the Galician Government (ED431C2025/55). This work has received funding from the Swiss State Secretariat for Education, Research and Innovation (SERI) under contract number 24.00511.

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