THERMAL-HYDROLOGIC-CHEMICAL-MECHANICAL MODELING OF DEEP BOREHOLE DISPOSAL

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Disposal of high-level radioactive waste, including spent nuclear fuel, in deep (3 to 5 km) boreholes is a potential option for safely isolating these wastes from the surface and near-surface environment. Coupled thermal-hydrologic-chemical-mechanical processes induced by heat from the radioactive waste may impact fluid flow, properties of the host rock near the borehole, and borehole wall stability.

Numerical simulations of these coupled processes were conducted at large and small scales using the FEHM, Calorie JAS3D, Aria, and Adagio software codes and unstructured grids to evaluate the potential impacts on a deep borehole disposal system.

Simulation results show that peak temperature increases at the borehole wall by about 30 °C for disposal of nuclear fuel assemblies and increases by about 180 °C for vitrified waste. Peak upward groundwater flow rates in the borehole disturbed zone vary with depth and are related to the thermal expansion of groundwater and focusing of flow within the assumed higher-permeability zone near the borehole. Smaller-scale simulation results show that the host rock near the borehole is placed under additional compression from the input of waste heat and thermal expansion. Significant increases in stress and volumetric strain near the borehole are relatively short lived. Under anisotropic ambient horizontal stress conditions the simulated maximum compressive stress at the borehole wall likely exceeds the compressive strength of granite, which could result in borehole instability and the formation of borehole breakouts.

I. INTRODUCTION

Deep borehole disposal of high-level radioactive waste has been considered as an option for geological isolation for many years, including original evaluations by the U.S. National Academy of Sciences in 1957.[1] International efforts over the last half-century toward disposal of high-level waste and spent nuclear fuel have primarily focused on mined repositories. Nonetheless, evaluations of deep borehole disposal have periodically continued in several countries.[2-8] An updated conceptual evaluation of deep borehole disposal and a preliminary performance assessment have also recently been completed.[9] None of these studies have identified any fundamental flaws regarding safety or implementation of the deep borehole disposal concept.

The deep borehole disposal concept is illustrated in Figure 1. The concept consists of drilling a borehole (or array of boreholes) into crystalline basement rock to a depth of about 5,000 m, emplacing waste canisters of used fuel assemblies or vitrified radioactive waste from reprocessing in the lower 2,000 m of the borehole, and sealing the upper 3,000 m of the borehole. As shown in Figure 1, waste in the deep borehole disposal system is several times deeper than for typical mined repositories, resulting in greater natural isolation from the surface and near-surface environment. The disposal zone in a single borehole could contain about 400 waste canisters of approximately 5 m length. The borehole seal system would consist of compacted bentonite clay, asphalt, and concrete.

Several factors suggest that the deep borehole disposal concept is viable and safe. Crystalline basement rocks are relatively common at depths of 2,000 to 5,000 m in stable continental regions, suggesting that numerous appropriate sites exist.[2, 5] Existing drilling technology permits the reliable construction of sufficiently large diameter boreholes to a depth of 5,000 m at a cost of about $US 20 million each.[9] The projected waste inventory from the current fleet of nuclear reactors in the U.S. could be disposed as spent fuel assemblies in about 950 boreholes. Low permeability and high salinity in the deep continental crystalline basement at many locations suggest extremely limited interaction with shallow fresh groundwater resources (a typical lower boundary is shown by the dashed blue line in Figure 1), which is the most likely pathway for human exposure. The density stratification of groundwater would also oppose thermally induced groundwater convection from the waste to the shallow subsurface. Geochemically reducing conditions in the deep subsurface limit the solubility and enhance the sorption of many radionuclides in the waste, leading to limited mobility.

