

## **Advances in Thermal-Hydrologic Modeling of Nuclear Waste Disposal in Deep Boreholes - 16303**

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### **ABSTRACT**

Deep borehole disposal is one of the potential options for safely isolating high-level radioactive waste. It is expected that existing drilling technology can provide reliable and cost-effective construction of suitable deep boreholes. In addition, favorable disposal conditions such as low permeability host rock, high salinity, and geochemically reducing conditions, exist at depth in many locations. Coupled thermal-hydrologic processes induced by heat from the radioactive waste may impact fluid flow and the associated migration of radionuclides. This work looks at those processes as was also done with recent studies. Simulations of thermal-hydrology for the emplacement of cesium and strontium capsules in a deep borehole are presented. The simulations looked at disposal options such as different disposal configurations and 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 temperatures, and fluxes above the disposal zone.

### **INTRODUCTION**

Studies have shown that disposal in deep (about 5 km) boreholes is a viable option for long term isolation of high level nuclear waste [1, 2]. Crystalline basement rocks in many locations possess natural barriers that help limit migration of radionuclides to the accessible environment.

Recent numerical modeling studies of thermal-hydrology in deep boreholes have shown that decaying heat from the nuclear waste results in thermal convection causing vertical-upwards movement of water, mainly in the borehole and surrounding disturbed rock zone [2, 3, 4]. A good understanding of the thermal regime and the resulting upwards flow are of importance due to the potential to transport radionuclides away from the disposal zone. Previous simulations looked primarily at disposal of spent nuclear fuel (SNF) in deep boreholes [2, 3, 4]. The basic concept used in these studies is to drill a 5 km deep borehole in a formation with basement crystalline rock below the depth of 2 km. The basic concept also included waste emplacement in the bottom 2 km of the borehole and a seal system in the upper part of the borehole.

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 [3]. More recent modeling studies [4] 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.

Recent studies have pointed out limitations of deep borehole disposal because of the size of the maximum borehole diameter [5]. Due to the resulting limitations on waste package dimensions disposal in deep boreholes is more restricted than in mined geological repositories. However, even with the restrictions there are waste types that may be suitable for deep borehole disposal. One of these waste types is cesium and strontium capsules from the Hanford site, USA. The dimensions of the capsules are within the limits for deep borehole disposal. In this study we look at thermal-hydrologic processes for disposal of the cesium and strontium capsules in a single borehole.

## **METHOD**

Numerical simulations of thermal-hydrology in the deep borehole disposal system were carried out with waste emplaced in the disposal zone of a single borehole. The disposal zone, which is nominally assumed to be between depths of 3 km and 5 km, varies depending on type and quantity of the nuclear waste. The borehole includes the waste packages, casing and seal materials, and is surrounded by disturbed rock zone. For this study these materials are not modeled in detail. The geometry of the system includes a higher permeability material representing the borehole, seal materials and the disturbed rock, within an area of  $1\text{m}^2$ . To account for that permeability values of grid blocks in the specified area have been increased by a factor of 10 compared to adjacent host rock material. The area is surrounded by lower permeability host rock. The model includes realistic representation of the hydrogeological system typical of regions with crystalline bedrock. This includes depth-varying permeability and thermal conductivity.

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 1). Initial conditions and rock material properties used are mostly the same as in [4]. 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 I were used.

TABLE I. Parameter values of sedimentary rocks [4]

<b>Lithology</b>	<b>Permeability (m<sup>2</sup>)</b>	<b>Porosity (-)</b>	<b>Thermal Conductivity (W/m/K)</b>	<b>Heat Capacity (J/kg/K)</b>
sandstone	1 x 10 <sup>-12</sup>	0.30	3.5	840.
shale	1 x 10 <sup>-15</sup>	0.02	1.8	840.
limestone	1 x 10 <sup>-13</sup>	0.05	2.7	840.
dolomite	1 x 10 <sup>-13</sup>	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 permeability variation with depth in the granite rock is used [6]. 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:

$$\text{Log}(k) = -1.38 \log(z) - 15.4 \quad (\text{Eq. 1})$$

Where  $z$  is depth in km and  $k$  is permeability in m<sup>2</sup>. The permeability of the borehole and the surrounding disturbed rock within an area of 1 m<sup>2</sup> 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 [7]. 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 analysis average thermal output of the cesium and strontium capsules was used. Borehole emplacement was assumed to be in 2020.

Simulations were run with PFLOTRAN, an open source, state-of-the-art massively parallel subsurface flow and reactive transport code [8] in a high-performance computing environment.

