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Hydrologic Modeling of Subsurface Brine Density Stratification for Deep Borehole Disposal - 20213

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ABSTRACT

Density-dependent and topographically-driven subsurface brine flow was modeled in regional-scale and Deep Borehole Disposal-scale domains under varying conditions. These conditions included variable basement permeability, brine density, and hydraulic head. Findings revealed the possibility of hydraulic isolation of deep basement for at least 1 million years under appropriate conditions, which supports the viability of the Deep Borehole Disposal concept.

1. INTRODUCTION

Deep borehole disposal (DBD) has been proposed as a viable approach for the safe disposal of radioactive wastes (Freeze et al., 2019). The DBD concept consists of drilling a large-diameter borehole into crystalline basement rock to a depth of about 5 km, placing waste packages in the lower, waste emplacement zone portion of the borehole, and sealing and plugging the upper portion of the borehole. Other rock types could also be adequate. Although there is some reliance on the engineered components of the system, the safety of the concept relies primarily on the depth of burial and the assumed hydraulic isolation of the groundwater at the depth of the emplacement zone.

Groundwater salinity generally increases with depth in crystalline basement, resulting in density-stratified fluids. This study was done to analyze the influence of density stratification on groundwater flow in a generic rock domain under varying conditions.

Park et al. (2009) performed simulations of regional-scale, density-dependent flow to illustrate how density stratification can inhibit fluid flow at depth and maintain hydraulic isolation of deep basement fluids. Flow in these cases was topologically-driven. In this study, the results of Park et al. (2009) are replicated and expanded upon.

2. METHODOLOGY

2.1 PFLOTRAN

Simulations were performed using PFLOTRAN, an open-source, massively parallel porous-medium flow and reactive transport simulator (Lichtner et al., 2019). Domains modeled were treated as isothermal and fully-saturated with water that has concentration-dependent density. The equation of state for the density and viscosity of water was a function of salinity, pressure and temperature (Batzle and Wang, 1992). Brine density is calculated based on an inert tracer with the same molecular weight as NaCl.

2.2 Regional-Scale Studies

The 2-D model domain (**Figure 1**) is 10 km wide and 3 km deep with grid cell dimensions of 10 m by 10 m. Simulations are run to 1,000,000 years. Pressure and flow boundary conditions are such that recharge and discharge occur five km away from each other. In the base case, the permeability of the model domain is $k = 10^{-14}$ m^2, and the hydraulic head difference between the inflow and outflow locations is ΔH = 50 m. Groundwater down to 500 m below the surface is treated as freshwater ($\rho_o \approx 1.00$ g/cm^3) and the remaining groundwater is treated as brine ($\rho_{bo} \approx 1.20$ g/cm^3).

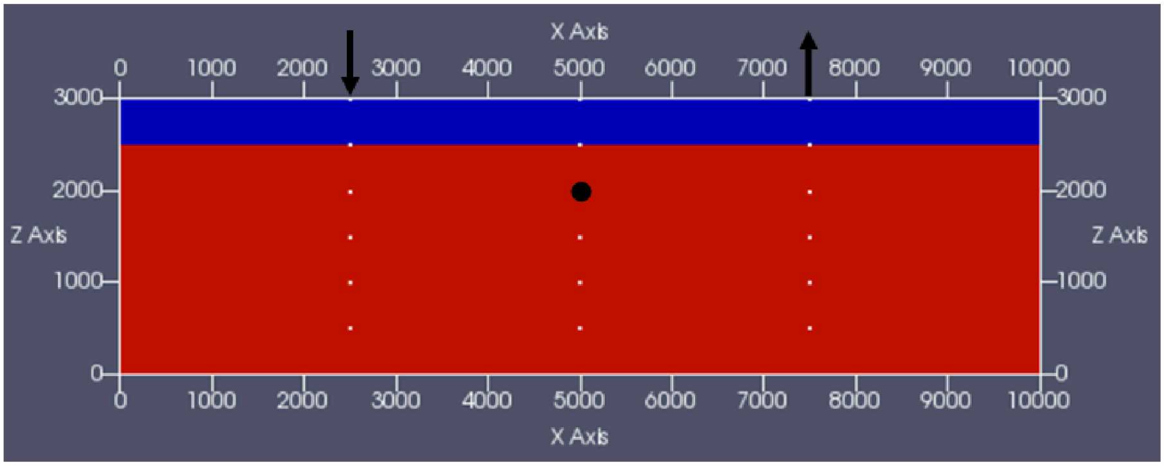

Figure 1. Domain and initial density stratification. Red indicates brine, blue indicates freshwater. Arrows indicate inlet and outlet locations. The dark circle indicates the location of the observation point of interest (modified from Freeze et al. 2019).

Tests were run to observe the effects of permeability, brine density, and hydraulic head difference. Variations were as follows:

- Permeability Study: The base case was re-run at $k = 10^{-15}$, 10^{-16}, and 10^{-17} m^2. In the latter two, the $k = 10^{-15}$ m^2 case was first run to 400 years to establish a flow pattern, then run for the 1 million observed years at the new permeability.
- Density Study: The density at depth was changed from $\rho_{bo} \approx 1.20$ g/cm^3 to $\rho_{bo} \approx 1.00$, 1.03, or 1.10 g/cm^3. Each of these three cases was run at $k = 10^{-14}$ m^2 and $k = 10^{-15}$ m^2.
- Hydraulic Head Study: The hydraulic head difference was changed from $\Delta H = 50$ m to $\Delta H = 25$, 100, or 500 m. These correspond to head gradients of 0.01, 0.005, 0.02, and 0.1 m/m, respectively. Each of these three cases was run at $k = 10^{-14}$ m^2 and $k = 10^{-15}$ m^2.

2.3 DBD-Scale Study

This model was then applied to a domain more relevant to DBD, which is 10 km wide and 5 km deep. In this scenario, two different homogeneous rock layers are present: a sediment layer in the upper two kilometers with a permeability of either $k = 10^{-14}$ m^2 or $k = 10^{-15}$ m^2, and a crystalline basement in the lower three kilometers with a permeability of $k = 10^{-18}$ m^2. The sediment layer contains freshwater and the crystalline basement contains brine. All other assumptions and boundary conditions from the base case of the previous model remain, as well as the domain discretization.

