SAND2022-8387C

Sandia National Laboratories

Effects of Fracture Transmissivity Relationship on Repository Performance Characteristics

Mariah Smith, Teresa Portone, Laura Swiler

3rd International Discrete Fracture Network Engineering Conference

June 30th, 2022

U.S. DEPARTMENT OF ENERGY NNSA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

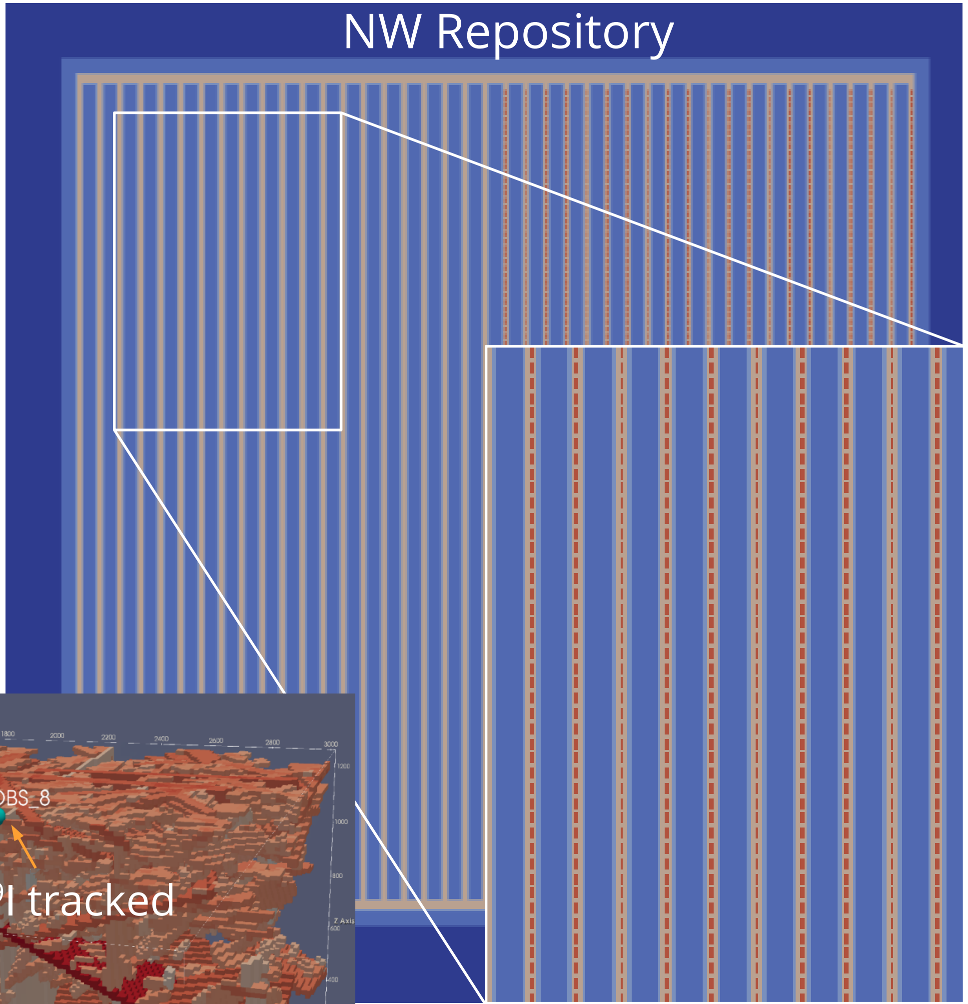
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

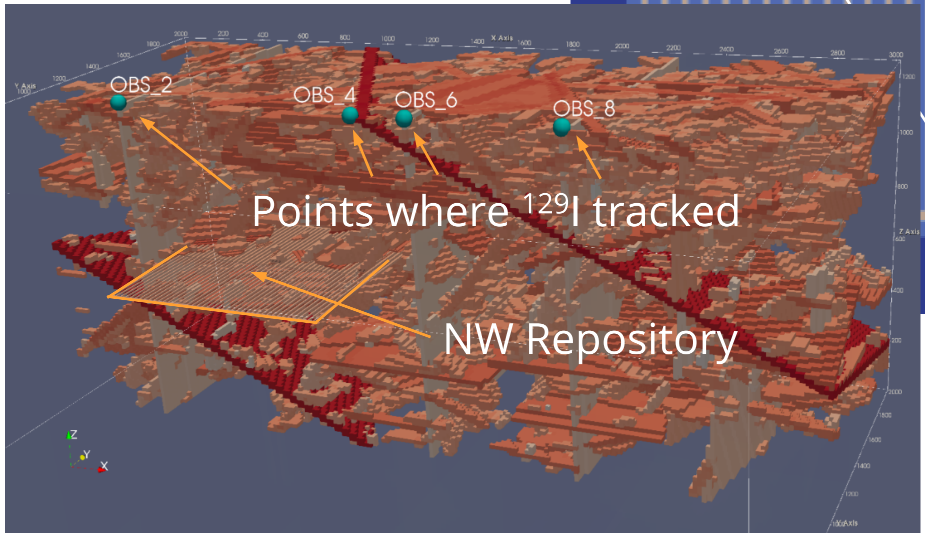
Performance assessment for nuclear waste repository site

Performance assessment involves a set of evaluations to provide reasonable assurance that a repository system will achieve sufficient safety and meet the relevant requirements for the protection of humans and the environment over a prolonged period.