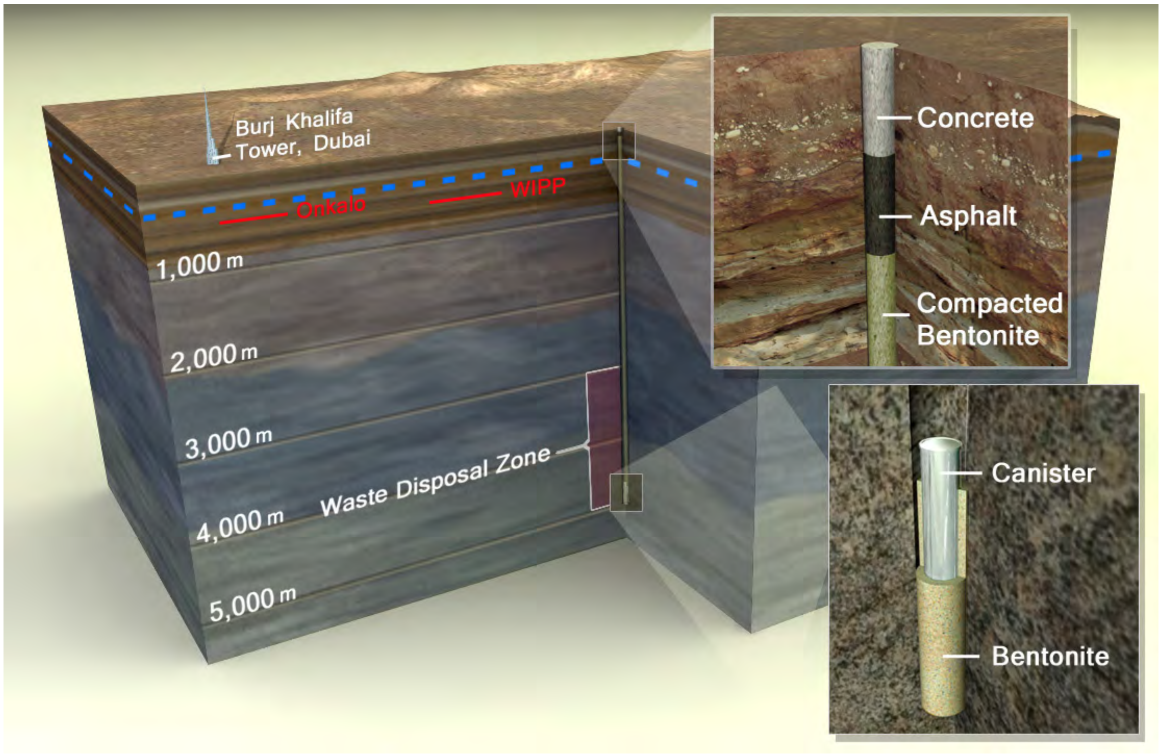

Figure 1. Concept for Deep Borehole Disposal of High-Level Radioactive Waste.

The nominal design used in these analyses consists of a borehole with a diameter of about 44 cm in the waste disposal zone. Emplacing intact spent fuel assemblages, without pre-consolidation, is one of the simplest approaches to borehole disposal, and is the one considered here.[10] Alternatively, canisters could be filled with vitrified waste from reprocessing. The thermal output histories from canisters containing either a representative pressurized water reactor fuel assembly that has been aged for 25 years or vitrified waste from reprocessing that has been aged 10 years[11] are evaluated in this study.

II. MODELING OF THERMAL-HYDROLOGIC-MECHANICAL PROCESSES

II.A. Coupled Processes Near the Disposal Borehole

The objectives of near-borehole model included evaluation of mechanical stress and strain near the borehole and comparison of software codes for thermal-mechanical simulations. Stress and strain were evaluated for disposal of used fuel assemblies and vitrified waste, and for both isotropic and anisotropic ambient horizontal stress conditions. Software codes compared were (1) FEHM, (2) Calorie coupled to JAS3D, and (3) Aria coupled to Adagio.