3. RESULTS AND DISCUSSION

3.1 Base Case

The model shows the establishment of a flow path between the recharge and discharge points by 1,000 years. The flow pattern established by recharge and discharge has also caused the transport of brine out of the system. Some disturbance of the deep brine occurs by this time, as shown in **Figure 2A**. These results were expected based on Park et al. (2009), indicating that this model is comparable to the model developed by Park. More significant brine flushing occurs by 1,000,000 years as shown in **Figure 2B**.

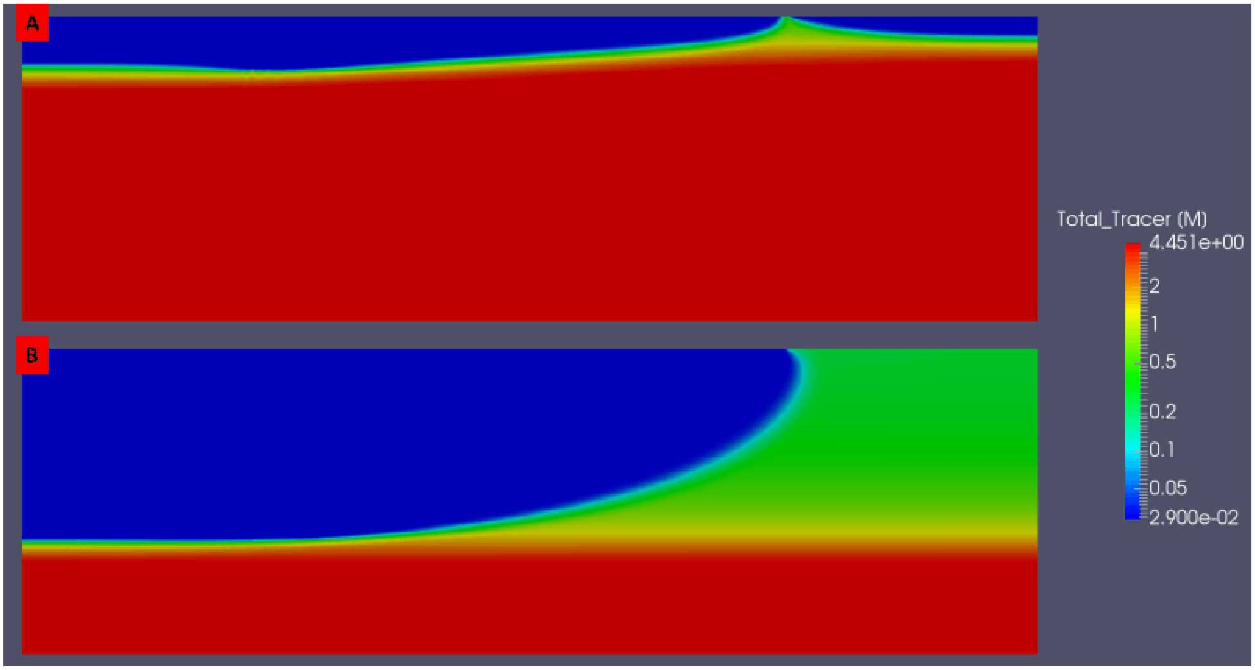

Figure 2. Tracer concentrations in the base case. A) Time = 1000 years. B) Time = 1 million years.

3.2 Permeability Study

Permeabilities below 10^{-14} m^2 exhibited less displacement of brine by 1 million years (**Figure 3**). No notable differences were found across these lower permeabilities, indicating a threshold permeability below 10^{-14} m^2. Further studies only investigated $k = 10^{-14}$ m^2 and $k = 10^{-15}$ m^2 for this reason.

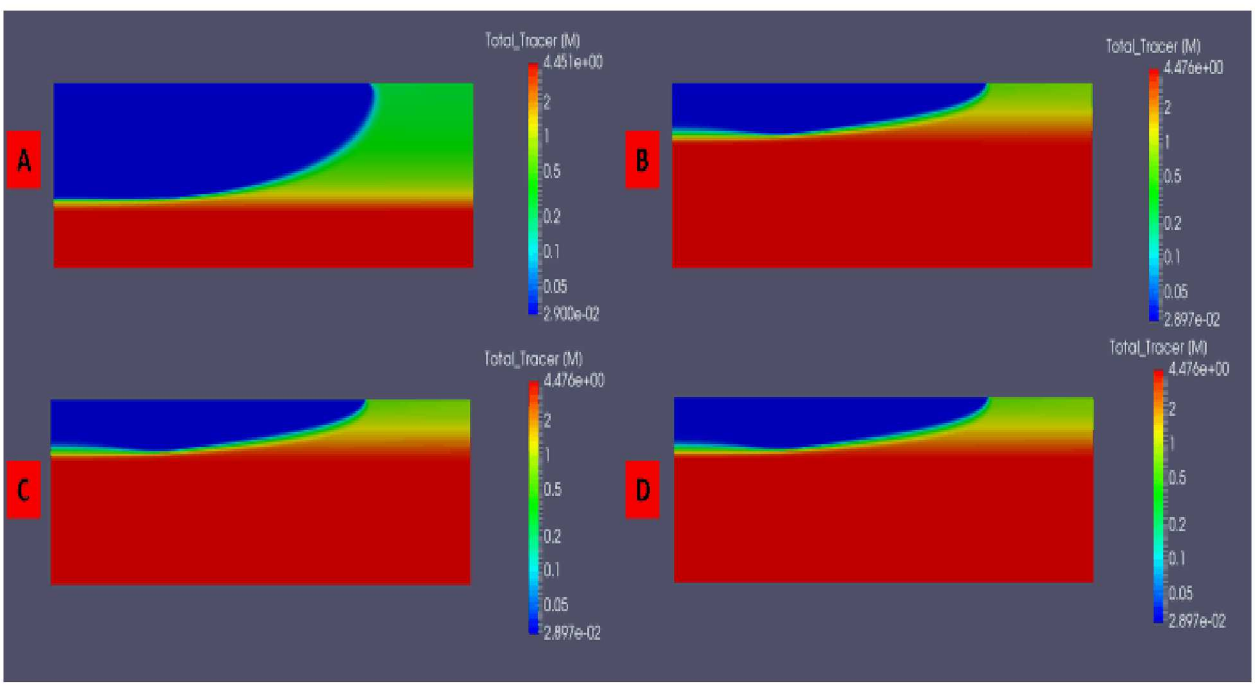

Figure 3. Tracer concentrations at 1 million years. A) $k = 10^{-14}$ m^2. B) $k = 10^{-15}$ m^2. C) $k = 10^{-16}$ m^2. D) $k = 10^{-17}$ m^2.