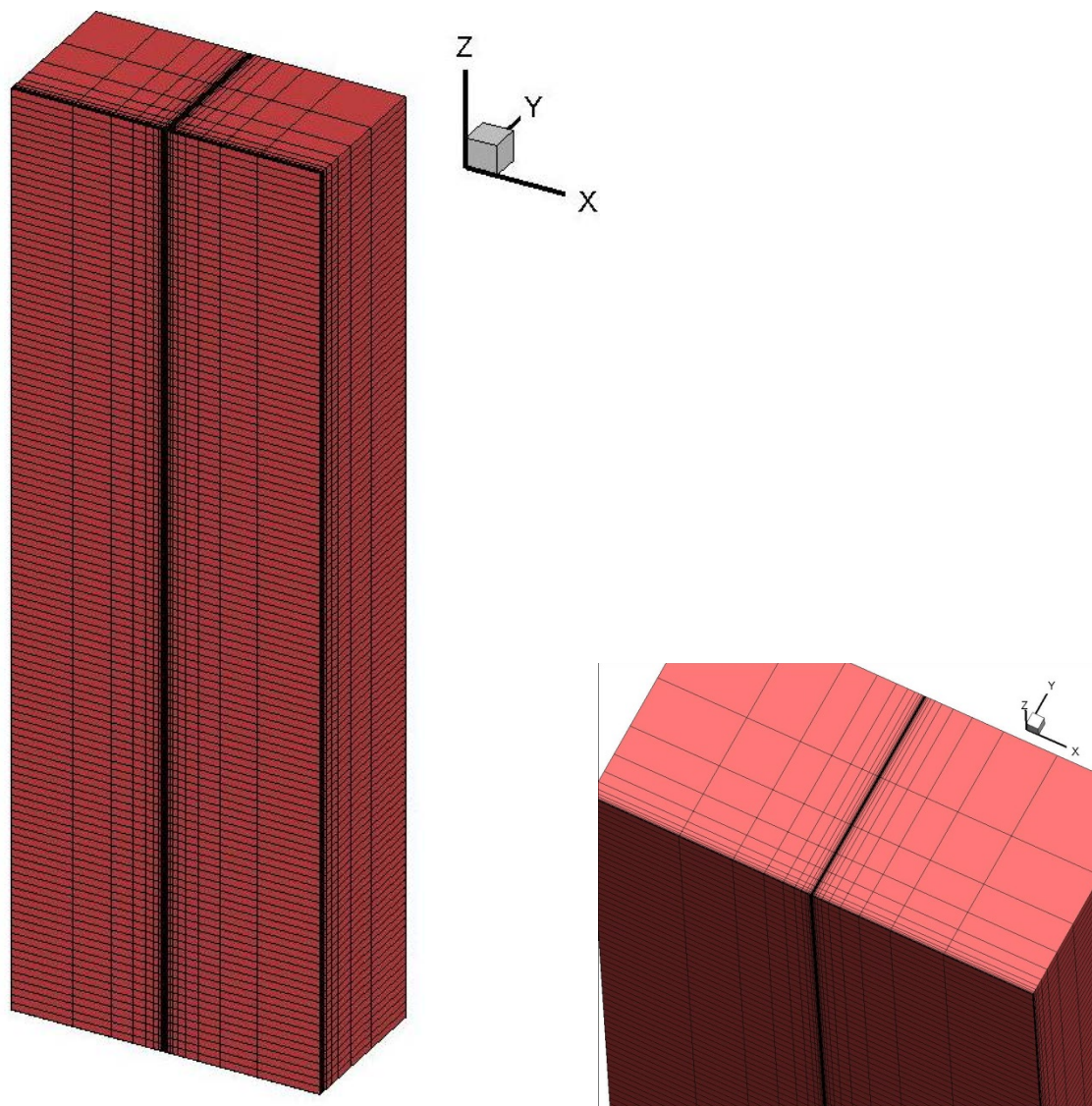


Figure 1. Numerical mesh of the thermal-hydrologic model.

## RESULTS AND DISCUSSION

Thermal-hydrologic simulations were carried out for the disposal of cesium and strontium capsules in a single borehole. The inventory of cesium and strontium capsules includes 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 three possible configurations are considered. The baseline case (2-capsule case) has two capsules arranged end-to-end within a waste package or disposal overpack. For this case the assumption is 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). For case 2 or 6-capsule case, the waste package contains 2 layers of 3 capsules each. 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. Case 3 or 14-capsule case 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. Thus, a two-layer canister could hold 14-capsules. In this analysis we assumed this would have the same length as the 2-capsule and 6-capsule canisters described above. Simulations were carried out for the three cases, for bottom hole disposal above 5000 m as well as disposal below 3000 m. The simulations also looked at different surface storage periods.

### Case 1: Canisters with two capsules

For the 2-capsule modeling case capsules were first placed in the lower part of the borehole between 5000 m and 3700 m depth. Half of the thermal output was applied because of symmetry considerations. Thermal-hydrology simulations were run to total time of  $10^5$  years. Figure 2 shows temperature distribution in the bottom part of the borehole after 10 years simulation time. 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 3 shows predicted borehole center temperature at 4000 m depth for emplacement at 2020 (base case) and 2030. For the delayed emplacement case (2030) simulations show that the peak temperature is reduced by about 10 °C, resulting in a smaller temperature increase. Figure 4 shows the predicted groundwater flux at the center of the borehole for the two emplacement periods. As shown in the figure, delaying emplacement to 2030 would reduce the simulated peak flux to about 0.025 m/yr.

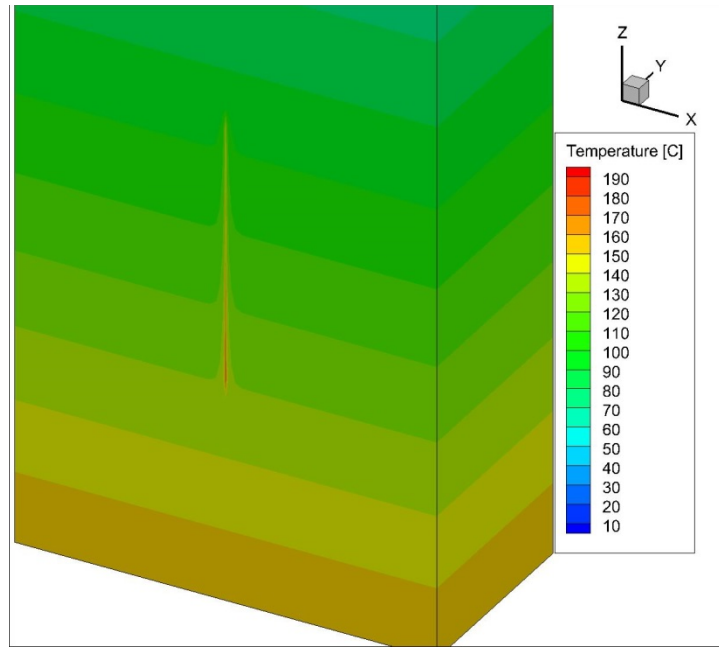


Figure 2. Temperature distribution in the bottom part of the borehole for the 2-capsule case at 10 years simulation time. Emplacement at bottom of borehole.

