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Thermal-Hydrology Simulations of Disposal of High-Level Radioactive Waste in a Single Deep Borehole

Teklu Hadgu, Emily Stein, Ernest Hardin, Geoff Freeze and Glenn Hammond

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Teklu Hadgu, Emily Stein, Ernie Hardin, Geoff Freeze and Glenn Hammond

Nuclear Waste Disposal research and Analysis

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Abstract

Simulations of thermal-hydrology were carried out for the emplacement of spent nuclear fuel canisters and cesium and strontium capsules using the PFLOTRAN simulator. For the cesium and strontium capsules the analysis looked at disposal options such as different disposal configurations and surface aging of waste to reduce thermal effects. The simulations studied temperature and fluid flux in the vicinity of the borehole. Simulation results include temperature and vertical flux profiles around the borehole at selected depths. Of particular importance are peak temperature increases, and fluxes at the top of the disposal zone. Simulations of cesium and strontium capsule disposal predict that surface aging and/or emplacement of the waste at the top of the disposal zone reduces thermal effects and vertical fluid fluxes. Smaller waste canisters emplaced over a longer disposal zone create the smallest thermal effect and vertical fluid fluxes no matter the age of the waste or depth of emplacement.

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The authors would like to thank Robert McKinnon (6224) for technical interest and programmatic support.

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NOMENCLATURE

DOE	Department of Energy
HLW	High-Level Radioactive Waste
PWR	Pressurized Water Reactor
SNF	Spent Nuclear Fuel
SNL	Sandia National Laboratories

1. INTRODUCTION

Thermal-hydrologic modeling of disposal of high-level radioactive waste in deep boreholes has been the subject of recent studies. Previous simulations looked primarily at disposal of spent nuclear fuel (SNF) in deep boreholes (Arnold et al., 2011; Arnold and Hadgu, 2013). Arnold et al. (2014) looked at disposal of cesium and strontium capsules in a single deep borehole. The basic concept of deep borehole disposal is to drill a 5 km deep borehole in a formation with basement crystalline rock below the depth of 2 km. The base case also includes waste emplacement in the bottom 2 km of the borehole and a seal system in the upper part of the borehole. Previous modeling studies used the FEHM numerical code (Zyvoloski, 2007) for thermal-hydrology modeling.

Earlier thermal-hydrologic simulations represented the host rock with a single low permeability, and seals and the surrounding disturbed rock zone with a single relatively higher permeability. Sensitivity studies were also carried out to understand the effect of the rock and near-borehole permeability on performance of the disposal option (Hadgu et al., 2012). More recent modeling studies (Arnold and Hadgu, 2013) have used more realistic geological and hydrogeological conditions. These include permeability and thermal conductivity variations with depth and salinity stratification representative of relevant formations. The studies also looked at representations of different arrays of boreholes and spacing between them.

This study is a continuation of previous work with the objective of studying the thermal-hydrology of a single borehole for different waste using the PFLOTRAN simulator (Hammond et al., 2014). The analysis assumed that either spent nuclear fuel (SNF) or a combination of cesium and strontium capsules is emplaced in the borehole. For the emplacement of SNF, it was assumed that 400 PWR assemblies of 40 GW-d/MT burn-up are emplaced in a borehole. The thermal decay curve for a single PWR assembly is shown in Figure 1. The thermal output of Cs-137 and Sr-90 capsules is shown in Figure 2, which includes large variations. For the thermal-hydrology analysis the average thermal output (weighted by number of each canister type) was considered, as was also done in Arnold et al. (2014). Using the average thermal output per canister results in the correct total heat source for the disposal zone, because all 1936 cesium and strontium capsules will fit in a single borehole (Arnold et al., 2014). Borehole emplacement was assumed to be in 2020.

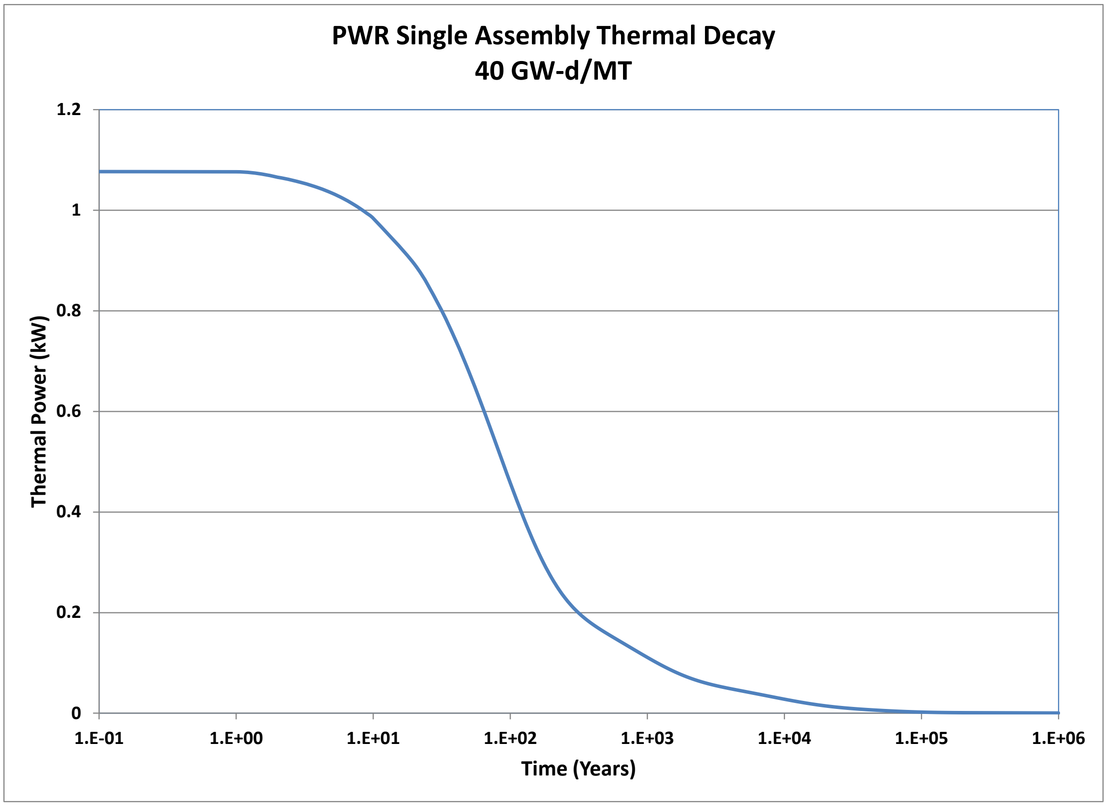

Figure 1. Thermal decay history of PWR Single Assembly with 40 GW-d/MT burn-up

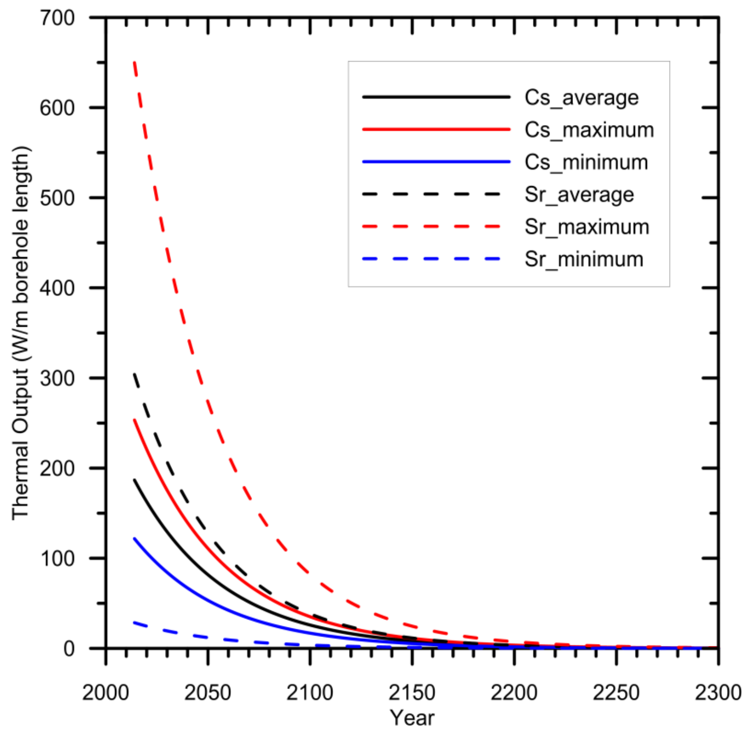

Figure 2. Projected thermal output from Cesium and Strontium capsules (From Arnold et al., 2014, based on DOE 2014)

Disposal concepts for the disposal of cesium and strontium capsules in a deep borehole are discussed in Arnold et al. (2014, Section 3.2.2). The inventory includes 1,335 Cs-137 capsules and 600 Sr-90 capsules, for a total of 1935 capsules. Different configurations are possible for the disposal of the capsules in a deep borehole depending on the size of canisters, borehole diameter and depth. In this analysis four of the possible configurations considered in Arnold et al. (2014) were adopted. The four possible options are summarized in Table 1. The 2-capsule case has the capsules arranged end-to-end within a 1.083-meter long waste package or disposal overpack. Arnold et al. (2014) assumed that the disposal borehole contains 1.5 capsules per linear meter. Thus, the entire inventory could be disposed of in a single borehole over 1300 m disposal length. This configuration could be emplaced in a borehole with disposal zone diameter of 8.5 inches (0.216 m). In the 6-capsule case, a 1.083-m long waste package contains 2 layers of 3 capsules each (Figure 3a). This configuration requires a larger disposal zone diameter of 12.25 inches (0.311 m) and a shorter disposal zone length (433 m) than the 2-capsule case.

Arnold et al. (2014) also considered a concept based on the SNL reference design for the disposal of SNF in deep boreholes. The SNL reference design is based on a 17-inch (0.432-m) diameter borehole. The larger borehole would allow canisters that can accommodate 7 capsules in a layer (Figure 3b). Thus, a two-layer canister could hold 14-capsules. If the SNL reference design canister is used, it could accommodate eight layers for a total of 56 capsules. In this analysis we assumed the two-layer case would have the same length as the 2-capsule and 6-capsule canisters described above. We also assumed that the thermal analysis of the 14-capsule case would also cover the 56-capsule case because the configuration is likely to lead to about the same total length of canisters. Thus, we did not conduct thermal analysis of the 56-capsule case.