This is further exemplified in **Figure 4**. The concentrations at 1 km depth at the middle of the domain for the $k = 10^{-15}$ m^2, 10^{-16} m^2, and 10^{-17} m^2 cases were nearly identical over the observed period, and so plot on top of each other. Brine flushed out of this location in the base case ($k = 10^{-14}$ m^2) by 400,000 years, a behavior not seen in either of the other three cases. There is a slight decrease in the concentration of tracer at this point in the latter cases.

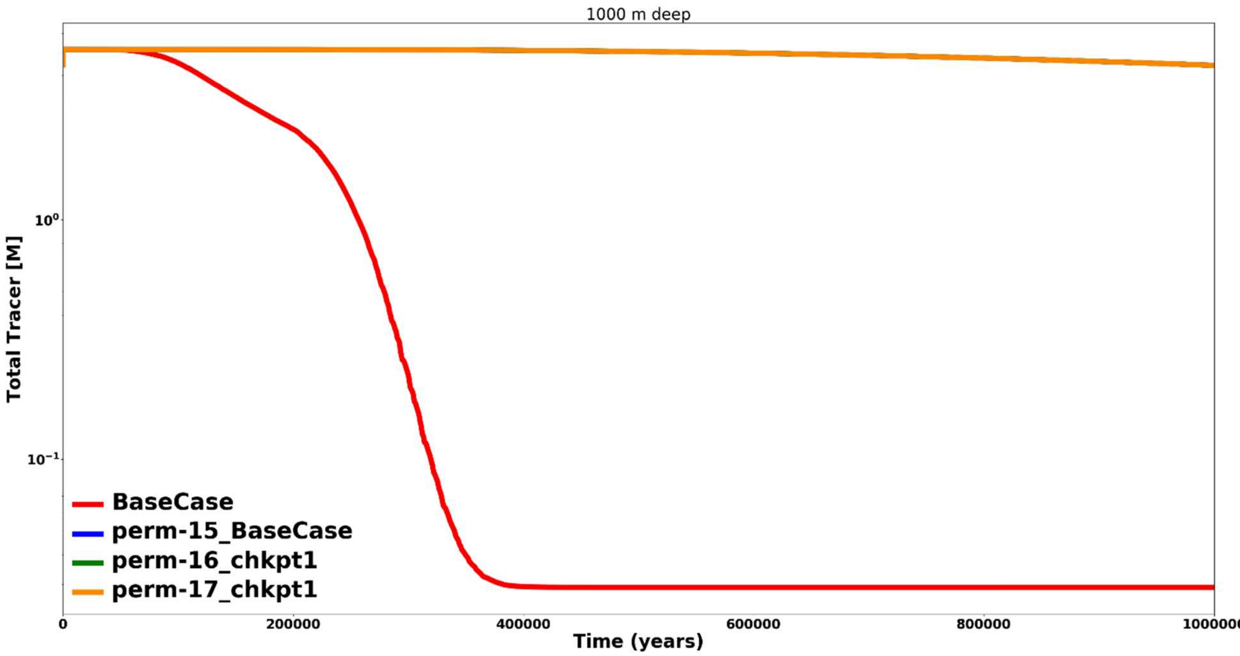

Figure 4. Tracer concentration as a function of time in the four permeability cases at the observation point from Figure 1.

3.3 Density Study

3.3.1 Permeability $k = 10^{-14}$ m^2

The density of the brine at depth directly correlated with the transport behavior of the brine, as expected. When $\rho_{bo} \approx 1.00$, the tracer flushed out of the domain completely by 1 million years (**Figure 5A**). At $\rho_{bo} \approx 1.03$, a significant amount of brine has been drained by this time (**Figure 5B**). At $\rho_{bo} \approx 1.10$, a layer of undisturbed brine remained at the bottom of the domain (**Figure 5C**), an observation that was comparable to the findings in the base case ($\rho_{bo} \approx 1.20$, **Figure 5D**). The selected observation point saw complete flushing of brine in all four cases (**Figure 6**), though increasing densities slowed the amount of time required for this to occur.