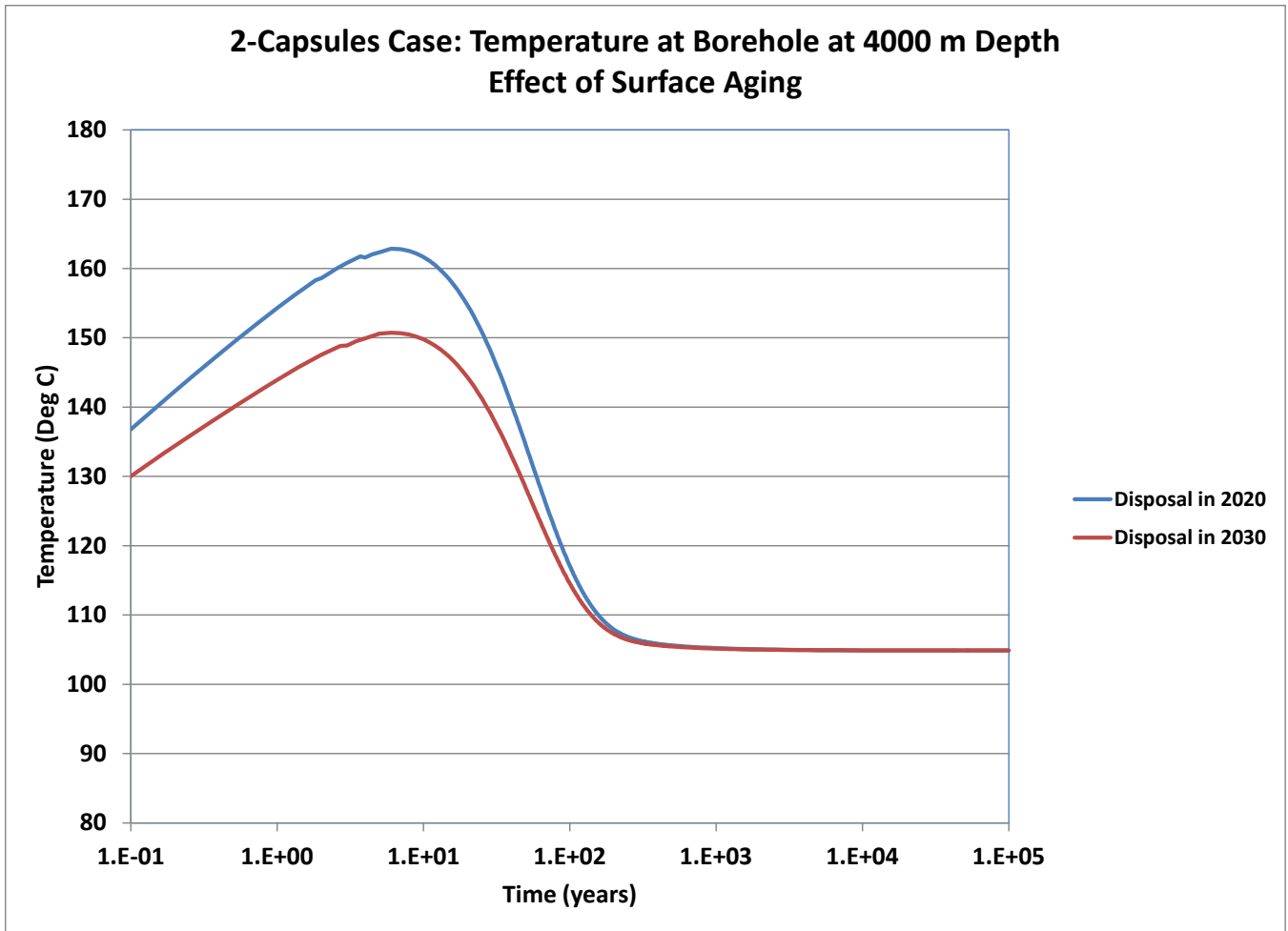


Figure 3. Simulated temperature vs. time in the borehole for the 2-capsule case at 4000 m depth. Effect of surface storage to 2020 and 2030. Emplacement at bottom of borehole.