Table 1. Possible alternative deep borehole disposal concepts for CsCl and SrF_2 capsules (From Arnold et al., 2014, Table 3-4)

	2-Capsule (Baseline)	6-Capsule	SNL Reference SNF Canisters	
Borehole Diameter (m)	**0.216**	**0.311**	**0.432**	**0.432**
(in)	8.5	12.25	17	17
DZ Casing O.D. (m)	0.178	0.273	0.340	0.340
DZ Casing I.D. (m)	0.162	0.245	0.321	0.321
Canister O.D. (m)	0.114	0.191	0.273	0.273
Canister I.D. (m)	0.089	0.165	0.212	0.212
Capsules per Layer	1	3	7	7
Number of Layers	2	2	2	8
Capsules per Canister	2	6	14	56

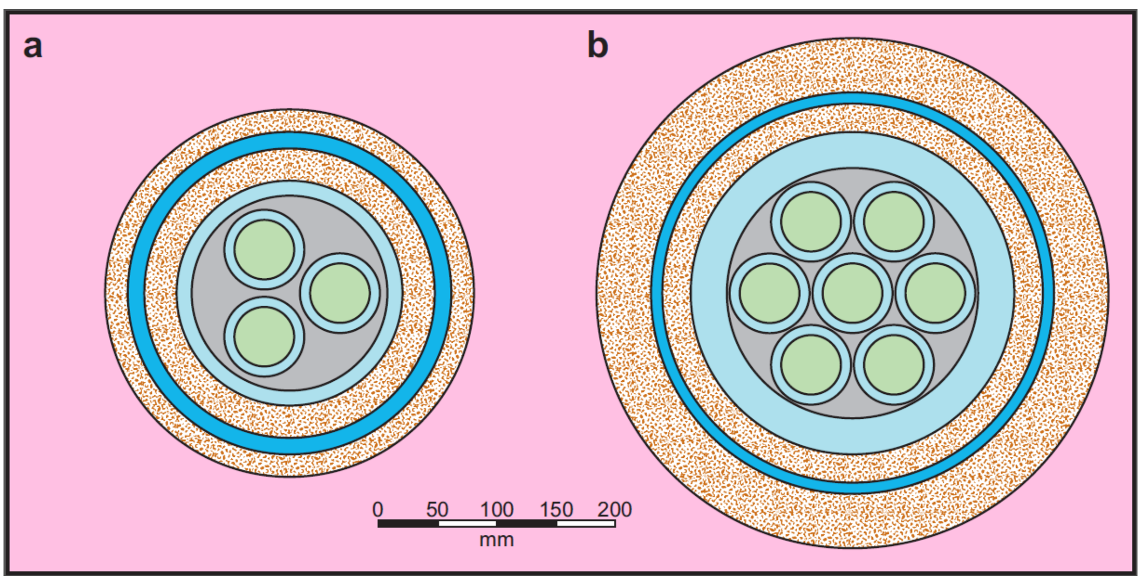

Figure 3. Representation of 6-capsule (a) and 14-capsule (b) canister geometries for the disposal of CsCl and SrF_2 capsules (Arnold et al., 2014, Figure 3-4)

2. MODEL SET-UP

For model set-up a single borehole with a total depth of 5 km was assumed. The model geometry includes an area of 2 km x 2 km and a depth of 6 km. To reduce the computational burden a mesh with half-symmetry was made. The resulting mesh includes 54,000 grid blocks (Figure 4). Initial conditions and rock material properties used are mostly the same as in Arnold and Hadgu (2013). The stratigraphy includes sedimentary rock above 1500 m depth, underlain by granite rock to total depth. For sedimentary formations above the crystalline bedrock, parameters given in Table 2 were used.

Table 2. Parameter values of sedimentary rocks (Arnold and Hadgu, 2013)

Lithology	Permeability (m^2)	Porosity (-)	Thermal K (W/m/K)	Heat Capacity (J/kg/K)
sandstone	1×10^{-12}	0.30	3.5	840.
shale	1×10^{-15}	0.02	1.8	840.
limestone	1×10^{-13}	0.05	2.7	840.
dolomite	1×10^{-13}	0.05	4.0	840.

For granite rock in the crystalline basement, porosity of 0.01 and heat capacity of 880 J/kg/K were used. For this study we have selected the relationship of Stober and Bucher (2007) for permeability variation with depth in the granite rock. The relationship is based on deep drilling into continental crystalline basement rock and thus is appropriate for thermal-hydrology analysis of nuclear waste disposal in deep boreholes. The relationship is given as:

$$\text{Log}(k) = -1.38 \log(z) - 15.4$$

Where z is depth in km and k is permeability in m^2. The permeability of the borehole and the surrounding disturbed rock within an area of 1 m^2 was increased by a factor of 10 to account for increased permeability in the disturbed rock zone and degradation of borehole seals. The analysis also used depth dependent thermal conductivity in the granite rock. The relationship of Vosteen and Schellschmidt (2003) was used. In this analysis salinity stratification was not included.

Boundary conditions include: constant pressure and temperature at the top surface (atmospheric pressure and 10 °C); no fluid flux and a constant temperature of 160 °C at the bottom surface; no fluid or heat flux at the sides of the model domain. The temperature boundary conditions represent an average geothermal gradient of 25 °C/km. The system is initially at hydrostatic pressure conditions and the temperature gradient. For the simulations the PFLOTRAN numerical software (Hammond et al., 2014) was used. Use of PFLOTRAN allowed for high performance parallel computing utilizing many processors.

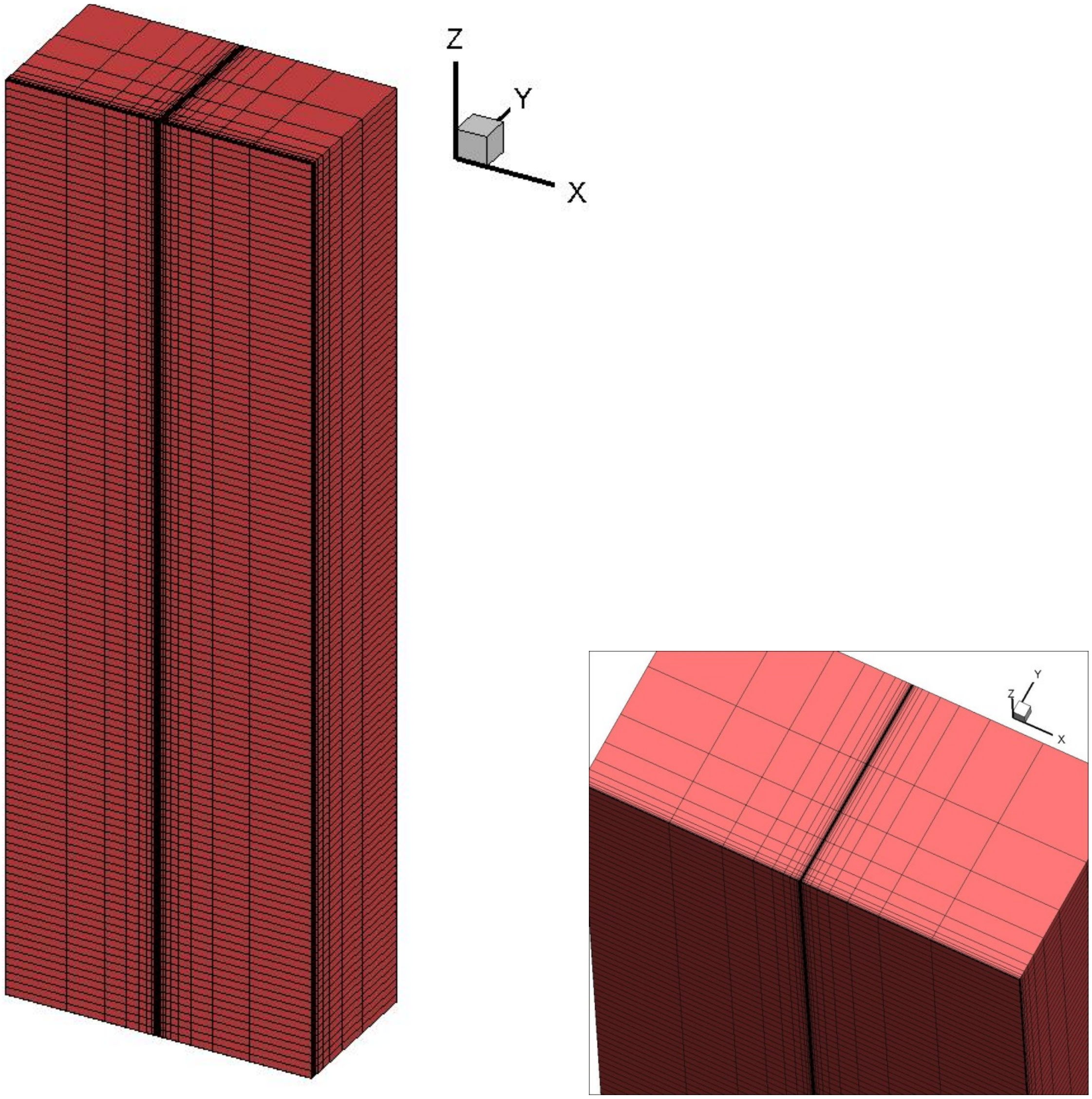

Figure 4. Numerical mesh of the thermal-hydrologic model.

3. RESULTS AND DISCUSSION

3.1. Modeling of Disposal of SNF Canisters

The analysis first looked at emplacement of SNF canisters in a single borehole between 3 km and 5 km depth. Thermal output of PWR single-assembly fuel rods used is the same as in Arnold et al. (2013). PFLOTRAN was run to generate temperature and fluid flux output using the Stober and Bucher (2007) permeability relations in granite rock. The results of the simulations are shown in Figures 5 and 6. Figure 5 shows temperature profiles inside the borehole at 4000 m depth. The predicted peak temperature is about 174 °C (~60 °C increase from ambient) at approximately 10 years.