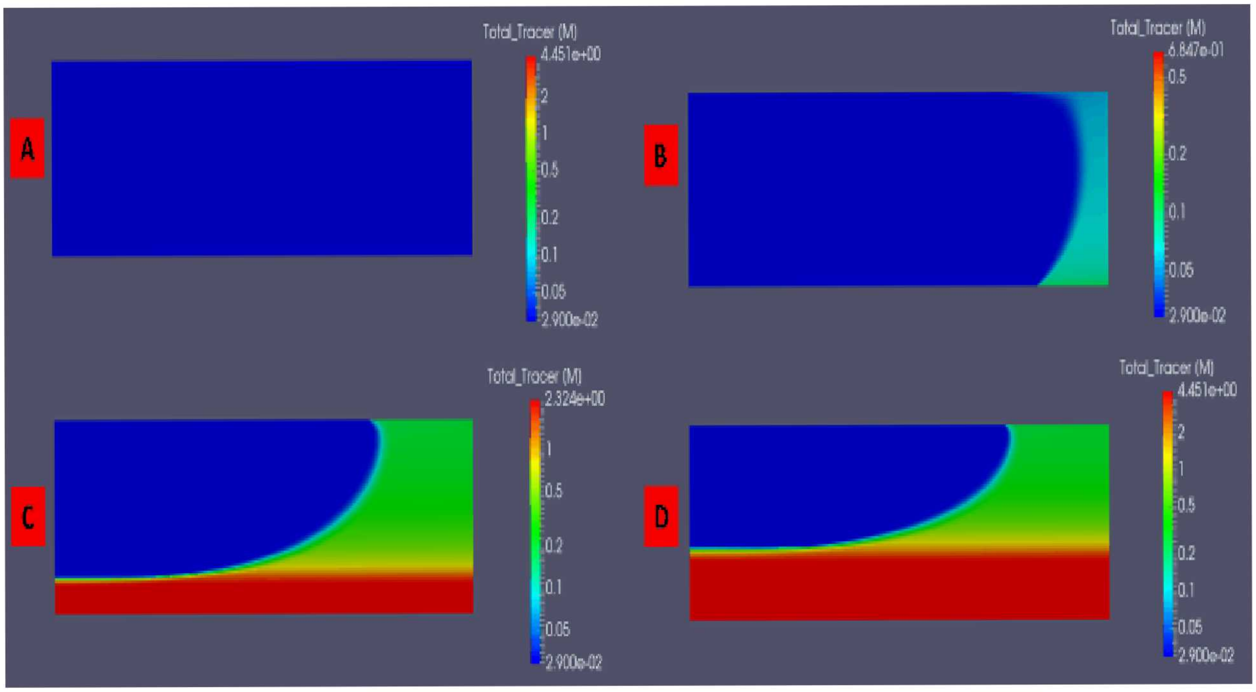

Figure 5. Tracer concentrations at 1 million years for $k = 10^{-14}$ m^2. A) $\rho_{bo} \approx 1.00$. B) $\rho_{bo} \approx 1.03$. C) $\rho_{bo} \approx 1.1$. D) $\rho_{bo} \approx 1.2$ (base case).

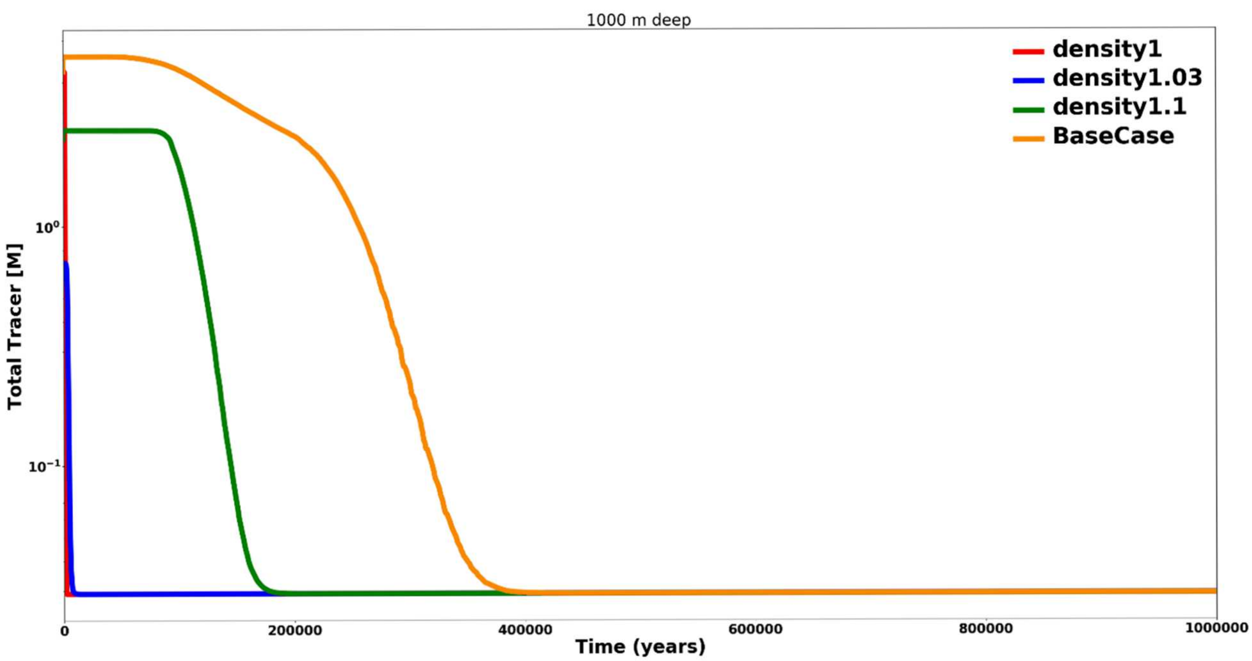

Figure 6. Tracer concentration as a function of time in the four salinity cases at the observation point from Figure 1. For $k = 10^{-14}$ m^2.

3.3.2 Permeability $k = 10^{-15}$ m^2

Trends as observed in the higher permeability cases for the salinity study are pervasive at $k = 10^{-15}$ m^2 as well. Increasing densities decreased the transport of brine out of the domain (**Figure 7**). The decrease in permeability further restricted this flow, and so, total flushing of brine at $\rho_{bo} \approx 1.00$ was not observed at 1 million years. More brine remained undisturbed in the remaining three cases by this time. At this permeability, the $\rho_{bo} \approx 1.1$ case exhibited very similar behavior to the $\rho_{bo} \approx 1.2$ case until approximately 600,000 years (**Figure 8**).