Multiphysics problem:

- subsurface multiphase flow and transport
- chemical reactions
- waste canister degradation and failure
- biosphere





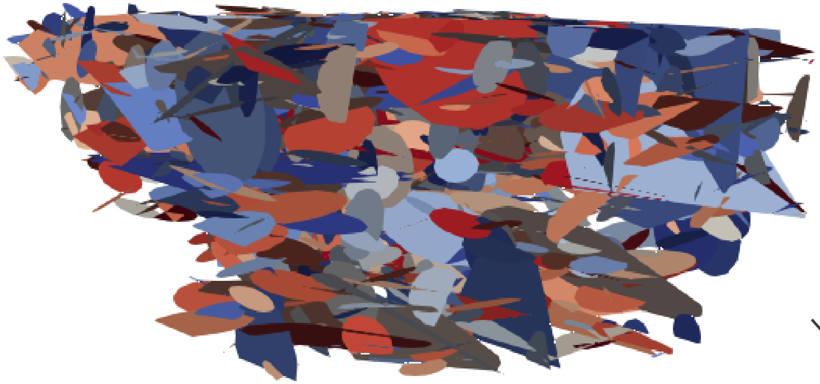
Representing spatial uncertainty in fractured crystalline rock

$$r \sim p_r(r)$$
$$\theta \sim p_\theta(\theta)$$
$$P_{32} \approx P_{32}^{target}$$

Statistical models

DFNWorks

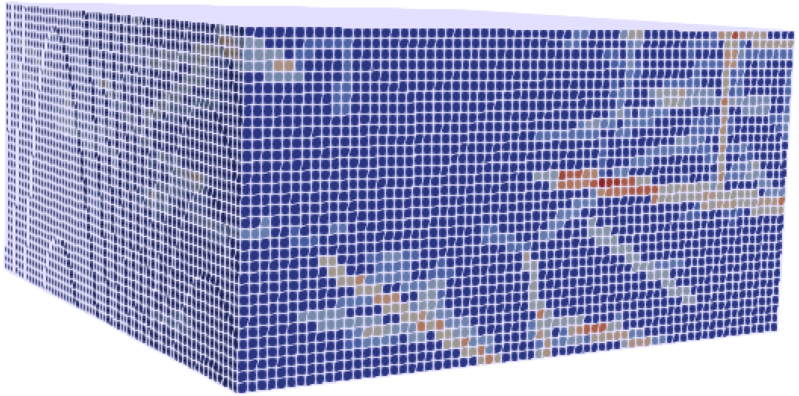
Los Alamos National Laboratory EST. 1943



Discrete Fracture Networks (DFNs)

mapDFN

Sandia National Laboratories



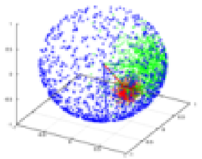
Equivalent Continuous Porous Media (ECPMs)

Converting to ECPM

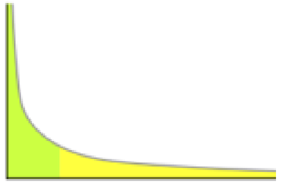
DFNWorks

Los Alamos NATIONAL LABORATORY EST. 1943

- Generate DFN
  - Orientation: Fisher distribution



  - Radius: Truncated power law



- Assign $T_f = k_f b_f$

Transmissivity Permeability Aperture

mapDFN

Sandia National Laboratories

- Define mesh and locate fractures in grid cells
- Rotate coordinates of T_f
- Calculate cell permeability k

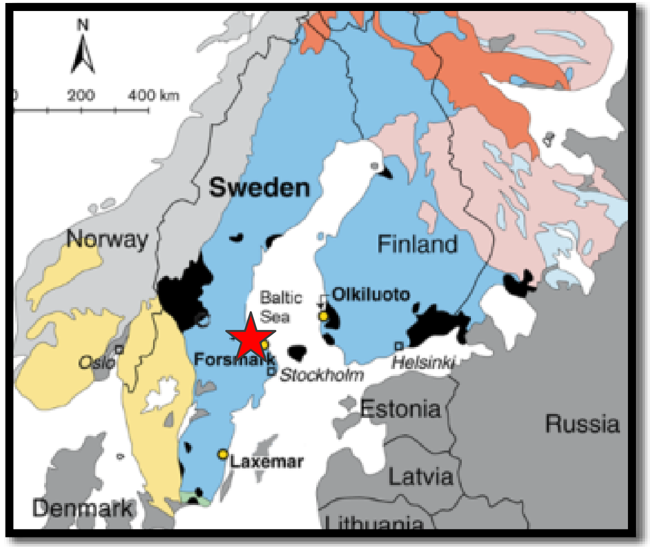
$$\begin{bmatrix} k_{xx} & & \\ & k_{yy} & \\ & & k_{zz} \end{bmatrix} = \frac{1}{d} \sum \begin{bmatrix} T_{xx} & & \\ & T_{yy} & \\ & & T_{zz} \end{bmatrix}_f$$

- Calculate cell porosity ϕ

$$\phi = \frac{1}{d} \sum b_f$$

Assumed transmissivity affects permeability of ECPM!