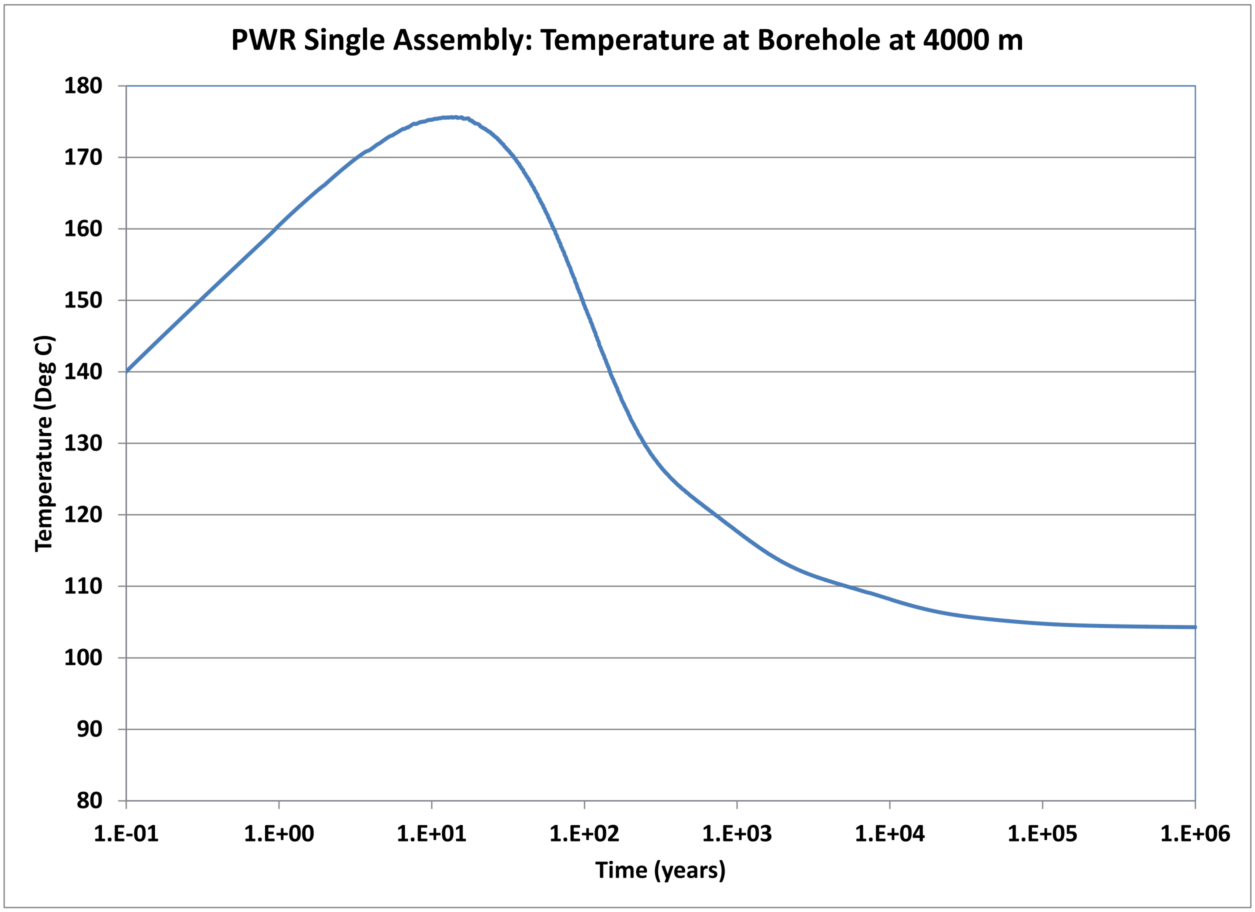

Figure 5. Simulated temperature vs. time in the borehole for the PWR single assembly case at 4000 m depth.

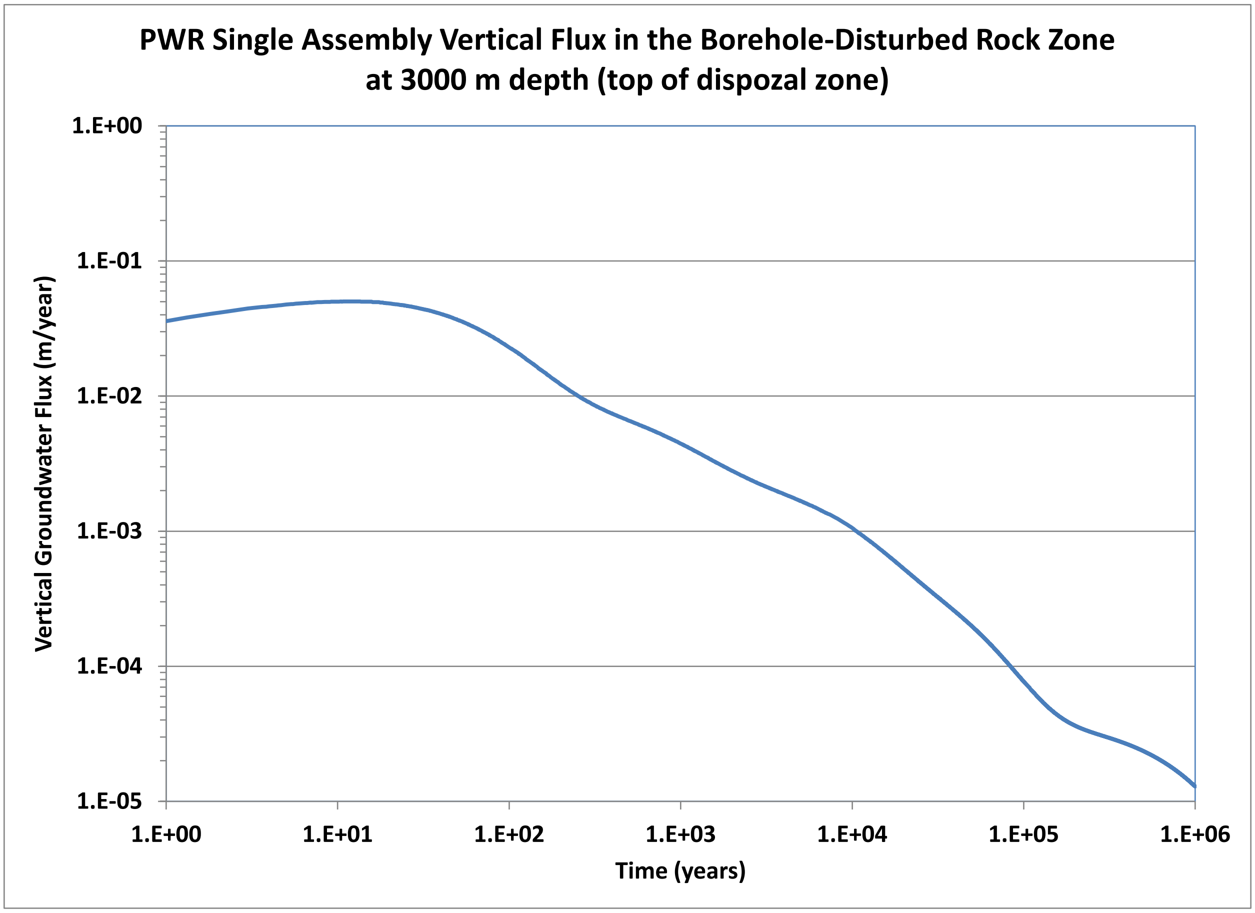

Figure 6. Simulated vertical groundwater flux vs. time in the borehole and disturbed rock zone for the PWR single assembly case at 3000 m depth (top of disposal zone).

3.2. Modeling Disposal of Cesium and Strontium Capsules

3.2.1. Canisters with Two Capsules

For the 2-capsule modeling case (Table 1) the Cs-137 and Sr-90 capsules were first placed in the lower part of the borehole between 5000 m and 3700 m depth, as was done in Arnold et al. (2014). Half of the thermal output was applied because of symmetry considerations. Thermal-hydrology simulations were run to total time of 10^5 years. Figure 7 shows temperature at 3700 m and 4000 m depths as a function of time. Peak temperatures occur within 10 years after emplacement. At both depths the maximum temperature increase is over 50 °C. Figure 8 shows the corresponding vertical ground water flux at the top of the disposal zone (3700 m depth), as a result of the thermal perturbation. A peak flux of about 0.035 m/yr is reached at about the same simulation time as the peak temperature, and quickly dissipates following the sharp heat decay.

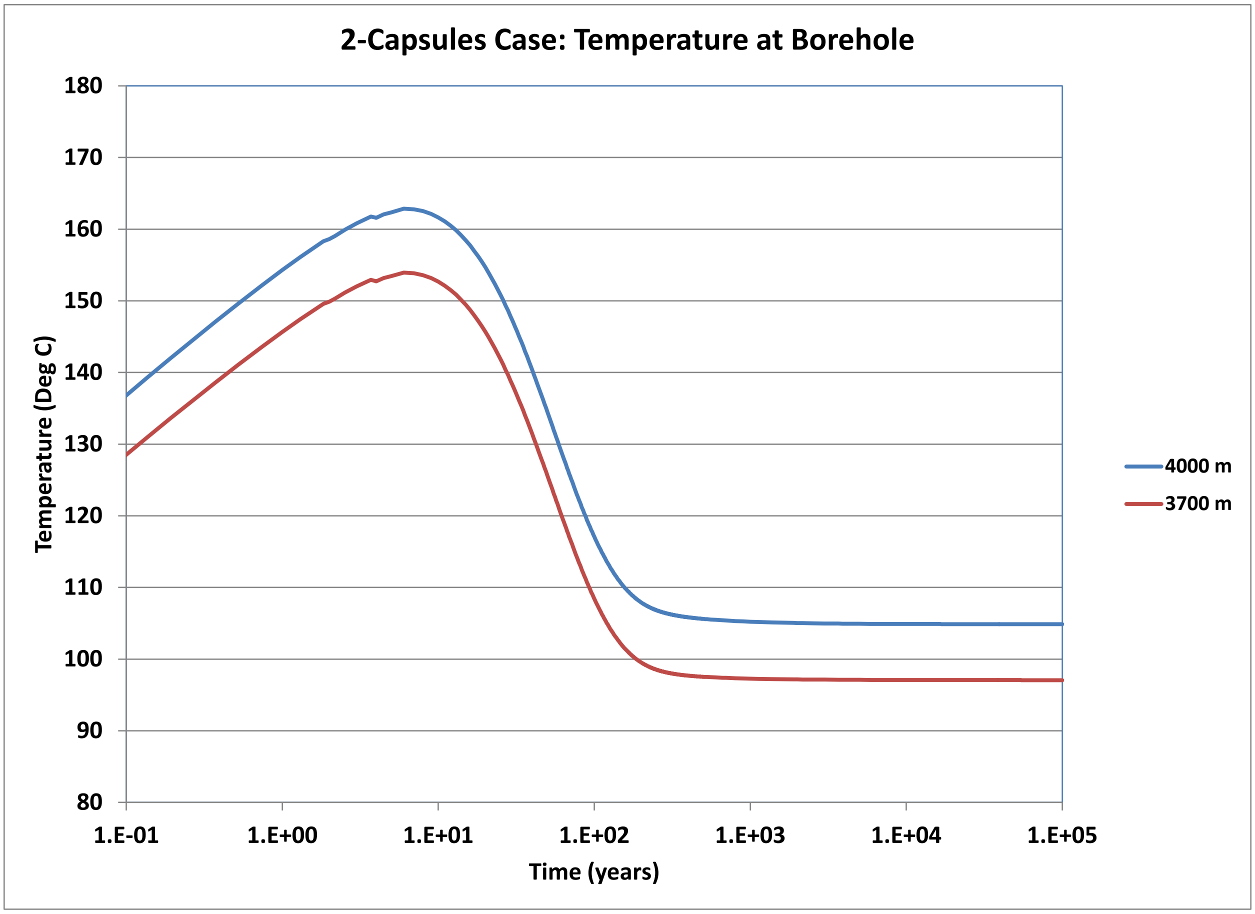

Figure 7. Simulated temperature vs. time in the borehole for the 2-capsule case at depths of 4000 m and 3700 m (top of the disposal zone). Emplacement at bottom of borehole.