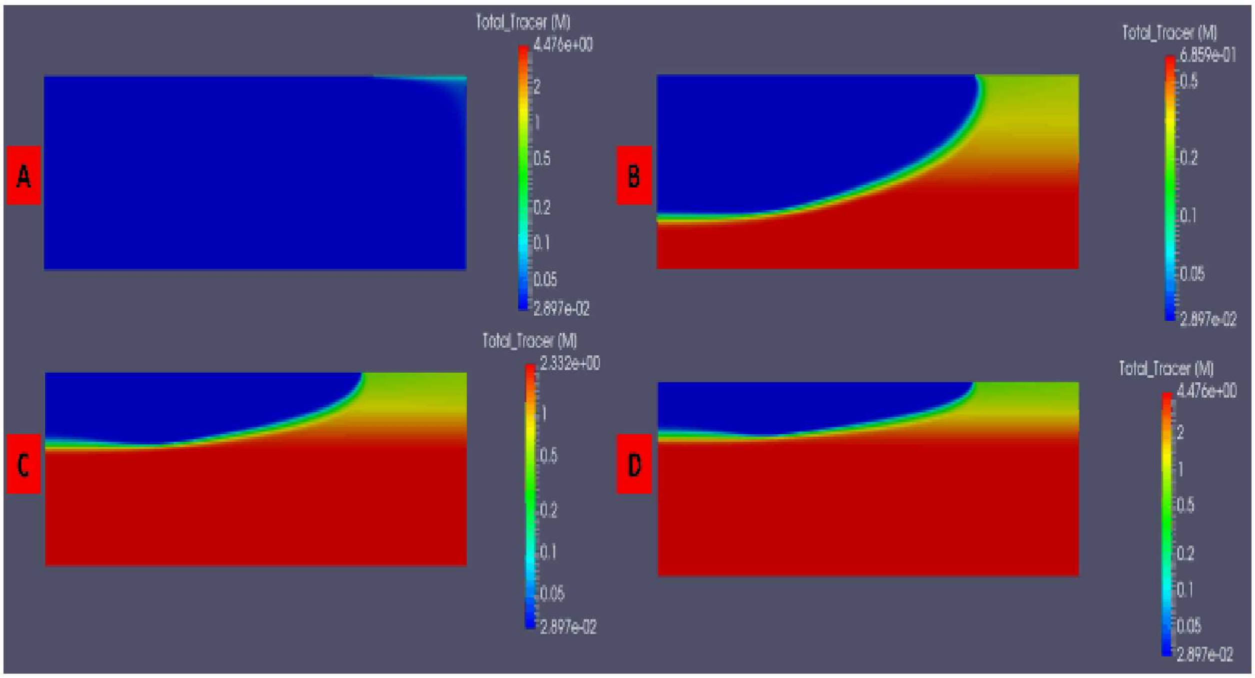

Figure 7. Tracer concentrations at 1 million years for $k = 10^{-15}$ m^2. A) $\rho_{bo} \approx 1.00$. B) $\rho_{bo} \approx 1.03$. C) $\rho_{bo} \approx 1.1$. D) $\rho_{bo} \approx 1.2$.

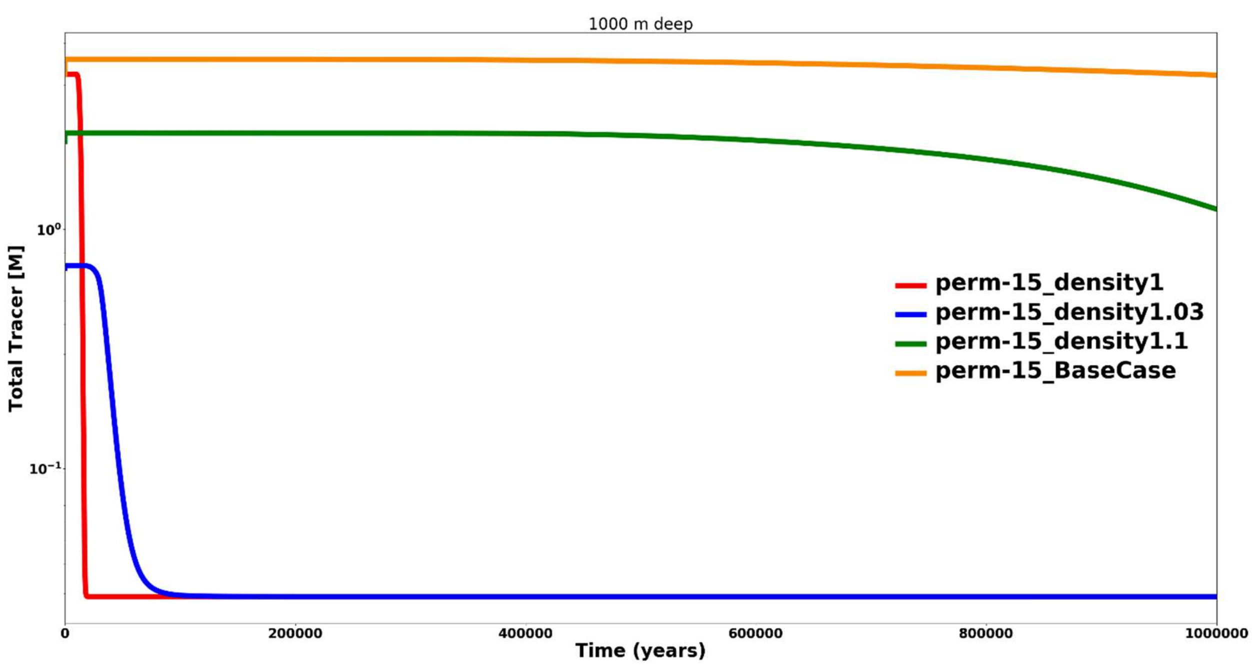

Figure 8. Tracer concentration as a function of time in the four salinity cases at the observation point from Figure 1. For $k = 10^{-15}$ m^2.

3.4 Hydraulic Head Study

3.4.1 Permeability $k = 10^{-14}$ m^2

The model continued to behave as expected in cases where the hydraulic head gradient between the recharge and discharge points was varied. **Figure 9** shows that, with the increase in magnitude of this gradient, more brine was discharged. **Figure 9D** specifically shows that significant enough transport driving force can develop a flow profile that will clear the domain of tracer by 1 million years; **Figure 10** further shows that a driving force ΔH = 500 m will evacuate the domain after a relatively small time. The observation point analyzed in **Figure 10** saw a marked decrease in brine evacuation when the driving force was halved from the value in the base case; this was the only case where the observation point was not completely devoid of brine at 1 million years.