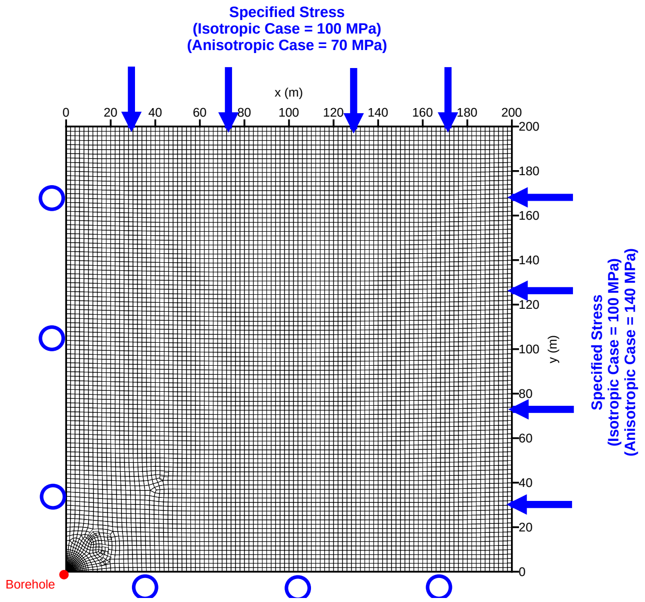

Figure 2. Model domain, numerical grid, and boundary conditions for thermal-mechanical simulations.

The model domain was set up for quarter symmetry in stress and thermal transport within a horizontal plane, as shown in Figure 2. Specified stress was applied to the outer boundaries and zero *x*-displacement along the *y*-axis boundary and zero *y*-displacement along the *x*-axis boundary. Thermal boundary conditions consisted of specified ambient temperature on the outer boundaries, zero heat flux along the inner boundaries, and time-varying, specified heat input at the borehole wall. Linear models of stress, thermal conductivity, and thermal expansion were used in the simulations. Parameter values representative of granite used in the model are shown in Table 1.

Table 1. Parameter values used in modeling.

Parameter	**Value**
thermal conductivity (W/m ^{o}K)	3.0
density (kg/m^3)	2750.
porosity (-)	0.01
specific heat (J/kg ^{o}K)	790.
linear coefficient of thermal expansion (^{o}K^{-1})	8×10^{-6}
Poison ratio (-)	0.25
elastic modulus (MPa)	5×10^4
permeability of host rock (m^2)	1×10^{-19}
permeability of borehole disturbed zone (m^2)	1×10^{-16}

An unstructured numerical grid was developed to conform to the borehole wall at a high resolution (Figure 3). This hexahedral grid transitions to an orthogonal mesh at greater distances from the borehole, as shown in Figure 2.

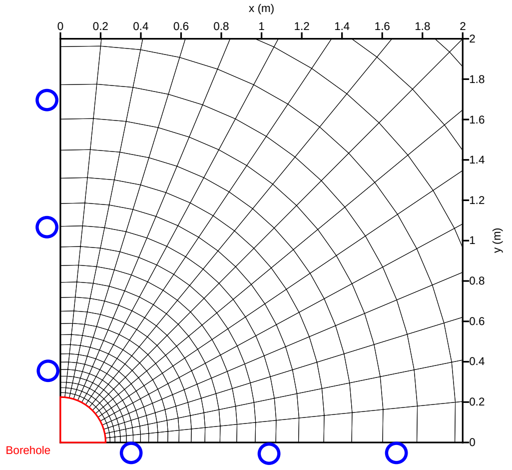

Figure 3. Detail of the thermal-mechanical numerical grid near the borehole.

II.B. Coupled Processes in the Far Field

The thermal-hydrologic model of heat transport and fluid flow in the far field was developed using the FEHM software code to evaluate the thermal impacts to fluid flow and sensitivity to the number of boreholes and spacing between boreholes. The 3D model domain extends from the ground surface to a depth of 6000 m and uses quarter symmetry boundary conditions to a distance of 1000 m from the central borehole. The thermal boundary conditions consist of specified temperature at the top, bottom, and outer boundaries of the domain, corresponding to a geothermal gradient of 25^{o}C/km, and specified heat flux in the boreholes at depths ranging from 3,000 to 5,000 m. The hydrologic boundary conditions are specified pressure on the top, bottom, and outer boundaries, corresponding to hydrostatic conditions. No flow boundary conditions for heat and fluid are assigned to the symmetry boundaries of the model domain. The numerical grid consists of hexahedral elements and includes higher resolution near the boreholes, as shown in Figure 4.

