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Coupled heat-mass transport modelling for safety assessment of deep borehole disposal of long-lived radioactive waste in a complex 3D petrophysical condition

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A potentially novel disposal pathway for small volumes of radioactive waste originating from reprocessing of spent nuclear fuels is in deep boreholes (DBs). The waste packages are stacked in a disposal zone at depths that would be considerably deeper than the typical depth of conventional mined repositories. DB disposal still requires considerable research and development to bring the science and technology to a similar level as the conventional disposal geological disposal facilities [1]. The half-life of several of the radionuclides in reprocessed spent nuclear fuel is on the order of 10^5 - 10^9 years. Such wastes generate heat for hundreds of years. Containers should have a lifetime long enough to survive at least the heat-production period [2]. In the geosphere surrounding the borehole, nonlinear interactions between transport phenomena and long time scales necessitate modelling as the most realistic tool to assess the risks. Coupling the flow, natural hydrostatic and temperature profiles with heat and solute mass transport is not computationally trivial.

We study a complex domain including geological faults, stratified lithology, and an engineered DB with its surrounding damaged zone and backfilling materials. The system has an assumed groundwater flow above the low-permeable host rock, a diagonally-oriented fault and a cylindrical representation of the borehole. Such objects require a domain which is neither axisymmetric nor 2D Cartesian. A structured mesh to represent such a domain in 3D, with the required fine-scale near-field resolutions essential for simulation of the slow advective and diffusive transport, significantly increases the computational cost. For the first time a fully-3D unstructured Voronoi mesh was developed to represent such a layout with various petrophysical features and engineering objects to conduct a preliminary safety assessment.

We present a coupled heat-solute mass transport modelling framework, subjected to depth-dependent temperature, pressure, and viscosity profiles - assuming an instantaneous release of radionuclides, as the most conservative “what if” scenario. Several scenarios of heat-generation were investigated to test if the additional heat produced by the waste affects radionuclide migration, e.g., by generating convection-driven transport. The state-of-the-art TOUGHREACT-OMP was run on the CSIRO supercomputer to model the 3D Cartesian domain 3 km in length, 400 m in width and 3 km in depth. We present our meshing approach through linking voro2mesh, T2Viewer and in-house codes to develop a fully-3D unstructured mesh, compatible with the core model [3].

We tested the effect of lithology on the diffusion process (effective diffusion) for quantifying the radionuclide concentrations and annual dose rates for a potential human receptor (e.g., through a well). We show the dose rate is highly sensitive to the diffusion parameter and fault configuration, while the effect of heat generation on convection-driven transport is of lesser importance.

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2-IAEA, *Geological disposal facilities for radioactive waste*. 2011, International Atomic Energy Agency: Viena.

3-Bonduà, S. and V. Bortolotti, *TOUGH2Viewer 2.0: A multiplatform tool for fully 3D Voronoi TOUGH grids.* SoftwareX, 2020. **12**: p. 100596.