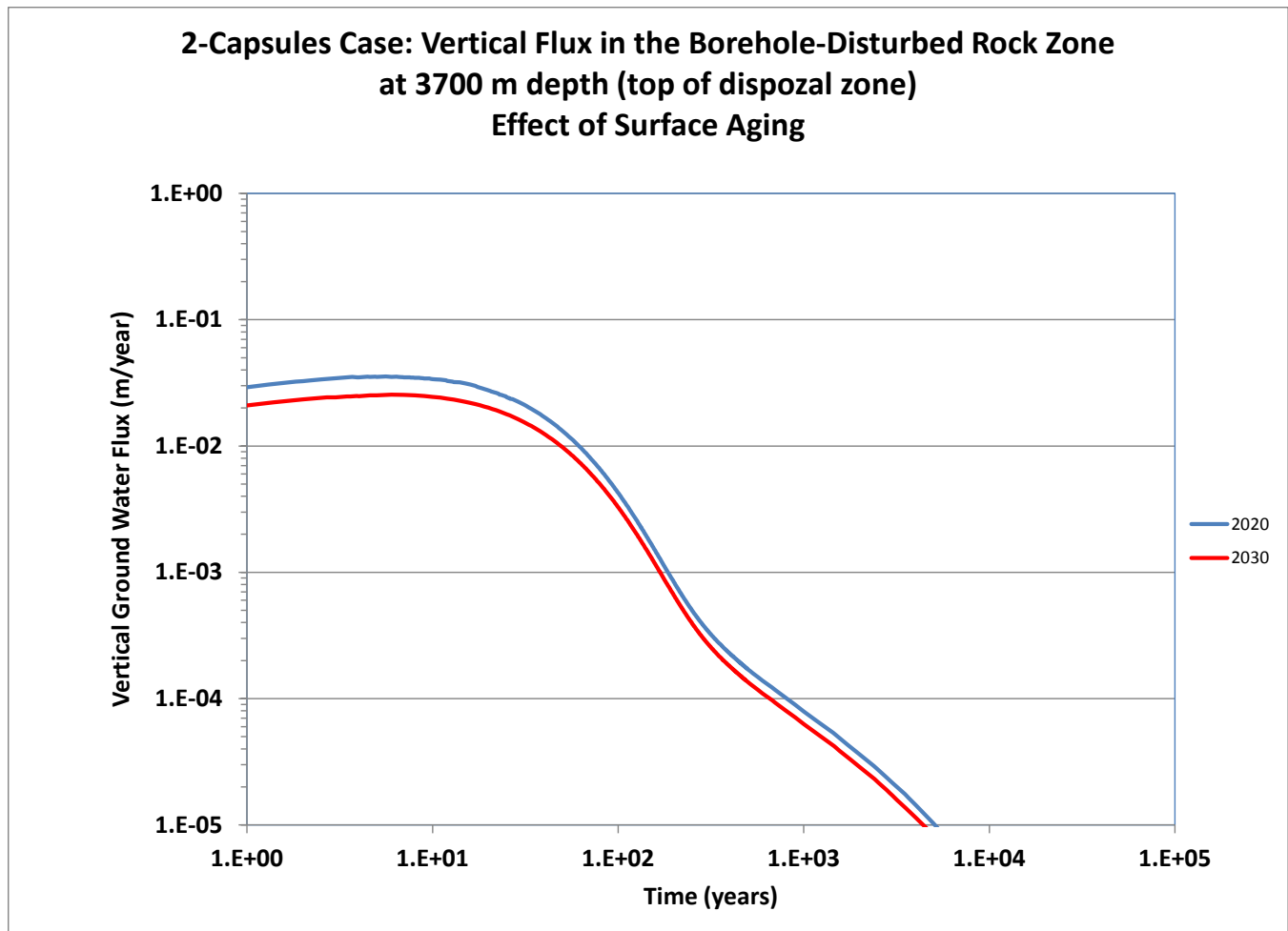


Figure 4. Simulated vertical groundwater flux vs. time in the borehole and the disturbed rock zone for the 2-capsule case at 3700 m depth (top of the disposal zone). Effect of surface storage to 2020 and 2030. Emplacement at bottom of borehole.

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 5 shows a comparison of predicted borehole center temperature for disposal in the upper part of the disposal zone (top emplacement) and disposal in the bottom part of the disposal zone (bottom displacement). The figure shows predicted temperature at the top of the disposal zone for both placement options. The figure indicates that placement in the upper part of the disposal zone reduces the peak temperature.