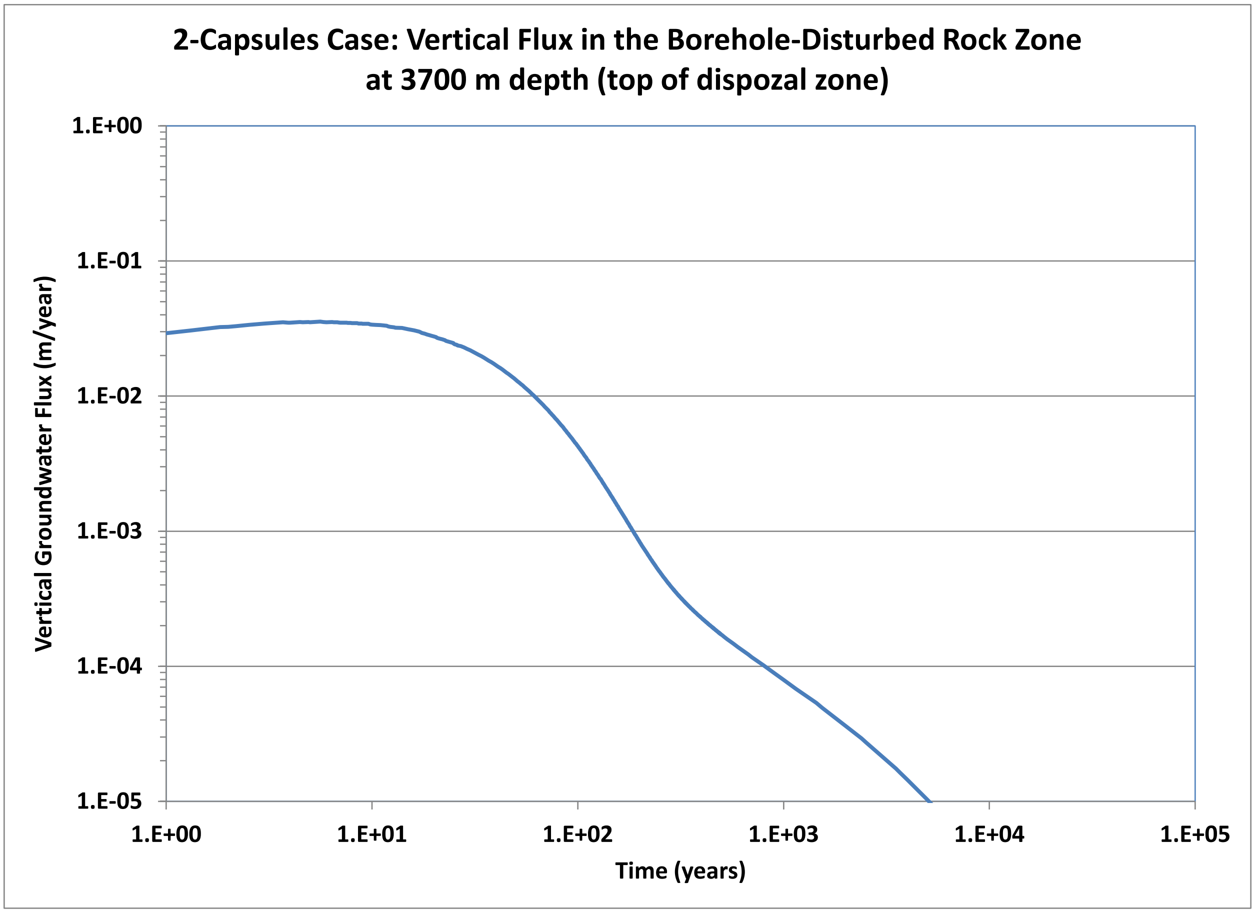

Figure 8. Simulated vertical groundwater flux vs. time in the borehole and the disturbed rock zone for the 2-capsule case at 3700 m depth (top of the disposal zone).

Delaying of borehole emplacement of the capsules would reduce the thermal output and thus reduce the maximum temperature increase which would be beneficial for borehole integrity. Figure 9 shows predicted temperature at 4000 m depth for emplacement at 2020 (base case) and 2030. For the delayed emplacement case (2030) the peak temperature is reduced by about 10 °C, resulting in a smaller temperature increase. Figure 10 shows the predicted groundwater flux for the two emplacement periods. As shown in the figure, delaying emplacement to 2030 would reduce the peak flux to about 0.025 m/yr.

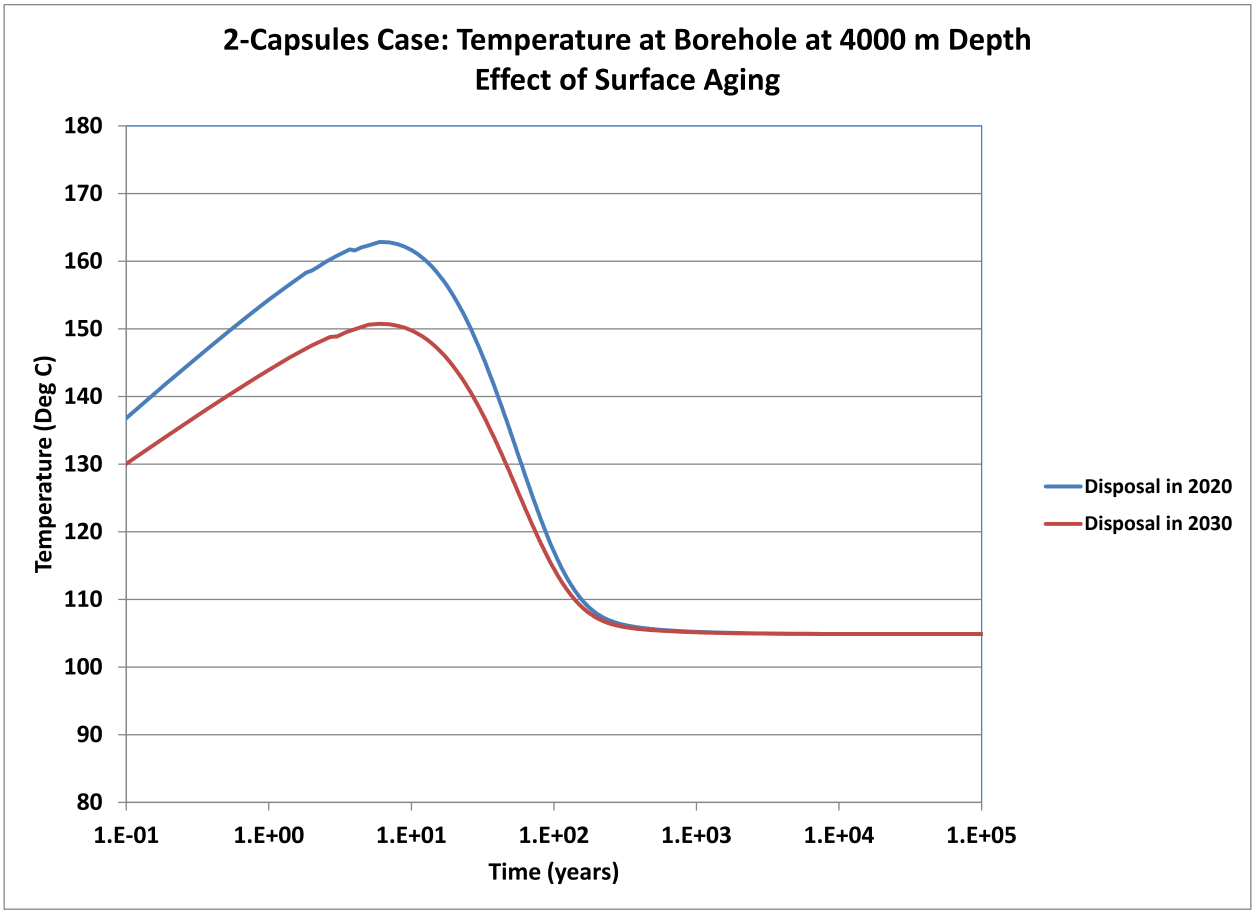

Figure 9. Simulated temperature vs. time in the borehole for the 2-capsule case at 4000 m depth. Effect of surface storage to 2020 and 2030. Emplacement at bottom of borehole.

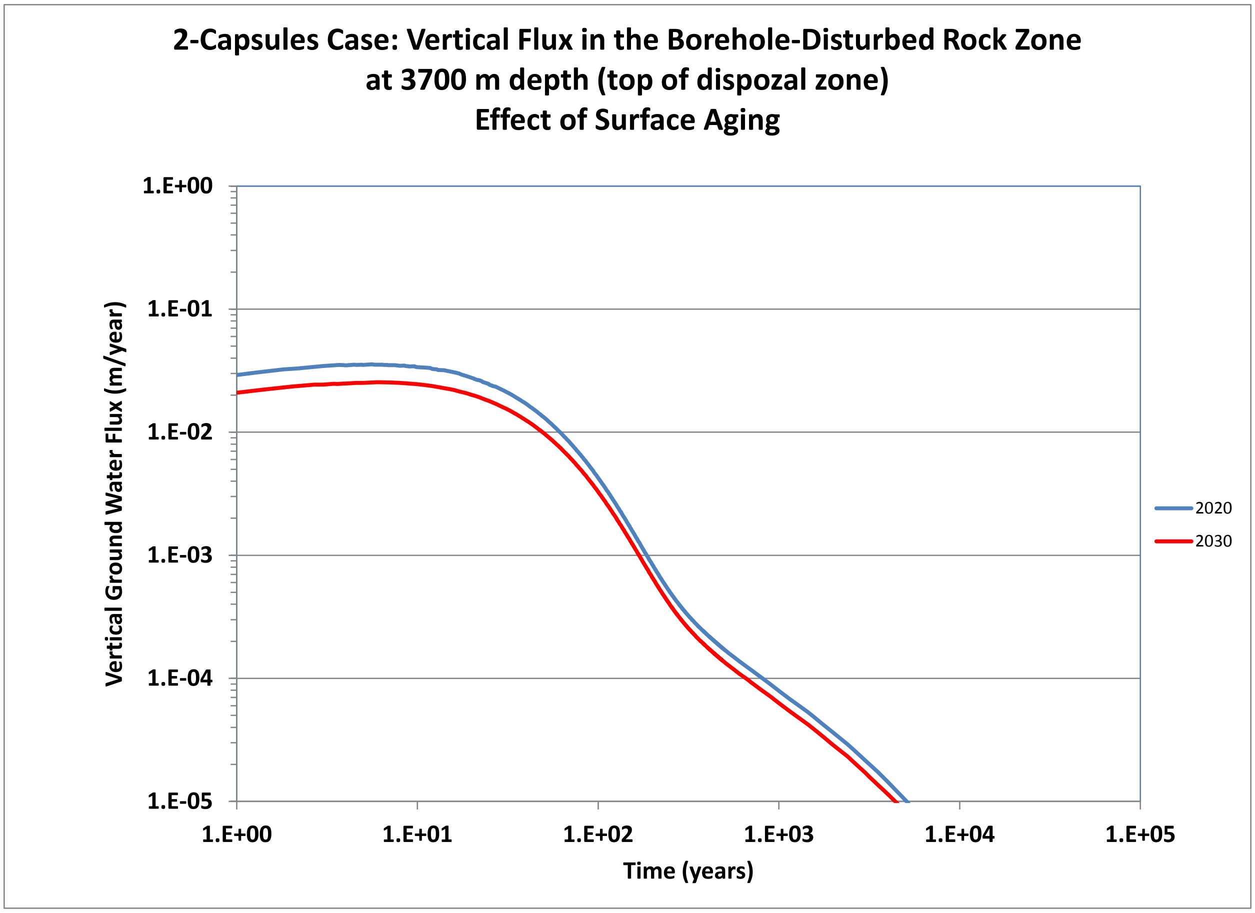

Figure 10. Simulated vertical groundwater flux vs. time in the borehole and the disturbed rock zone for the 2-capsule case at 3700 m depth (top of the disposal zone). Effect of surface storage to 2020 and 2030. Emplacement at bottom of borehole.