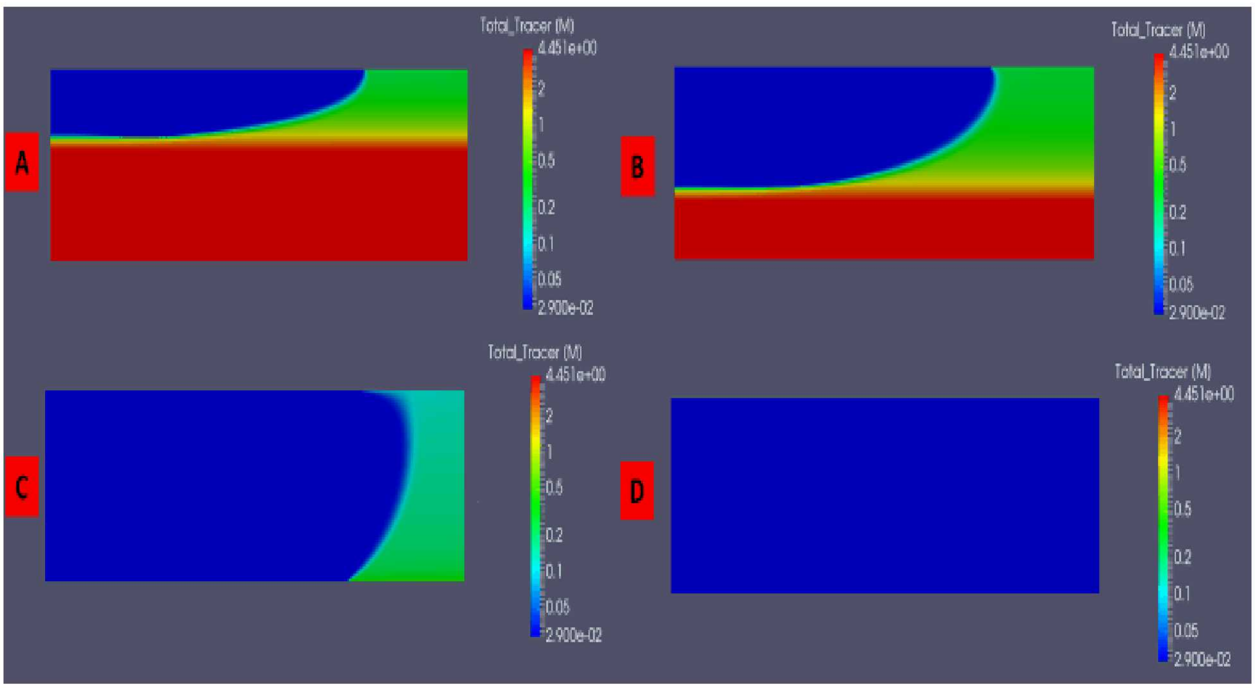

Figure 9. Tracer concentrations at 1 million years for $k = 10^{-14}$ m^2. A) ΔH = 25 m. B) ΔH = 50 m. C) ΔH = 100 m. D) ΔH = 500 m.

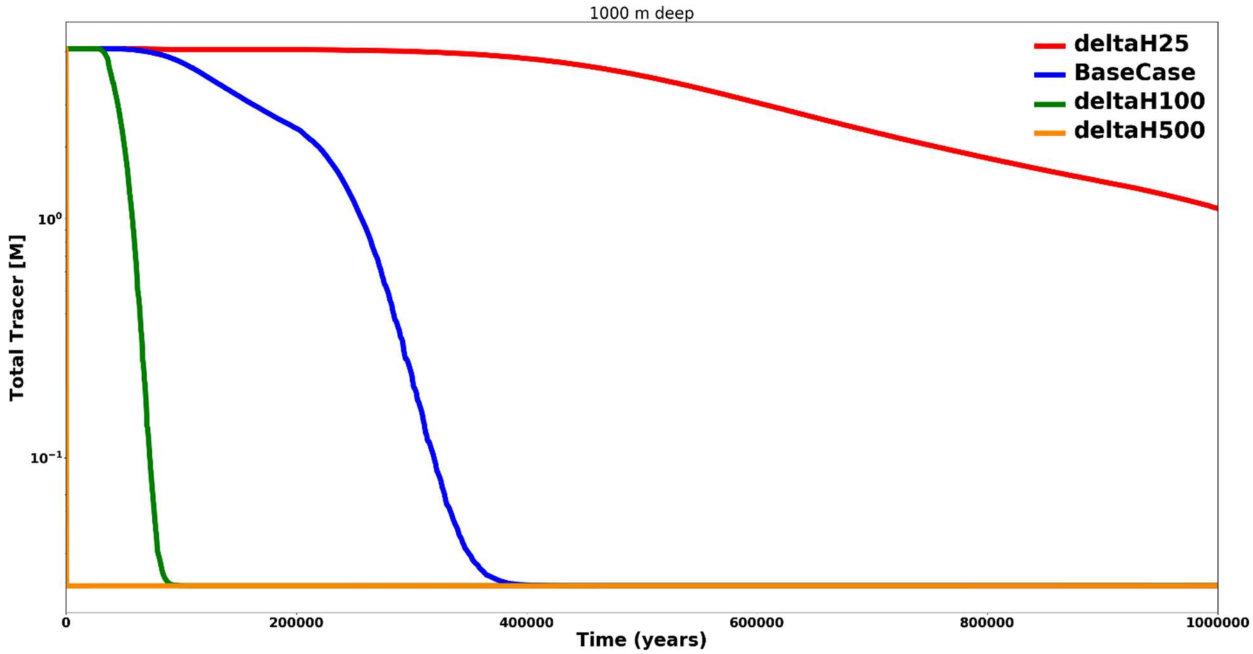

Figure 10. Tracer concentration as a function of time in the four hydraulic head cases at the observation point from Figure 1. For $k = 10^{-14}$ m^2.

3.4.2 Permeability $k = 10^{-15}$ m^2

The decrease of permeability in the hydraulic head study showed similar results to the decrease of permeability in the salinity study. The lower permeability notably slows the transport in the system, even despite the large magnitude of the head differences in cases such as is seen in **Figure 11D** (ΔH = 500 m). Total evacuation of brine does not occur in any case by 1 million years (**Figure 11**). In fact, in the case where ΔH = 25 m, very little disturbance of the deep brine occurs at all (**Figure 11A**). **Figure 12** shows that rapid brine flushing still occurs at the point of interest at ΔH = 500 m even if this is not the case throughout the rest of the domain. Total flushing at this point only occurs at ΔH = 100 m and ΔH = 500 m.