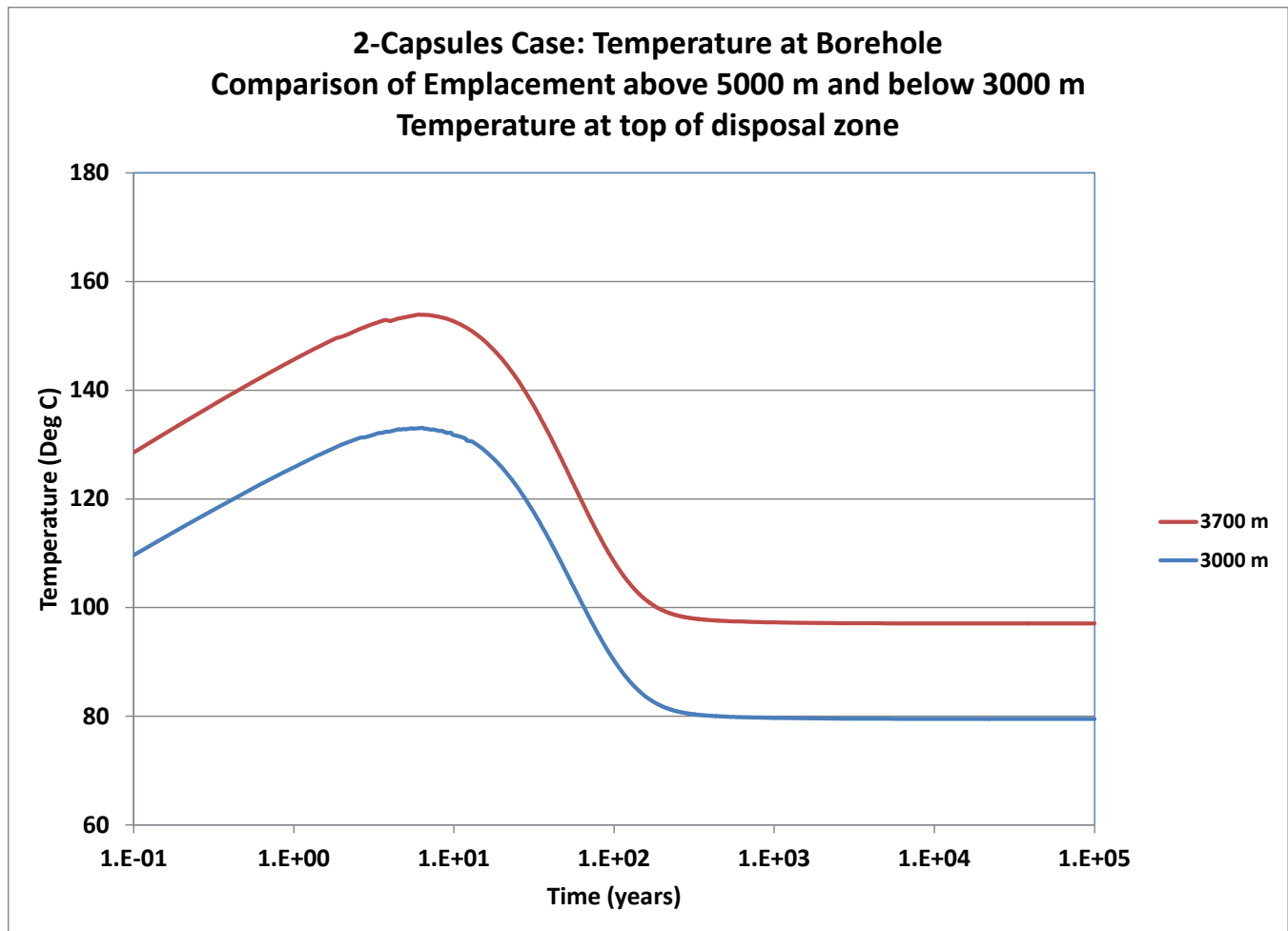


Figure 5. Simulated temperature vs. time in the borehole for the 2-capsule case at top of disposal zone. Effect of bottom and top of disposal zone emplacement.

### Case 2: Canisters with Six Capsules

For the 6-capsules case the total length required to emplace all capsules is assumed to be 433 m. For the case of bottom emplacement the 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. For this case three emplacement times were considered. Figure 6 shows predicted borehole center 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) significantly reduced the peak temperature, resulting in smaller temperature increases. Figure 7 shows the predicted borehole center 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.

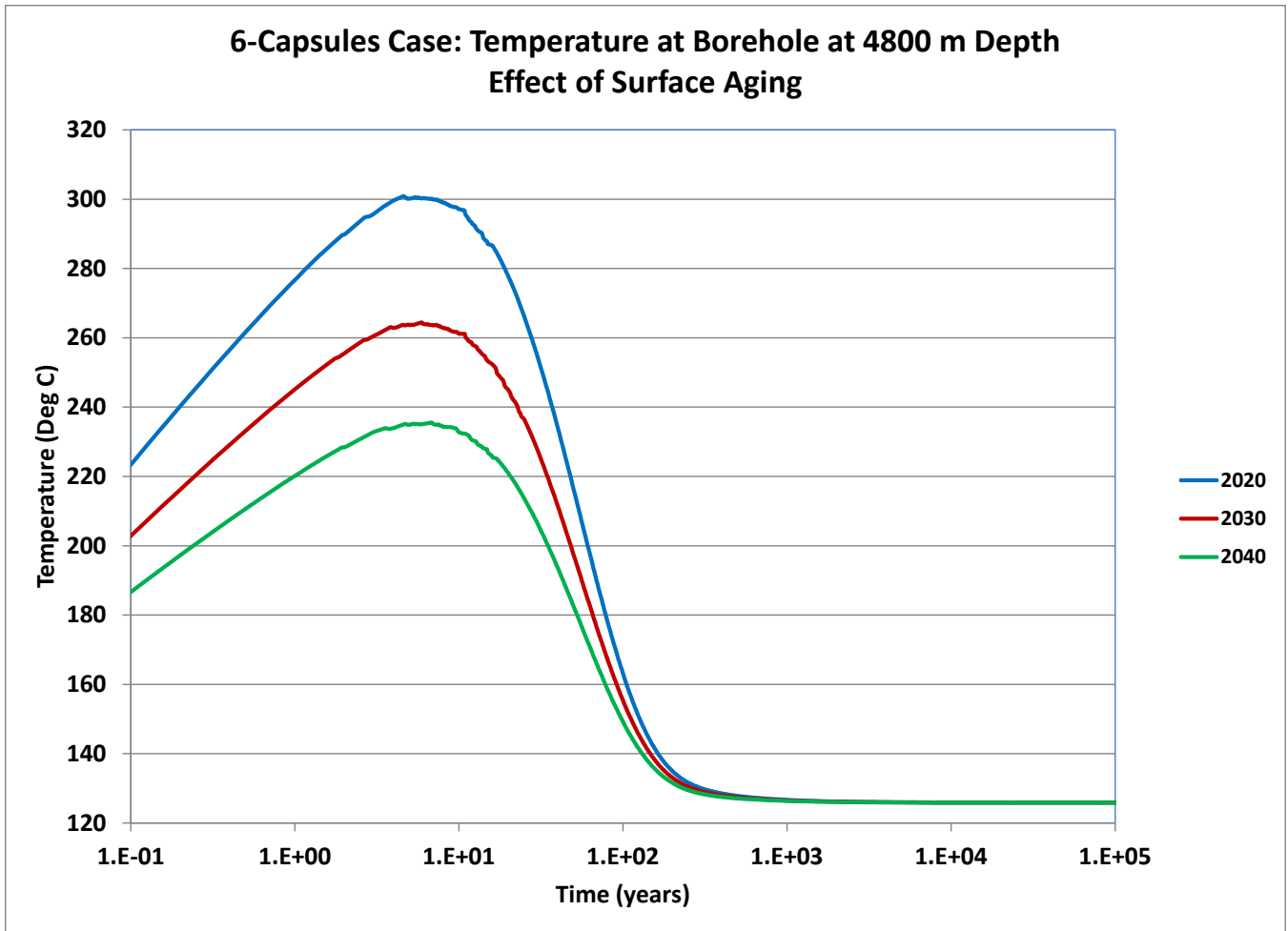


Figure 6. Simulated temperature vs. time in the borehole for the 6-capsule case at 4800 m depth. Effect of surface storage to 2020, 2030, and 2040. Emplacement at bottom of borehole.

