



Radioactive Contamination Risk Assessment in Long-Term Radioactive Waste Disposal: Actionable Data-Hub for Analysis-Readiness in Process and Impact Models

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Germany is currently conducting a site selection procedure with the quest for an optimal repository site for high-level radioactive waste in geological subsurface. The site selection procedure must be done in accordance with the Final Repository Safety Requirements Ordinance, which restricts the maximum allowable exposure for high-level radioactive waste released from the final repository site. One of the potential risks associated with the repository site is the release of radionuclides through groundwater flow. Therefore, a risk assessment regarding the environmental impact of different hazard scenarios is crucial to carefully select and ensure long-term safety of the repository site.

To assess the risk of radioactive contamination in the subsurface, physics-based process models are implemented to predict the spatial-temporal evolution of the radionuclide concentration associated with a given hazard scenario. The resulting radionuclide concentration provides the basis for impact modelling, namely estimating accumulated dose and subsequently quantifying potential radioactive contamination. Simulations are implemented through the OpenGeoSys software. A supporting Python package, Yaml2Solver, is developed to orchestrate process and impact modelling along with relevant parameters. The package centralizes simulation and material information in YAML files to define and adjust model parameters, and it enables simulating different coupled-level process models.

These data-integrated models, however, are built in the presence of uncertainties in material properties, including permeability of rock and groundwater flow. Accounting for uncertainties in physics-based simulations calls for an effective and reliable uncertainty management tool. We therefore developed an analysis-ready and actionable data-hub. The data-hub consists of a database integrated with a graphic user interface (GUI). The database provides material properties along with their uncertainty margins and sensible defaults in YAML files for analysis readiness of simulation models. The material properties are associated with synthetic, reference, and candidate sites, enabling the compilation of site-specific scenarios for simulations. The GUI provides detailed visualization for each site, including a three-dimensional geostructural model, a chronostratigraphic chart indicating the geological formation time of each stratum, and a table

providing information on rock properties and attributes of sensible defaults. The data-hub framework supports for systemic and uncertainty-informed model-based assessment as well as subsequent model-based decision-making tasks. We further integrated the data-hub with Yaml2Solver for efficient uncertainty management across various scenarios.

Data-hub integrated process and impact modelling offers benefits for managing long-term uncertainties and improving reproducibility, and thereby increasing the transparency and reliability of decision-making. Depending on the material properties with their marginal values sourced from different sites, we construct various site-specific process models. Subsequently, the process models are extended to impact models, describing spatial-temporal evolutions of radiation. The resulting uncertainty-informed impact models enable us to quantify potential radioactive contamination in specific sites and offer valuable insights in repository site selection and safety assessments.