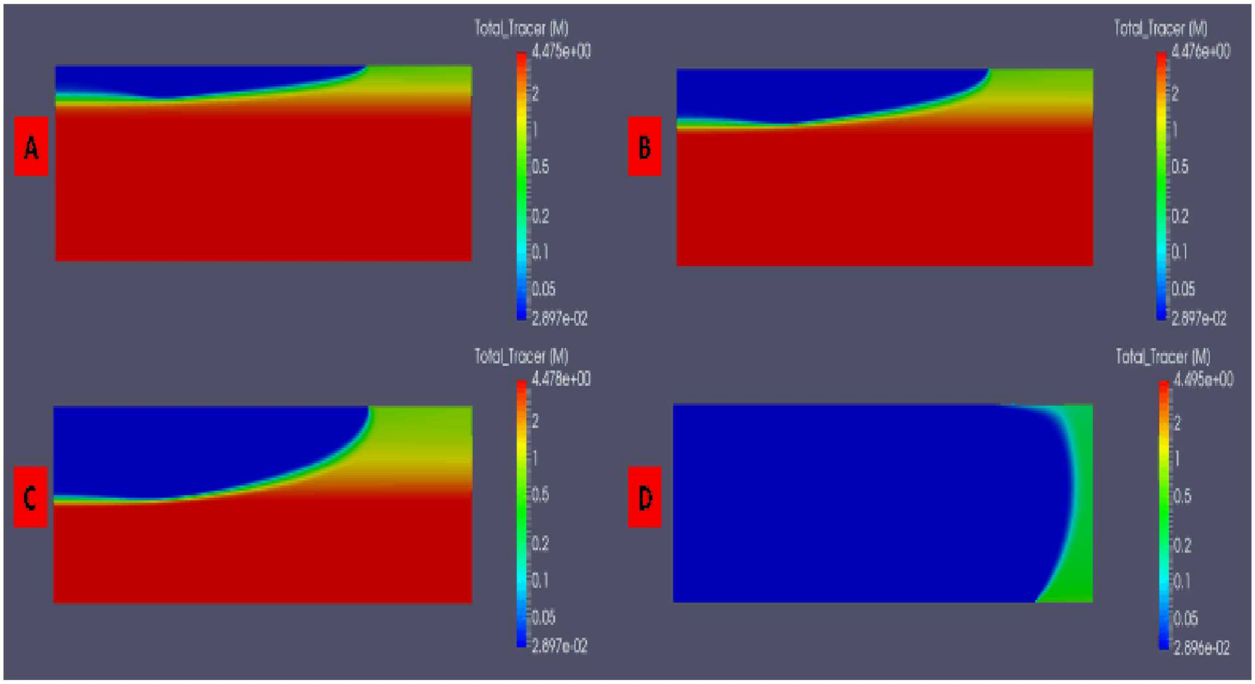

Figure 11. Tracer concentrations at 1 million years for $k = 10^{-15}$ m^2. A) ΔH = 25 m. B) ΔH = 50 m. C) ΔH = 100 m. D) ΔH = 500 m.

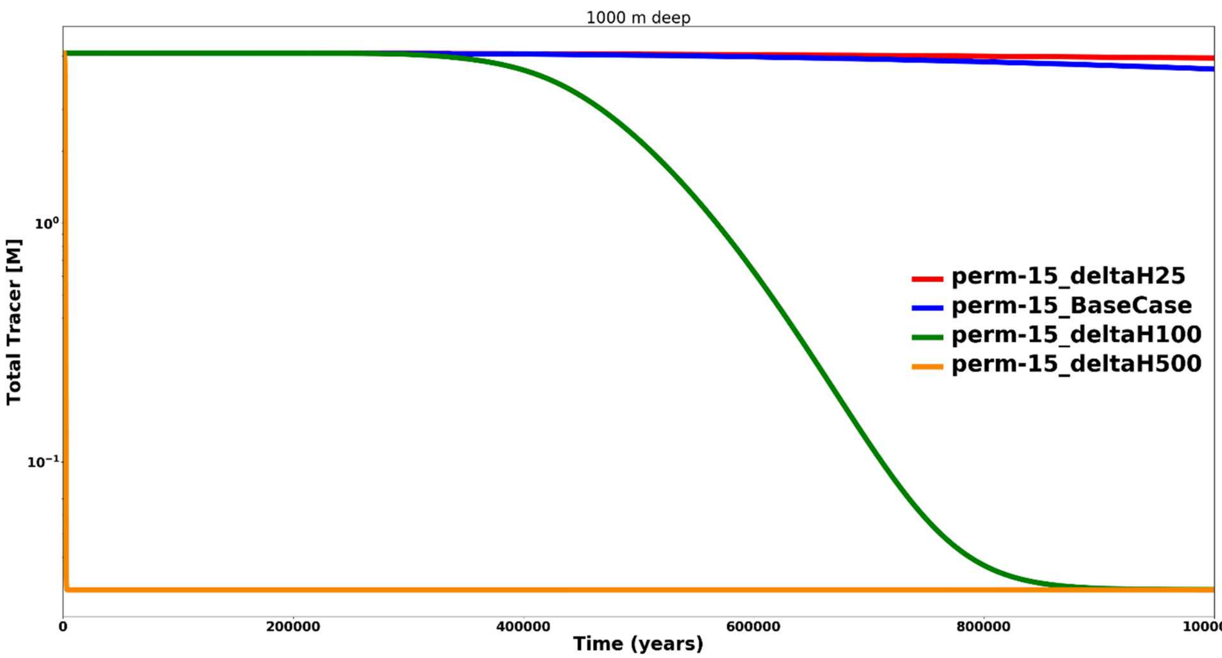

Figure 12. Tracer concentration as a function of time in the four hydraulic head cases at the observation point from Figure 1. For $k = 10^{-15}$ m^2.