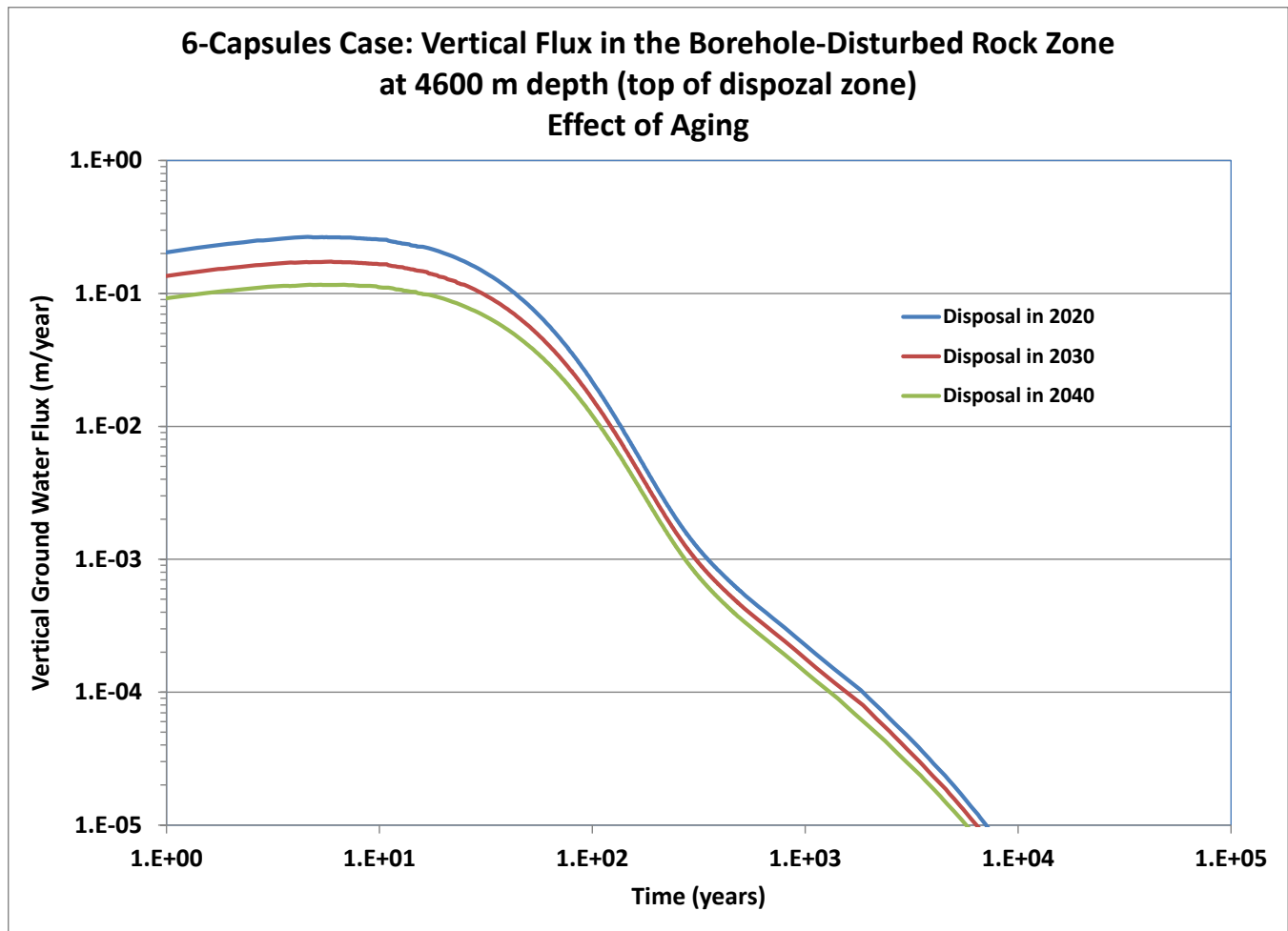


Figure 7. Simulated vertical groundwater flux vs. time in the borehole and the disturbed rock zone for the 6-capsule case at 4600 m depth (top of the disposal zone). Effect of surface storage to 2020, 2030, and 2040. Emplacement at bottom of borehole.

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 8 shows predicted temperature at the top of the disposal zone for both upper and lower placement options. The figure indicates that placement in the upper part of the disposal zone significantly reduces the peak temperature just as for the 2-capsules case.