Another way of reducing peak temperature is to emplace the capsules in the upper part of the disposal zone, which would reduce the in-situ ambient temperature compared to the lower part of the borehole. For the 2-capsule modeling case, that would be emplacement between 3000 m and 4300 m depth. Figure 11 shows predicted temperature at 4000 m and 3000 m (top of disposal zone) depths. Figure 12 shows the corresponding groundwater flux. The peak flux (about 0.035 m/yr) at 3000 m depth is about the same as the peak flux at the top of the disposal zone for the bottom emplacement option (Figure 8). The slightly smaller temperature increase at the top of the disposal zone (3000 m) for this case would reduce the vertical ground water flux. But the permeability relations of Stober and Bucher (2007) show increased permeability at shallower depths, resulting in increased vertical flow.

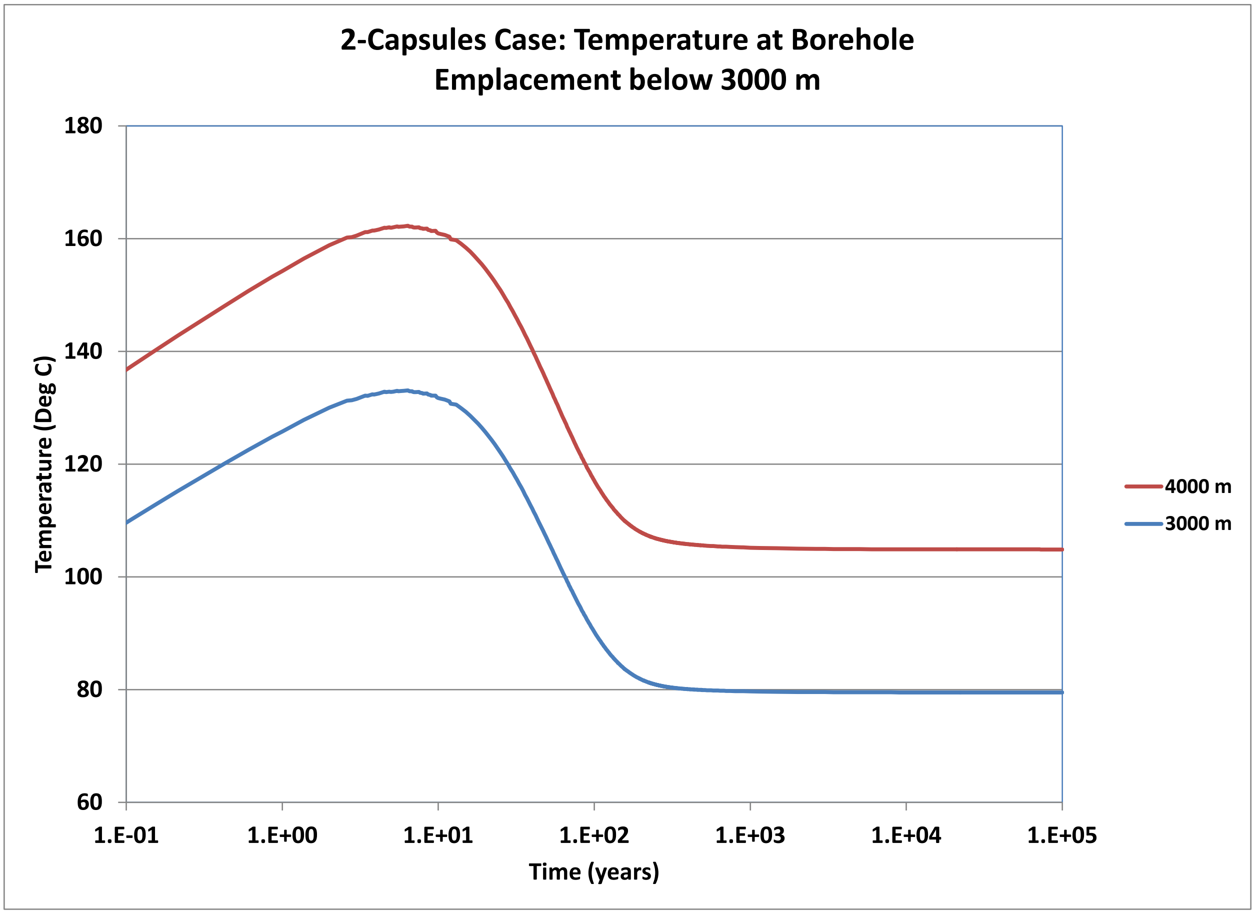

Figure 11. Simulated temperature vs. time in the borehole for the 2-capsule case at 4000 m depth. Effect of emplacement in the upper part of the borehole. Emplacement of waste between 3000 m and 4300 m depth.

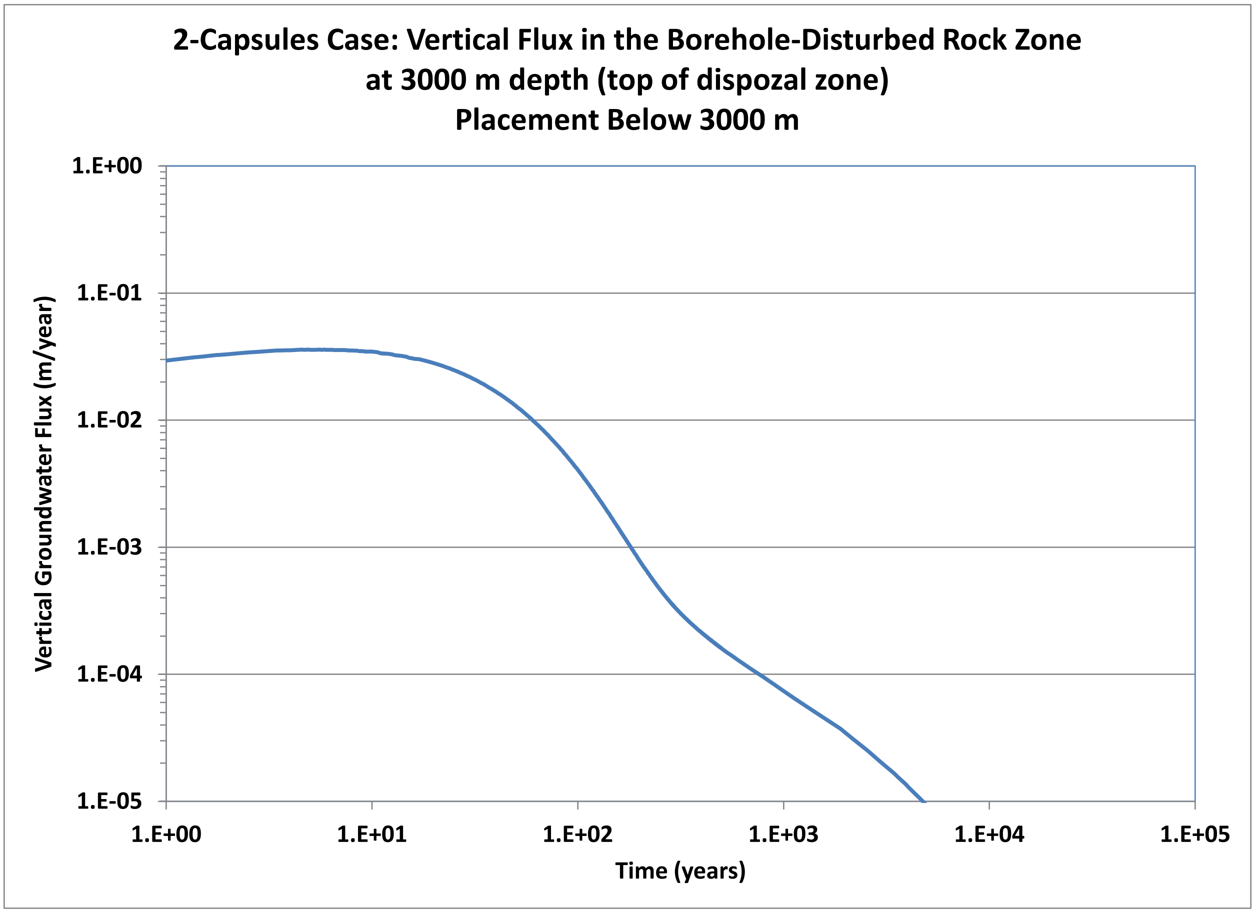

Figure 12. Simulated vertical groundwater flux vs. time in the borehole and the disturbed rock zone for the 2-capsule case at 3000 m depth (top of the disposal zone). Emplacement below 3000 m.

3.2.2. Canisters with Six Capsules

For the 6-capsule case (Table 1) a canister contains three capsules in a layer and two layers. Assuming the canister for the 6-capsule case has the same length as the 2-capsule canister, the total length required to emplace all capsules would be 433 m. For the case of emplacement at bottom part of the borehole (base case) the Cs-137 and Sr-90 capsules were placed in the lower part of the borehole between 5000 m and 4567 m depth. Thermal-hydrology simulations were run to a total time of 10^5 years. Figure 13 shows predicted temperature at selected depths as a function of time. As in the 2-capsule case, peak temperatures occur within 10 years after emplacement. The simulated peak temperature (about 300 °C at 4800 m depth) for the 6-capsule case is higher than that in the 2-capsule case due in part to the higher ambient temperature and in part to the more concentrated heat source, which results in a temperature increase of about 175 °C above ambient. Figure 14 shows the corresponding vertical ground water flux near the top of the disposal zone. As a result of the large temperature increase, peak vertical fluxes for this case (about 0.27 m/yr) are approximately 8 times greater than those predicted by the 2-capsule case.