3.5 DBD-Scale Study

In the DBD-scale study, very little brine disturbance occurs over the 1-million-year timeframe. Previous analyses showed that the permeabilities used in the top layer were conducive to the transport of brine, and that permeabilities lower than $k = 10^{-15}$ m^2 failed to develop a flow profile at this time that would be sufficient to drive transport. It follows that the basement permeability preferentially dictated transport. These observations hold true for this case.

Figure 13 shows that the top layer permeability had a negligible effect on the flow of brine. Though a flow pattern is established, it is not sufficient in magnitude to more than slightly disturb the deep brine at geologic time (**Figure 14**); the lower permeability of the crystalline basement region results in fluxes that are several orders of magnitude lower than those of the sediment region. Freshwater does not enter the crystalline region (though there is some mixing with the brine at the interface), and density stratification persists.

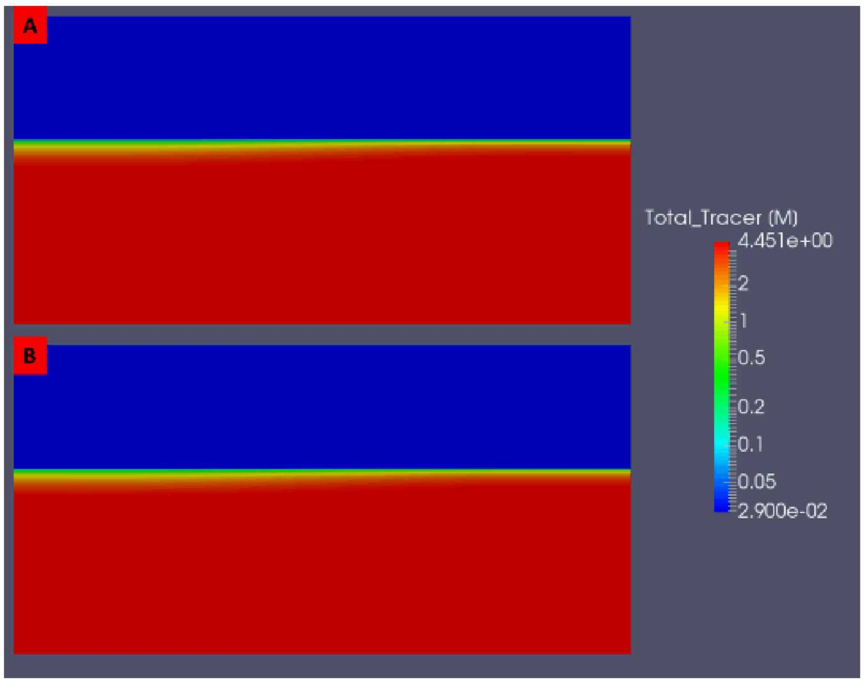

Figure 13. Tracer concentrations at 1 million years in the DBD-scale domain. A) Top layer permeability $k = 10^{-14}$ m^2. B) Top layer permeability $k = 10^{-15}$ m^2.

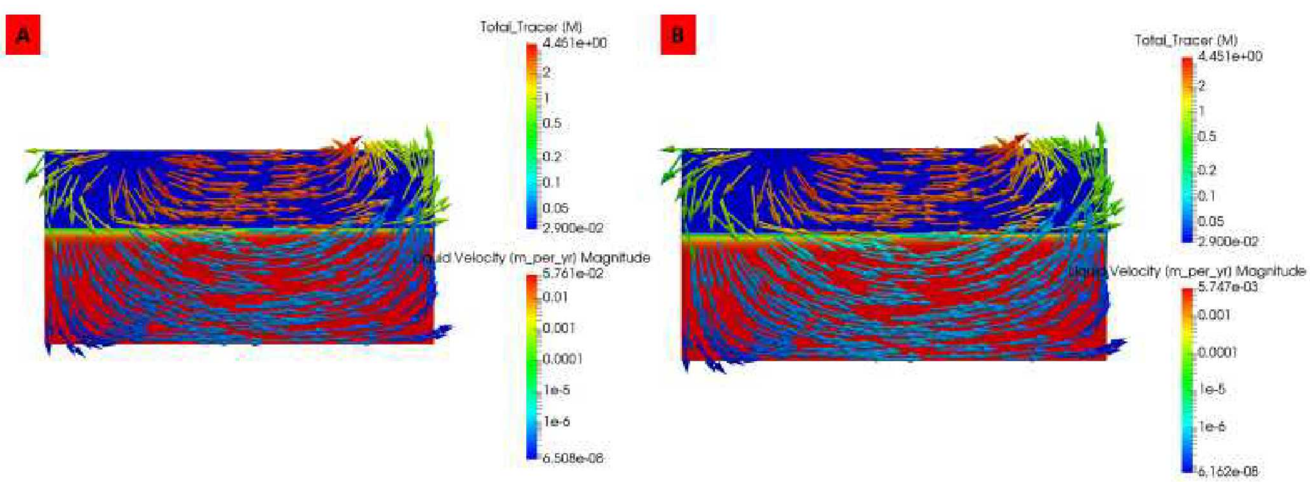

Figure 14. Liquid velocities and tracer concentrations at 1 million years in the DBD-scale domain. A) Top layer permeability $k = 10^{-14}$ m^2. B) Top layer permeability $k = 10^{-15}$ m^2.

4. CONCLUSIONS

This modeling shows that in a 2-D system with a homogenous permeability structure, hydraulic isolation of deep basement can be maintained for 1 million years, given sufficiently-high density contrast and sufficiently-low permeability and driving force. Such domains would be desirable for deep borehole disposal.

This is further illustrated by the layered model domain that more closely resembles a DBD-suitable site, wherein minimal transport occurs and the brine in the crystalline basement remains largely unperturbed across the million-year simulation.

Further studies could analyze the effects of heterogeneous permeability, discrete fractures, more complex brine stratification, environments with more complex recharge/discharge, and the effects of fluid-rock interactions at depth on the persistence of subsurface brine. Additionally, a further study could also analyze the interactions of an environment with a region similar to a disposal borehole.

5. REFERENCES

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6. ACKNOWLEDGEMENTS

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