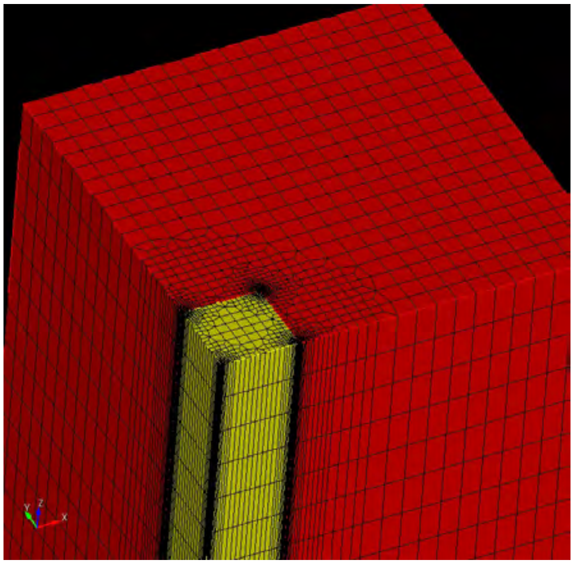

Figure 4. Numerical grid for the 3D thermal-hydrologic model of the far field.

Parameter values are shown in Table 1, with the permeability of the borehole disturbed zone applied to a 1 m^2 area around the borehole. A hexahedral, unstructured grid with higher resolution around the boreholes was used in the model.

III. RESULTS AND DISCUSSION

III.A. Results of Thermal-Mechanical Modeling Near the Borehole

Simulated temperature increases from radioactive decay in the waste indicate a transient response in the host rock that decrease rapidly with distance from the borehole and time. Figure 5 shows a peak temperature increase of about 30 °C at the borehole wall for disposal of used fuel assemblies over the assumed ambient temperature of 110 °C in the host rock at a depth of 4,000 m. This increase in temperature is approximately consistent with previous calculations for the disposal of used fuel assemblies that have been aged for 10 years.[2] Peak temperatures predicted by the model occur within 10 years of waste emplacement for distances of less than 1 m from the borehole center, with the time of peak temperature occurring later with greater distance. Alternatively, peak temperatures are significantly higher for the disposal of vitrified waste from reprocessing, with peak temperatures of about 180 °C above ambient temperature occurring within 10 years.

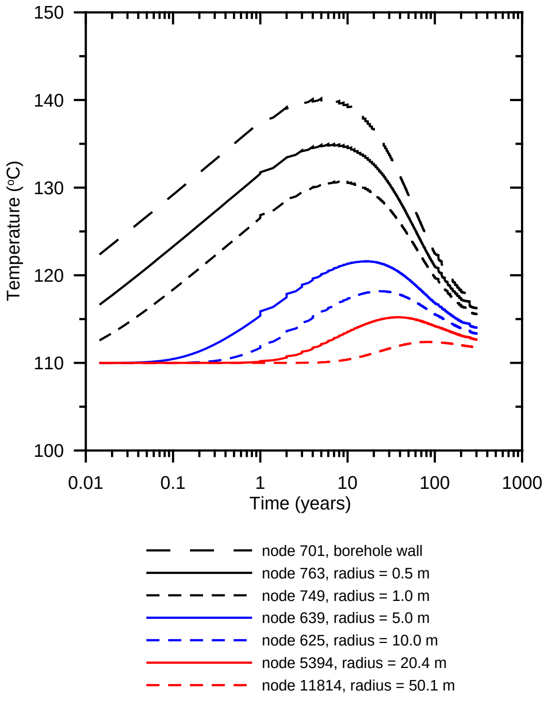

Figure 5. Simulated temperature histories at various distances from the borehole for disposal of used nuclear fuel assemblies.

The initial conditions for the thermal-mechanical simulations were determined by calculating the distribution of equilibrium horizontal stress around the borehole opening. Equilibrium stress conditions are zero stress in the *x*-direction on the side of the borehole normal to the *x*-direction and twice the ambient stress on the side of the borehole parallel to the *x*-direction. The simulated change in the *x*-direction stress due to thermal expansion at 10 years following emplacement of vitrified waste is shown in Figure 6. The maximum increase in stress of about 90 MPa occurs at the borehole wall at a location parallel to the *x*-direction. Note that this increase in stress is relative to equilibrium stress of 200 MPa for isotropic conditions.