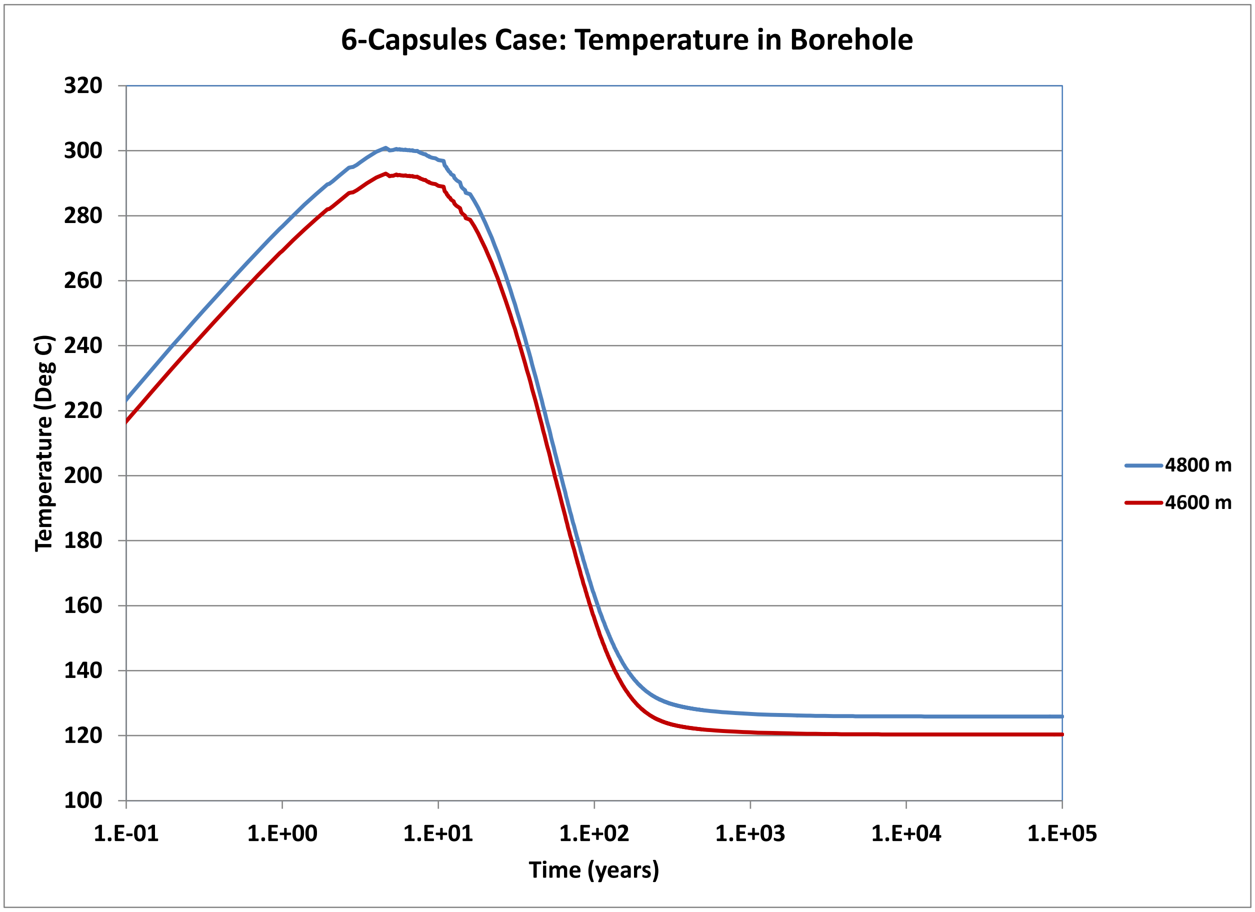

Figure 13. Simulated temperature vs. time in the borehole for the 6-capsule case at depths of 4800 m and 4600m. Bottom emplacement case.

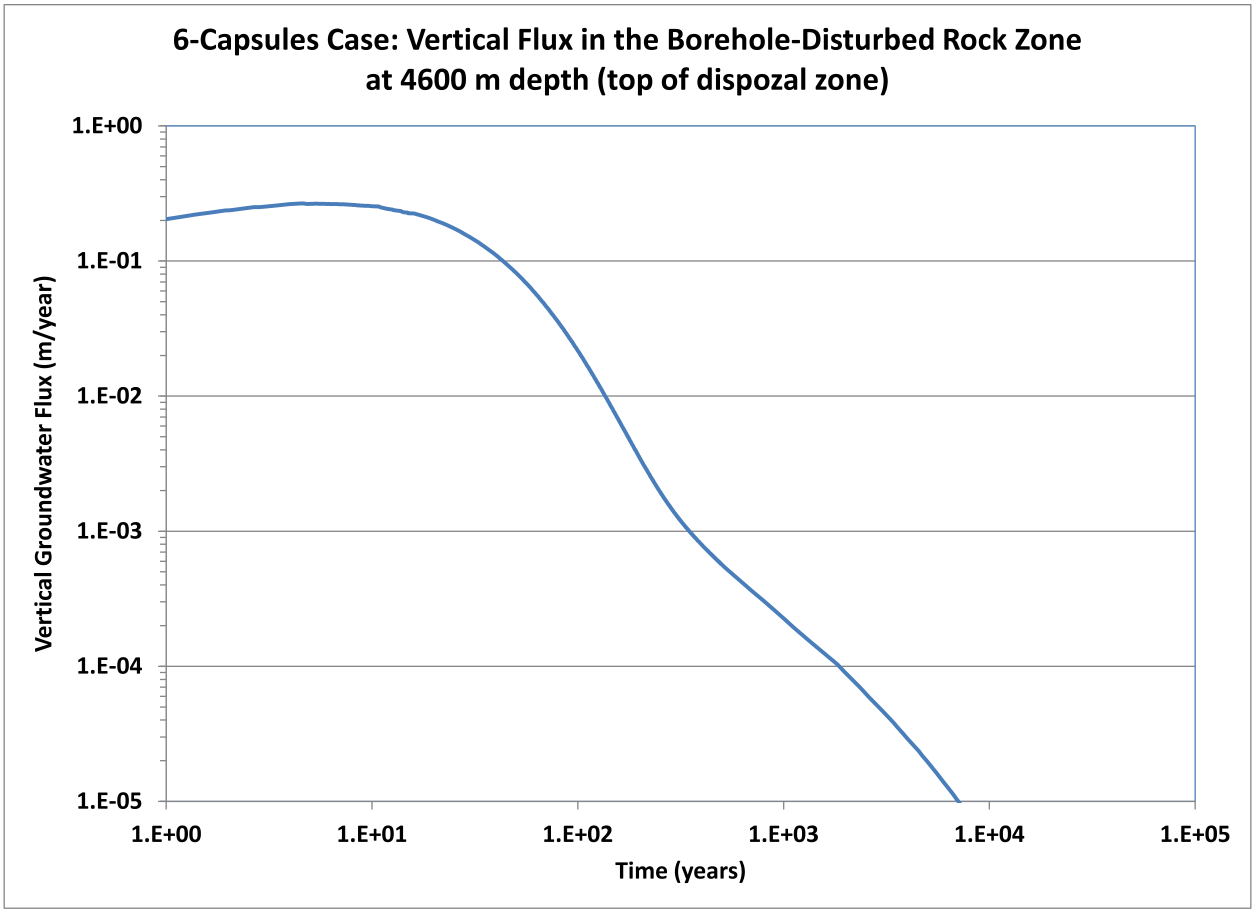

Figure 14. Simulated vertical groundwater flux vs. time in the borehole and the disturbed rock zone for the 6-capsule case at 4600 m depth (top of the disposal zone).

Peak temperatures could be reduced by delaying borehole emplacement of the capsules, as shown for the 2-capsule case. For this case we looked at three emplacement times. Figure 15 shows predicted temperature at 4800 m depth for emplacement at 2020 (base case), 2030 and 2040. As shown in the figure, both options of delayed emplacement (2030 and 2040) reduced the peak temperature, resulting in smaller temperature increases. Figure 16 shows the predicted groundwater flux for the three emplacement times. As shown in the figure, delaying emplacement to 2040 reduces peak fluxes by about a factor of 2.

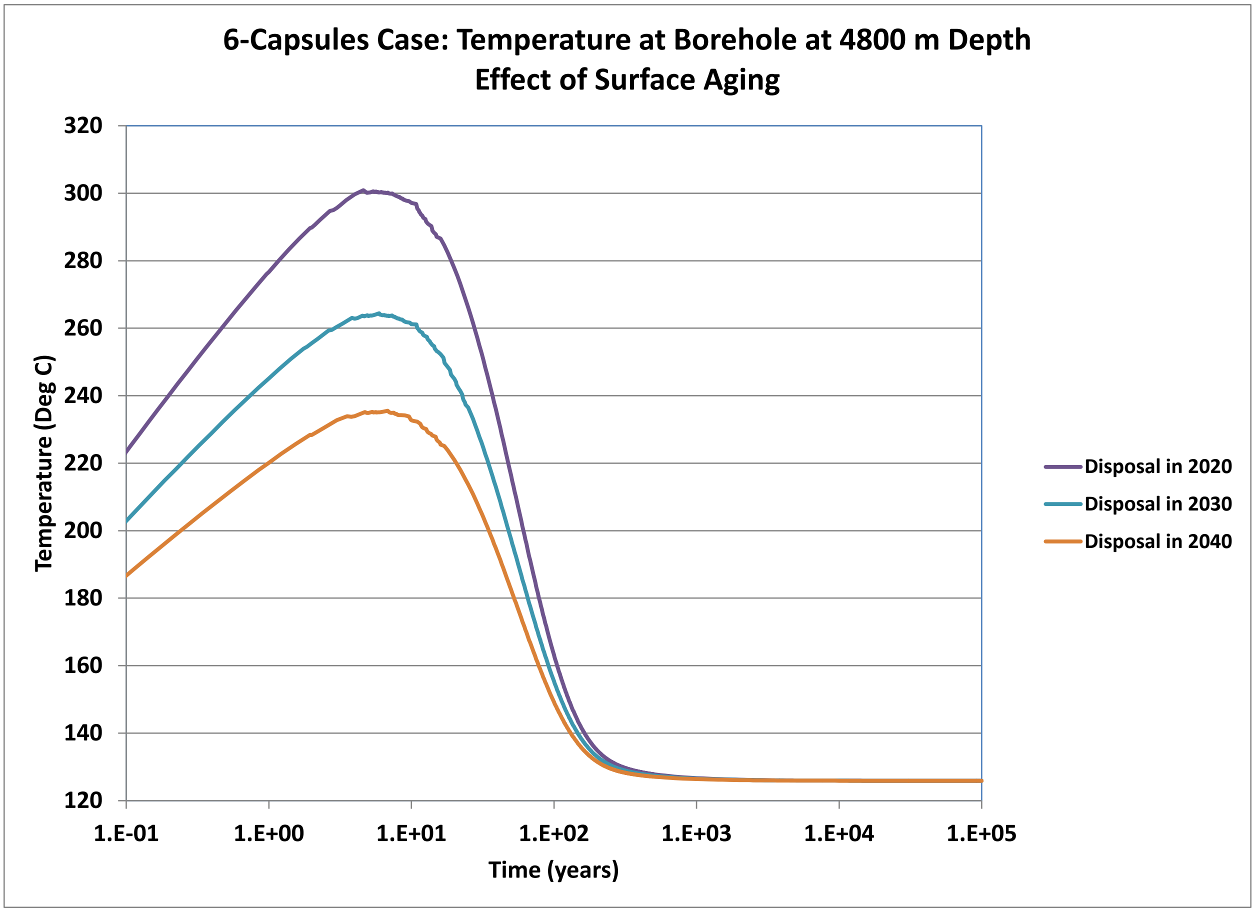

Figure 15. Simulated temperature vs. time in the borehole for the 6-capsule case at 4800 m depth. Effect of surface storage to 2020, 2030, and 2040. Emplacement at bottom of borehole.