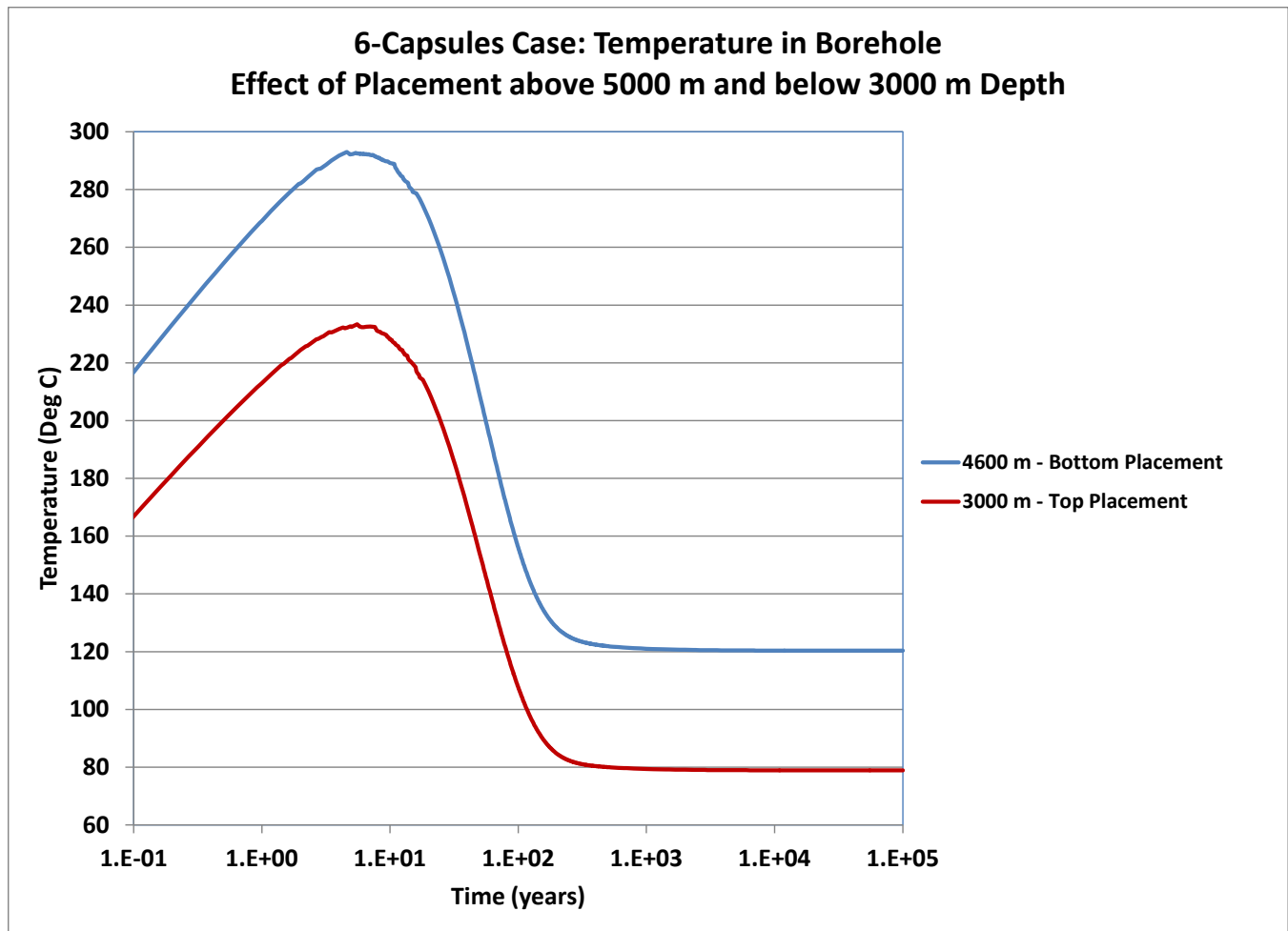


Figure 8. Simulated temperature vs. time in the borehole for the 6-capsule case at top of disposal zone. Effect of bottom and top of disposal zone emplacement.

### Case 3: Canisters with Fourteen Capsules

For the 14-capsule case the total length required to emplace all capsules would be 186 m. For the case of bottom emplacement the 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 PFLTRAN, whether the waste was aged to 2020, 2030, or 2040. For the case of top 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 9 shows predicted borehole center temperature (peak of about 300 °C) at 3100 m for surface storage to 2040. Figure 10 shows the corresponding borehole center vertical ground water flux (peak of about 0.47 m/yr) at 3000 m (top of the disposal zone).