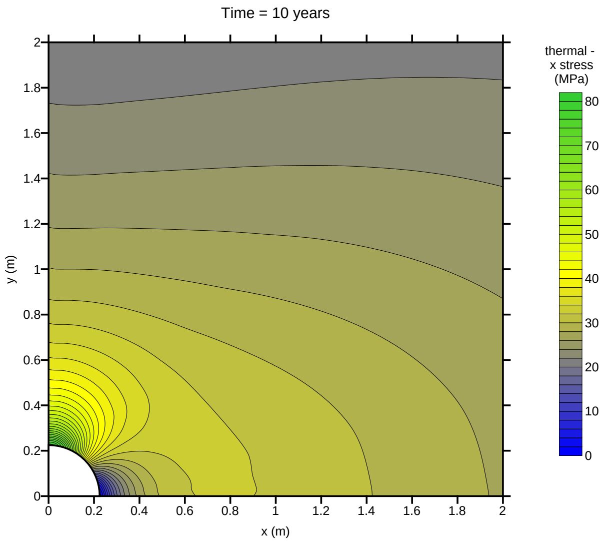

Figure 6. Change in stress in the *x*-direction at 10 years near the borehole simulated by the FEHM code for disposal of vitrified waste. Note that this is the change in stress from thermal input.

Simulations for anisotropic stress conditions, in which the ambient stress in the *x*-direction of 140 MPa exceeds the stress in the y-direction of 70 MPa by a factor of 2, were also performed. The maximum stress in the *x*-direction at 10 years for anisotropic stress conditions and vitrified waste is about 420 MPa, which greatly exceeds the average ambient horizontal stress in the model of 100 MPa.

The strain associated with the thermal input from the waste in the borehole is concentrated concentrically around the borehole and is compressive. The simulated volumetric strain as a function of time is shown for various distances from the borehole for the disposal of vitrified waste in Figure 7. The peak volumetric strain is approximately associated with peak temperature and peak stress in the simulations, with the strain declining toward zero after several hundred years. The magnitude of the peak strain near the borehole of greater than 1,000 microstrain could have significant impacts on fracture apertures and bulk permeability of the borehole disturbed zone and the low-porosity host rock. Compressive strain would tend to close fractures and reduce permeability in this critical area near the borehole during the thermal period.

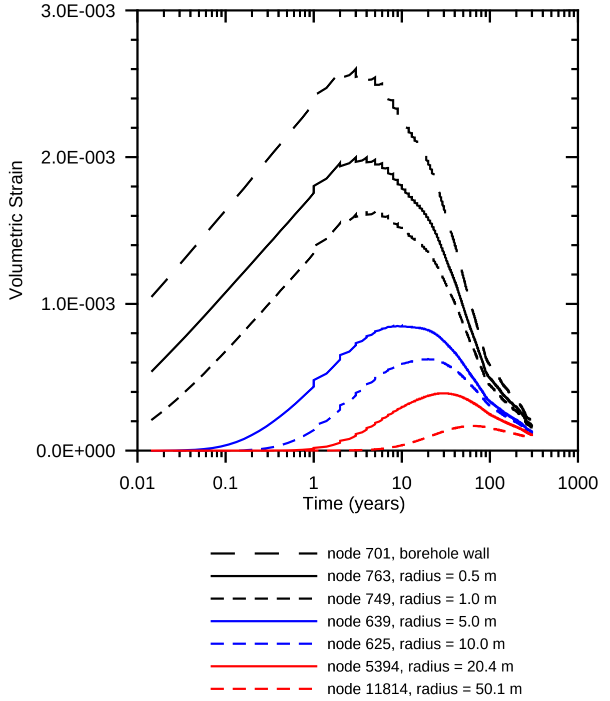

Figure 7. Histories of the volumetric strain at various distances from the center of the borehole simulated by the FEHM code for disposal of vitrified waste.

Comparison between the software codes used in the model, 1) FEHM, 2) Calorie coupled to JAS3D, and 3) Aria coupled to Adagio, indicated that the simulated spatial distributions of temperature, stress, displacement, and strain, and the time histories of these variables were generally similar near the borehole. One exception was the simulated stress and strain from the FEHM code at irregular grid cells where the curvilinear mesh transitions to the orthogonal mesh in the far field. FEHM calculated anomalous values at these grid locations, although these anomalies did not appear to impact the simulated values near the borehole. It should be noted that the FEHM code uses a non-deforming grid formulation, whereas JAS3D and Adagio include deformation of the grid in the mechanical calculations. Favorable comparison between the codes indicates that grid deformation is not an important factor in this problem.