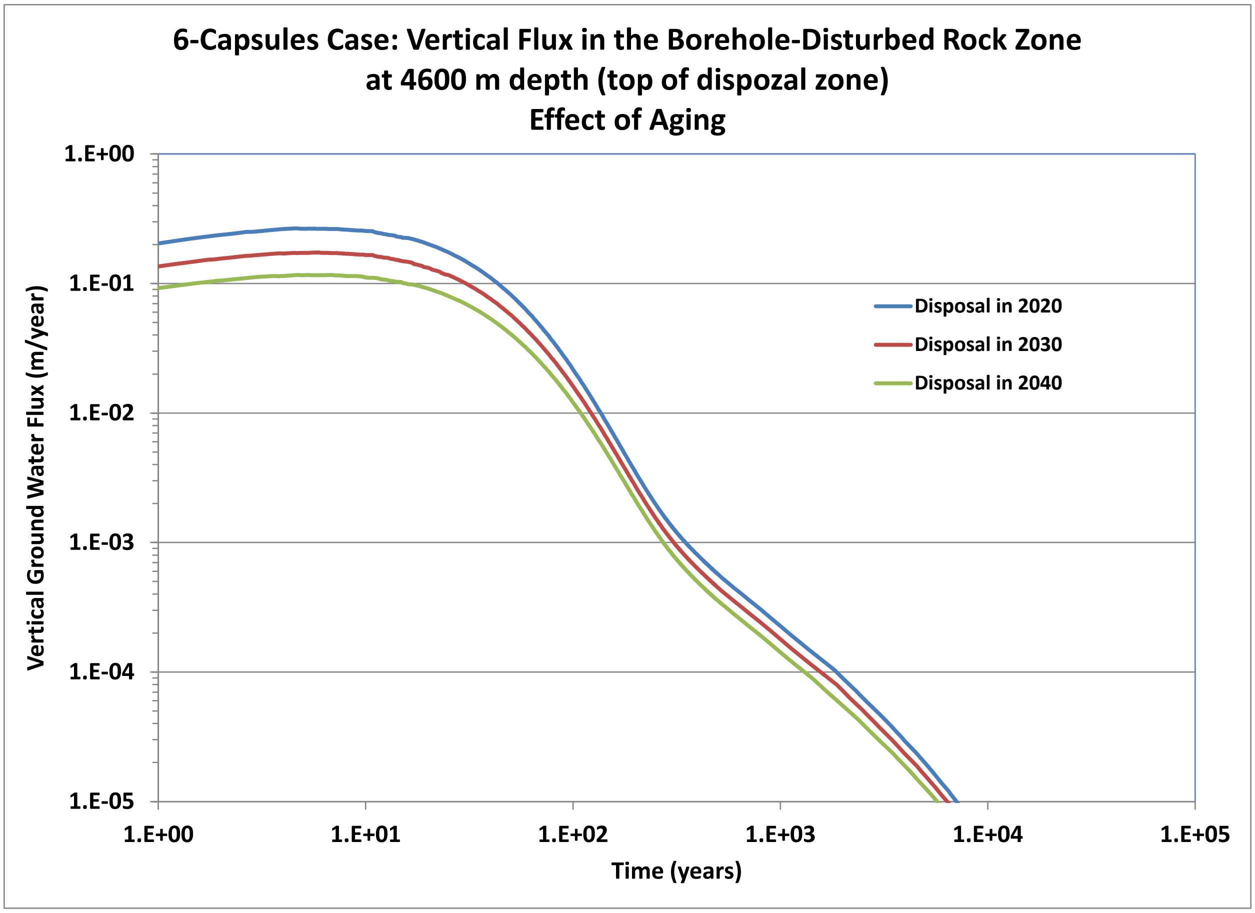

Figure 16. Simulated vertical groundwater flux vs. time in the borehole and the disturbed rock zone for the 6-capsule case at 4600 m depth (top of the disposal zone). Effect of surface storage to 2020, 2030, and 2040. Emplacement at bottom of borehole.

Simulations were also carried out for the emplacement of the capsules in the upper part of the borehole. For the 6-capsule modeling case, that would be emplacement between 3000 m and 3433 m depth. Figure 17 shows predicted temperature at 3200 m and 3000 m (top of disposal zone) depths. Figure 18 shows the corresponding groundwater flux. In this case, the peak temperature (about 242 °C) is substantially less than predicted for emplacement in the lower part of the borehole largely due to lower ambient temperatures. The temperature increase (about 158 °C) is somewhat smaller (Figure 13), and the peak vertical groundwater flux remains the same order of magnitude (about 0.23 m/yr).

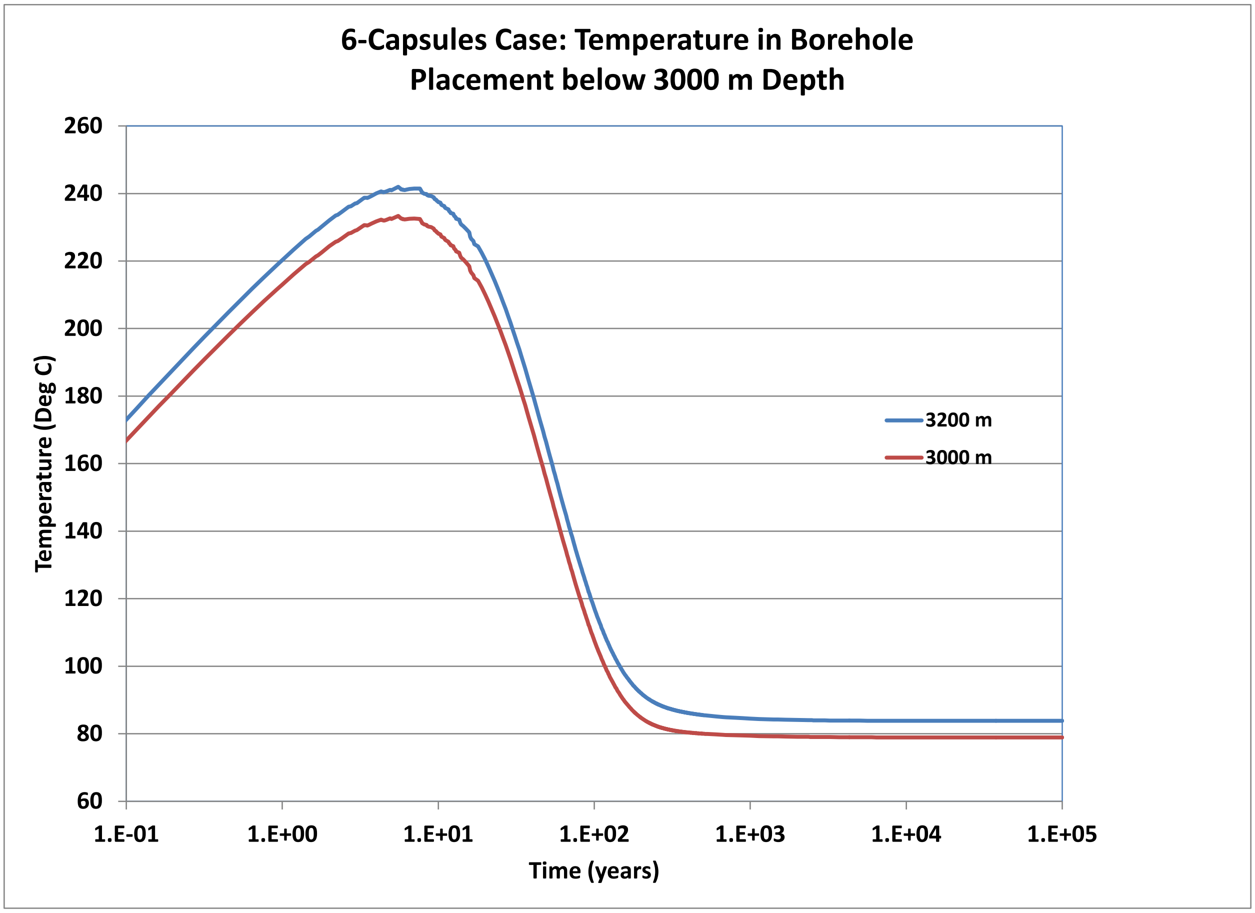

Figure 17. Simulated temperature vs. time in the borehole for the 6-capsule case at 3200 m and 3000 m depths. Effect of emplacement in the upper part of the borehole. Emplacement of waste between 3000 m and 3433 m depth.

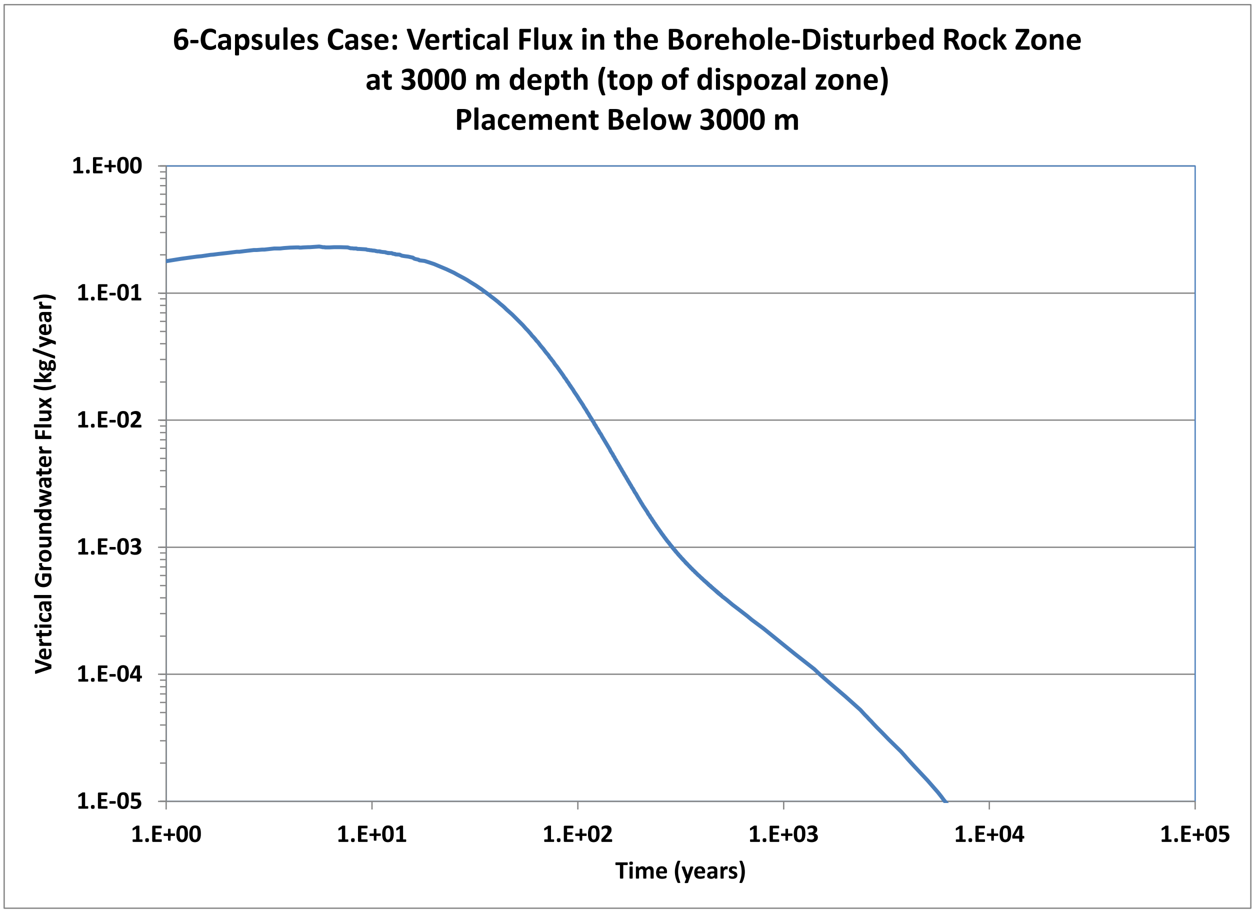

Figure 18. Simulated vertical groundwater flux vs. time in the borehole and the disturbed rock zone for the 6-capsule case at 3000 m depth (top of the disposal zone). Emplacement below 3000 m.