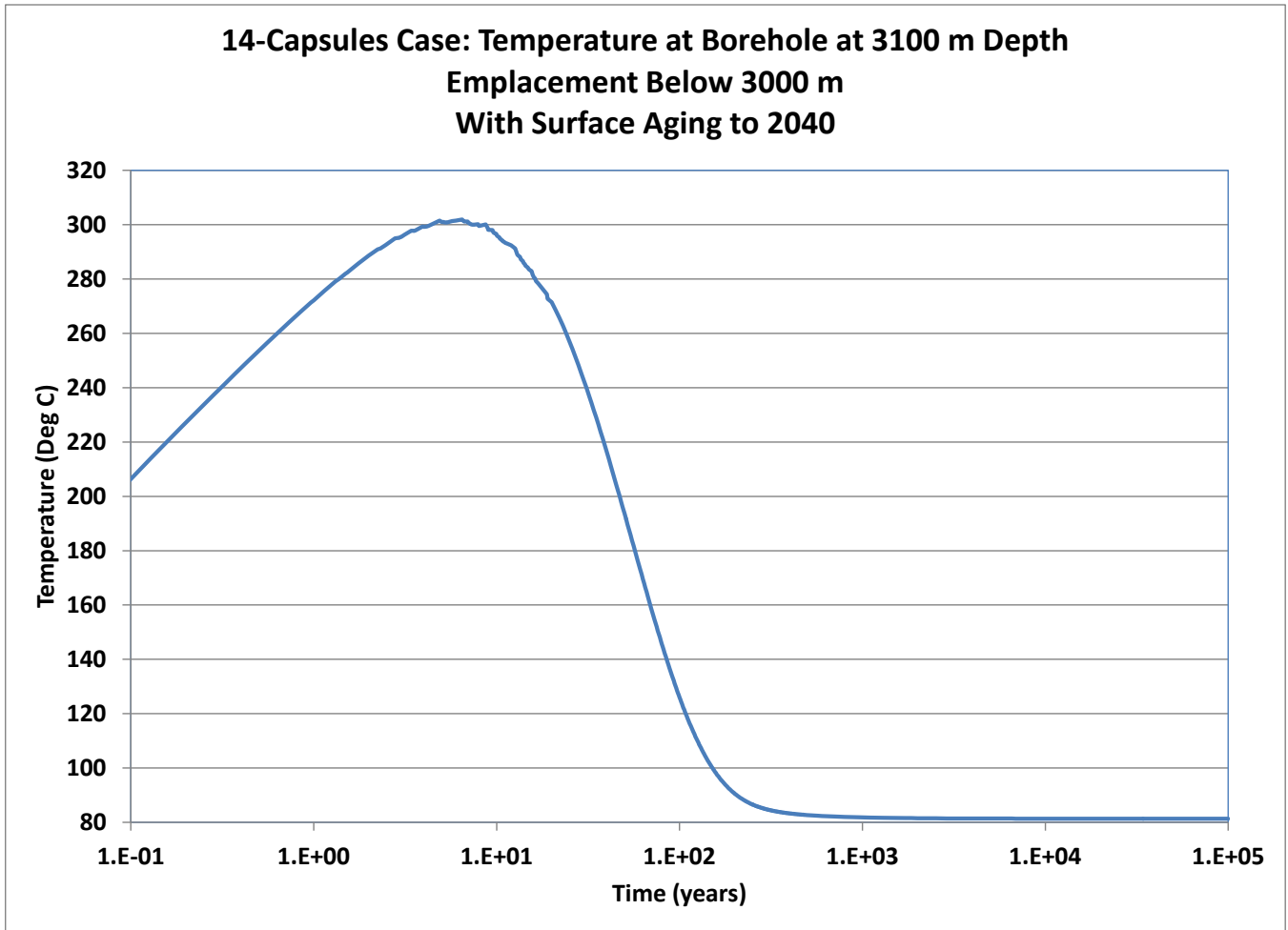


Figure 9. Simulated temperature vs. time in the borehole for the 14-capsule case at 3100 m depth. Effect of emplacement in the upper part of the borehole and surface aging to 2040. Emplacement of waste between 3000 m and 3186 m depth.

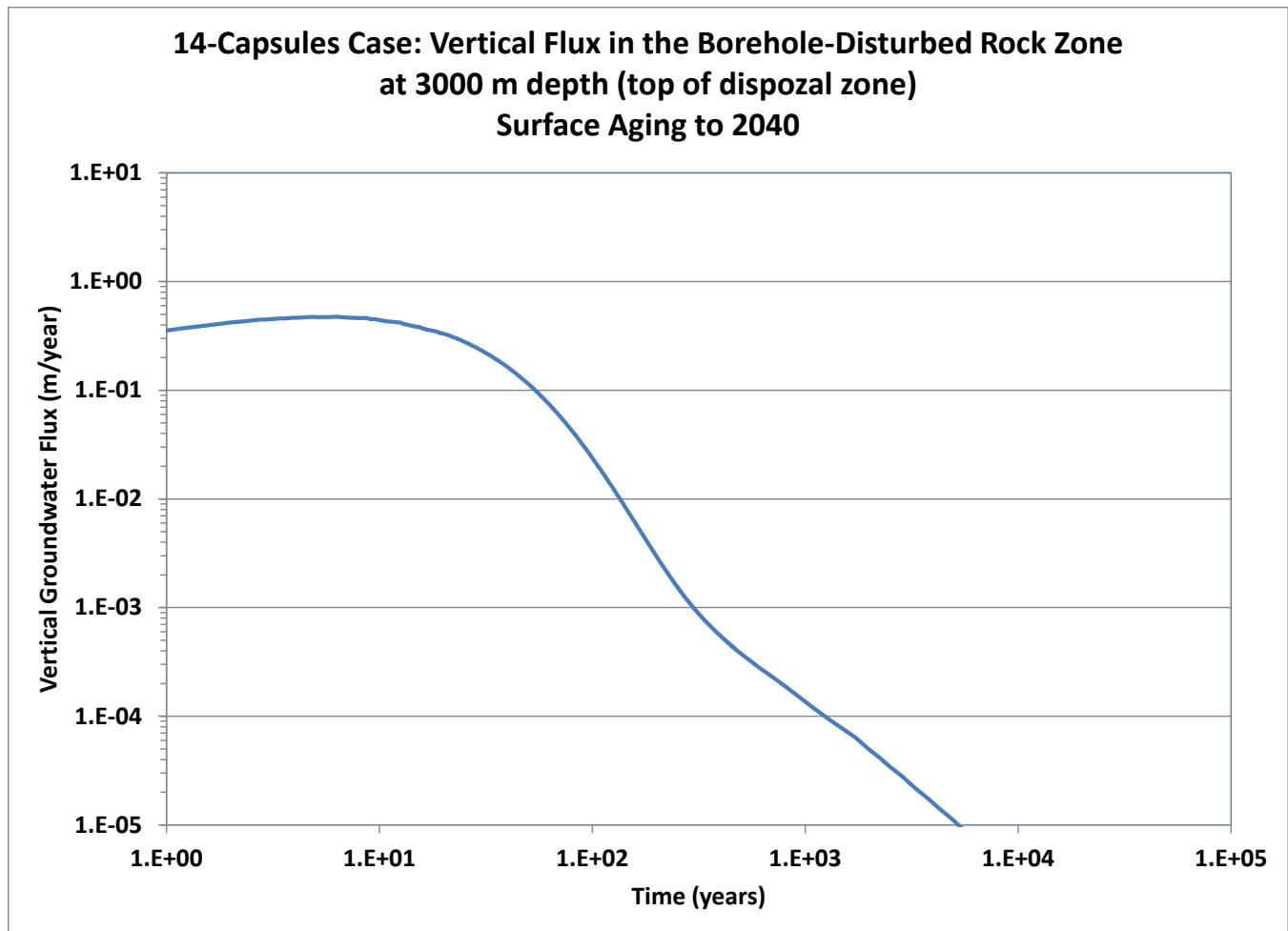


Figure 10. Simulated vertical groundwater flux vs. time in the borehole and the disturbed rock zone for the 14-capsule case at 3000 m depth (top of the disposal zone), with surface storage to 2040: Emplacement below 3000 m.

## CONCLUSIONS

Thermal-hydrology simulations of deep borehole disposal options presented in this paper include three configurations for disposal of cesium and strontium capsules. The different configurations together with the surface storage periods provide different disposal options. 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 (e.g. 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. The simulations show that the entire inventory of the cesium and strontium capsules can be emplaced in a single deep borehole with acceptable temperature rises and vertical upwards groundwater fluxes.

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