III.B. Results of Thermal-Hydrologic Modeling in the Far Field

The 3D far-field thermal-hydrologic model was run for cases in which the number of boreholes was 1, 9, and 25; the spacing between boreholes was 50, 100 or 200 m, and the waste was used nuclear fuel assemblies or vitrified waste. The simulated temperature history for the single-borehole case was similar to the temperatures simulated by the 2D thermal-mechanical model. This result indicates that heat transport in the coupled thermal-hydrologic system is dominated by conductive heat transport, with only minor transport of heat by convection. The simulated temperature in a horizontal plane at a depth of 3000 m for 9 disposal boreholes at 10 years following waste emplacement is shown in Figure 8.

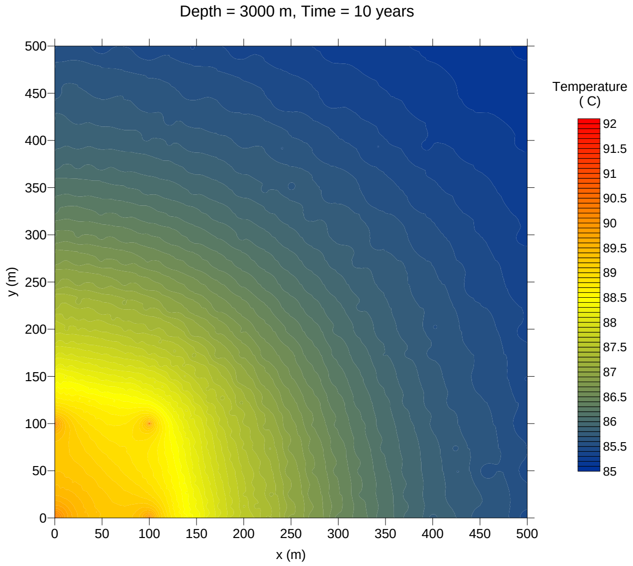

Figure 8. Simulated temperature at 3000 m depth for disposal of used fuel assemblies in an array of nine boreholes 10 years after disposal.

Simulated peak temperatures near the boreholes were approximately the same for 1, 9, or 25 equally spaced boreholes. However, temperatures remained higher for longer periods of time following peak temperature for the multiple borehole cases. Similarly, simulated peak temperatures were also approximately the same for borehole spacing of 100 or 200 m, but the temperatures were somewhat greater at later times. The simulated peak temperature for a spacing of 50 m was about 10 ^{o}C higher for disposal of fuel assemblies and about 30 ^{o}C higher for disposal of vitrified waste than the 100 or 200 m spacing case. The peak temperature occurred at a later time (about 30 to 50 years) for the 50 m spacing case.

The simulations also indicate that groundwater near the boreholes will remain in the liquid state, even at the peak temperatures induced by the disposal of the higher heat producing vitrified waste. This is because of the high hydrostatic pressure at the depths of the waste disposal zone (e.g., approximately 39 MPa at 4,000 m depth).

Simulated groundwater specific discharge in the disturbed zone of the central borehole for the base case model conditions (nine boreholes with 200 m spacing) and the disposal of used fuel assemblies is shown in Figure 9. The simulated upward groundwater flux within the waste disposal zone at depths of 3,500 to 4,000 m exceeds 1 mm/year for up to about 1,000 years. At the top of the waste disposal zone (z = -3,000 m) the upward specific discharge is about 0.1 mm/year during the early thermal period, but declines rapidly after a few decades. The upward flow rates in the borehole disturbed zone above the waste disposal zone are orders of magnitude lower than those deeper in the system (note the log scale of vertical specific discharge in Figure 9). Although not shown in Figure 9, the simulated vertical groundwater flux toward the bottom of the waste disposal zone is downward, indicating that thermal expansion of fluid is forcing water in a focused manner, against buoyant forces. The upward flow from these simulations may overestimate flow rates because the model does not include the salinity stratification that would tend to suppress upward flow from depth.