3.2.3. Canisters with Fourteen Capsules

For the 14-capsule case (Table 1) a canister contains seven capsules in a layer and two layers. Assuming the canister for the 14-capsule case has the same length as the 2-capsule canister, the total length required to emplace all capsules would be 186 m. For the case of emplacement at the bottom part of the borehole (base case) the Cs-137 and Sr-90 capsules were placed in the lower part of the borehole between 5000 m and 4814 m depth. Thermal-hydrology simulations were run to a total time of 10^5 years. Emplacing the entire inventory in this short, deep disposal zone resulted in temperatures in excess of 350 °C, beyond the limits of the equation of state currently implemented in PFLOTRAN, whether the waste was aged to 2020, 2030, or 2040. For emplacement in the upper part of the borehole (between 3000 m and 3186 m), predicted temperatures for disposal at 2020 and 2030 exceeded the limits of the model, but predicted temperatures for disposal in 2040 remained within the limits of the equation of state. Figure 19 shows predicted temperature (peak of about 300 °C) at 3100 m for surface storage to 2040. Figure 20 shows the corresponding vertical ground water flux (peak of about 0.47 m/yr) at 3000 m (top of the disposal zone).

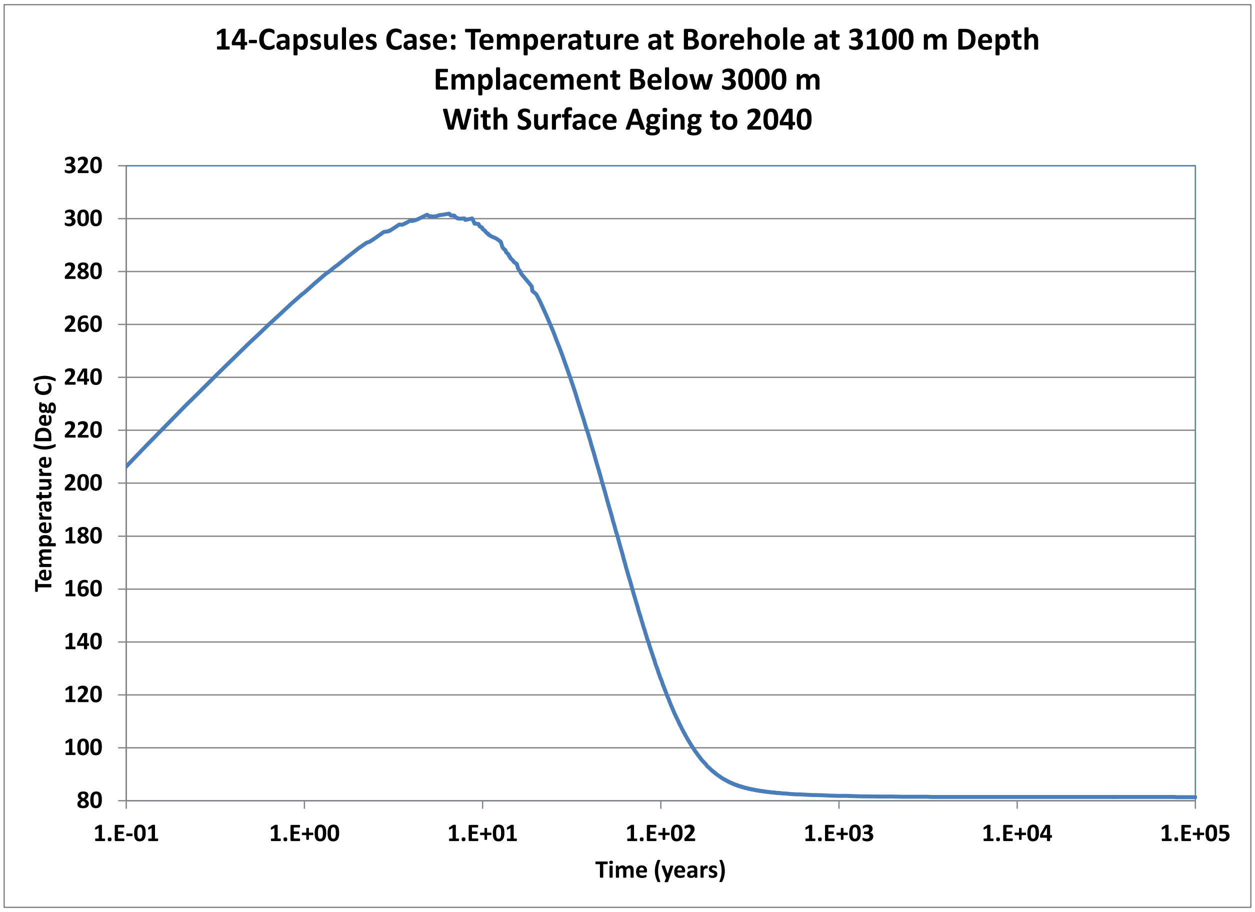

Figure 19. Simulated temperature vs. time in the borehole for the 14-capsule case at 3100 m depth. Effect of emplacement in the upper part of the borehole and surface aging to 2040. Emplacement of waste between 3000 m and 3186 m depth.

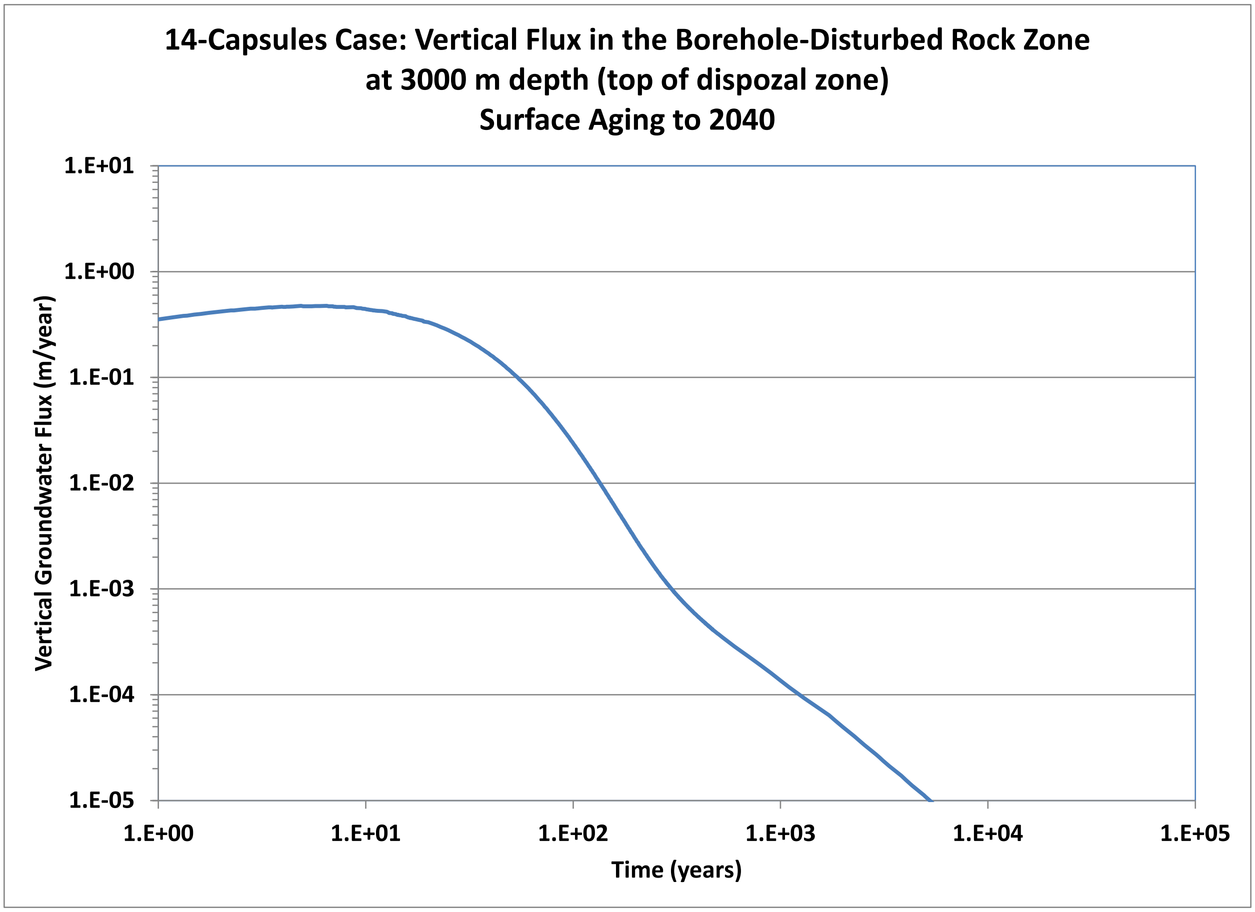

Figure 20. Simulated vertical groundwater flux vs. time in the borehole and the disturbed rock zone for the 14-capsule case at 3000 m depth (top of the disposal zone), with surface storage to 2040: Emplacement below 3000 m.

4. CONCLUSION

Thermal-hydrology simulations of deep borehole disposal options presented here include disposal of SNF and three configurations for disposal of cesium and strontium capsules. Simulations of cesium and strontium capsule disposal predict that smaller disposal canisters (2-capsule) emplaced over a longer disposal zone (1300 m) would result in smaller peak temperature increases and vertical fluid fluxes than larger disposal canisters (6-capsule) emplaced over a shorter disposal zone (433 m). These results hold true whether the capsules are emplaced at the base of the borehole (to 5000 m depth) or at the top of the acceptable disposal zone (from 3000 m depth) and no matter the age of the waste. Simulations involving 14-capsule disposal canisters emplaced over a very short disposal zone (186 m) tested the limits of current modeling capability. If the 14-canister disposal option is to be modeled accurately, future work will require the addition of an extended equation of state to PFLOTRAN.

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