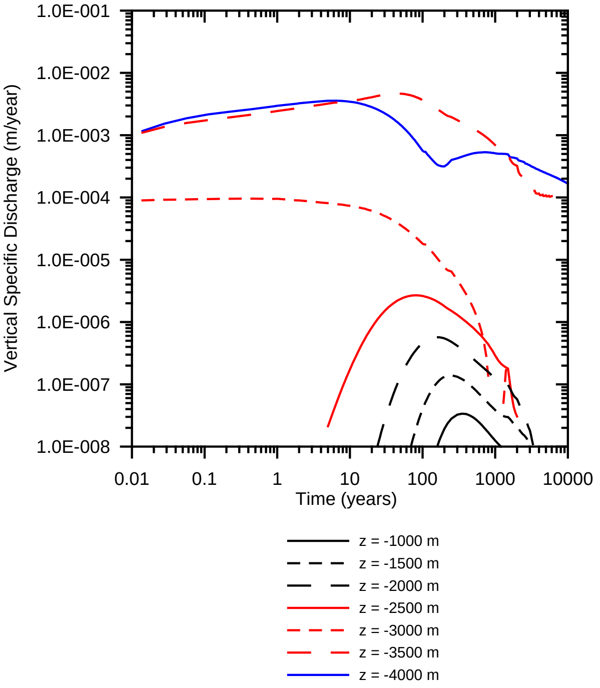

Figure 9. Histories of vertical groundwater specific discharge in the borehole disturbed zone at various depths for disposal of used nuclear fuel in an array of nine boreholes.

Groundwater flow induced by the waste heat includes flow from the thermal expansion of water and from free convection. The relative importance of these two effects depends on the contrast in permeability between the borehole disturbed zone and the surrounding host rock, and on the bulk permeability of the host rock. For the base case parameter values of permeability shown in Table 1 the effects of fluid thermal expansion and flow through the borehole disturbed zone dominate the flow near the waste. Increasing the permeability by three orders of magnitude significantly increases the flow rates in the borehole disturbed zone, but does not induce large-scale free convection in the host rock. Relatively rapid groundwater flow from convection after several hundred years is simulated to occur if the permeability in the disturbed zone and host rock is set to a value of $1\text{x}10^{-13}$ m^2. However, bulk permeability for crystalline basement rocks in the depth range of 3,000 to 5,000 m is not expected to be this high. Nonetheless, this sensitivity run demonstrates the model’s ability to simulate free convection from waste heat.

IV. CONCLUSIONS

Numerical modeling has been used to investigate the impacts of coupled processes on the disposal of high-level radioactive waste in deep boreholes. Coupled thermal-mechanical simulations were conducted with a 2D model of the host rock near the borehole. A 3D model of coupled thermal-hydrologic processes was constructed to simulate groundwater flow induced by waste heat.

Results of the thermal-mechanical model indicate significant increases in stress and compressive strain in the host rock near the borehole. Mechanical effects are associated with peak temperature increases and are thus much greater for the disposal of vitrified waste from reprocessing. Under anisotropic ambient horizontal stress conditions the simulated maximum compressive stress at the borehole wall likely exceeds the compressive strength of granite, which could result in borehole instability and the formation of borehole breakouts. The state of compression and associated strain near the borehole would lead to lower permeability in the disturbed zone around the borehole during the thermal period. The magnitude of the compressive strain suggests that fracture permeability could be significantly reduced in a sparsely-fractured, low-porosity granite. Software code comparisons indicate that there are multiple options for numerical modeling of coupled processes and that a deformable grid capability is probably not necessary for thermal-mechanical simulations of the borehole disposal system.

Results of the 3D thermal-hydrologic model of the far field provide information on the important flow processes induced by waste heat and the sensitivity to borehole disposal system design. Simulated temperatures from both the thermal-hydrologic and the thermal-mechanical model indicate that higher temperatures near the borehole are relatively short lived and decrease with distance into the host rock. Results of the thermal-hydrologic model show that pressure and temperature conditions are below boiling for all locations and times in the disposal system. At times from about 100 to 10,000 years simulated temperatures and groundwater flow rates are somewhat, but not dramatically, higher for closer borehole spacing of 100 m and up to 25 total boreholes. Heat transfer is dominated by conduction due to the low fluid flow rates. Peak upward groundwater flow rates in the borehole disturbed zone vary with depth, generally occur within 10 to 100 years, and are related to the thermal expansion of groundwater and focusing of flow within the assumed higher-permeability zone near the borehole. Flow rates that persist to longer times are much lower and caused by free convection. Sensitivity analyses indicate that the bulk permeability of the host rock would have to be higher than expected at depths of 3,000 to 5,000 m to support vigorous free convection of groundwater.

Overall, these results support the conclusion that deep borehole disposal of high-level radioactive waste is a viable potential option for the disposition of used nuclear fuel or vitrified waste.[9] The coupled modeling capabilities described in this paper, when augmented by some additional complexity, can be used to support disposal system design calculations, screening of features, events, and processes, and performance assessment analyses of risk.

Additional modeling will include the coupling of hydrologic processes in the 2D thermal-mechanical model near the borehole. Significant feedback may occur between decreased fracture permeability from compressive strain in the host rock and fluid pressure within the borehole. If fluid pressures within the borehole become sufficiently high from thermal expansion, this increased pressure would oppose the compressive strain as the pressure is transmitted into the host rock. The 3D thermal-hydrologic model will be extended to include the chemical stratification of salinity and associated variability in fluid density. The higher salinity at depth would tend to suppress the flow of groundwater from the waste disposal zone to the shallower subsurface by convection or thermal fluid expansion within the borehole disturbed zone.

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REFERENCES

1. NATIONAL ACADEMY OF SCIENCES, *The Disposal of Radioactive Waste on Land* (1957). http://www.nap.edu/openbook.php?record_id=10294
2. O'BRIEN, M.T, L.H. COHEN, T.N. NARASIMHAN, T.L. SIMKIN, H.A. WOLLENBERG, W.F. BRACE, S. GREEN, H.P. PLATT, *The Very Deep Hole Concept: Evaluation of an Alternative for Nuclear Waste Disposal*, Berkeley, CA, Lawrence Berkeley Laboratory, LBL-7089 (1979).
3. WOODWARD AND CLYDE CONSULTANTS, *Very Deep Hole Systems Engineering Studies*. Columbus, OH, ONWI (1983).
4. JUHLIN, C. AND H. SANDSTEDT, *Storage of Nuclear Waste in Very Deep Boreholes: Feasibility Study and Assessment of Economic Potential. Part I: Geological Considerations. Part II: Overall Facility Plan and Cost Analysis*., Svensk Karnbranslehantering AB (1989).
5. HEIKEN, G., G. WOLDEGABRIEL, R. MORLEY, H. PLANNERER, J. ROWLEY, *Disposition of Excess Weapon Plutonium in Deep Boreholes – Site Selection Handbook*. Los Alamos, NM, Los Alamos National Laboratory (1996).
6. NIREX, *A Review of the Deep Borehole Disposal Concept*, Report N/108, United Kingdom Nirex Limited (2004).
7. ANDERSON, V.K., *An Evaluation of the Feasibility of Disposal of Nuclear Waste in Very Deep Boreholes*, Dept. of Nuclear Engineering, Cambridge, MA, MIT (2004).
8. GIBB, F.G.F., N.A. MCTAGGART, K.P. TRAVIS, D. BURLEY, K.W. HESKETH, High-density support matrices: Key to the deep borehole disposal of spent nuclear fuel, *J. of Nuclear Materials* **374**: 370-377 (2008).
9. BRADY, P.V., B.W. ARNOLD, G.A. FREEZE, P.N. SWIFT, S.J. BAUER, J.L. KANNEY, R.P. RECHARD, J.S. STEIN, *Deep Borehole Disposal of High-Level Radioactive Waste*, SAND2009-4401, Albuquerque, NM, Sandia National Laboratories (2009).
10. HOAG, C.I., *Canister Design for Deep Borehole Disposal of Nuclear Waste*, Dept of Nuclear Engineering, Cambridge, MA, MIT (2006).
11. ANDRA (Agence nationale pour la gestion des déchets radioactifs), *Dossier 2005: Argile. Tome: Safety Evaluation of a Geological Repository* (2005).