Crystalline Reference Case based on Forsmark, Sweden



Joyce *et al.*, *Hydrogeology Journal* (2014) https://doi.org/10.1007/s10040-014-1165-6
Follin *et al.*, *Hydrogeology Journal* (2014) https://doi.org/10.1007/s10040-013-1080-2.

Orientation $\theta \sim p_\theta(\theta)$

Circular fractures, $r \sim p_r(r)$

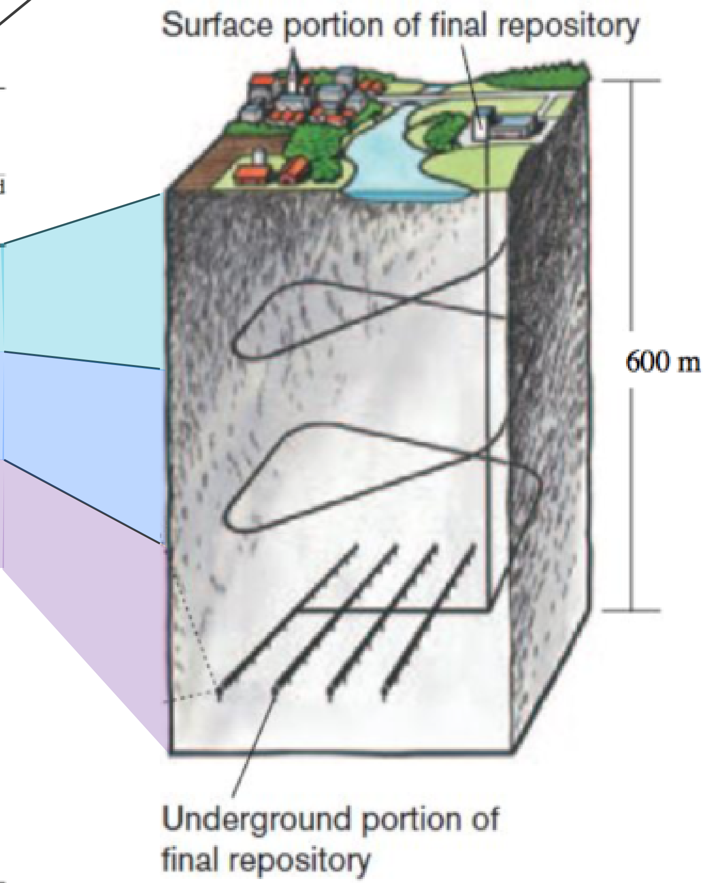
P_{32}

Transmissivity, e.g. correlated: $T = ar^b$

Table 2 Hydrogeological DFN parameters for each fracture domain, fracture set and depth zone

Fracture domain/elevation (m.a.s.l)[a]	Fracture set name	Orientation set pole: (trend, plunge), conc.	Size model, power-law (r_0, k_r) (m, −)	Intensity, (P_{32}), valid size interval: r_0 to 564 m (m^2/m^3)	Parameter values for the transmissivity models: Semi-correlated (a,b,σ)	Correlated (a,b)	Uncorrelated (μ,σ)
FFM01 and FFM06>−200	NS	(292, 1) 17.8	(0.038, 2.50)	0.073	$6.3 \cdot 10^{-9}$, 1.3, 1.0	$6.7 \cdot 10^{-9}$, 1.4	−6.7, 1.2
	NE	(326, 2) 14.3	(0.038, 2.70)	0.319			
	NW	(60, 6) 12.9	(0.038, 3.10)	0.107			
	EW	(15, 2) 14.0	(0.038, 3.10)	0.088			
	HZ	(5, 86) 15.2	(0.038, 2.38)	0.543			
FFM01 and FFM06 −200 to −400	NS	(292, 1) 17.8	(0.038, 2.50)	0.142	$1.3 \cdot 10^{-9}$, 0.5, 1.0	$1.6 \cdot 10^{-9}$, 0.8	−7.5, 0.8
	NE	(326, 2) 14.3	(0.038, 2.70)	0.345			
	NW	(60, 6) 12.9	(0.038, 3.10)	0.133			
	EW	(15, 2) 14.0	(0.038, 3.10)	0.081			
	HZ	(5, 86) 15.2	(0.038, 2.38)	0.316			
FFM01 and FFM06<−400	NS	(292, 1) 17.8	(0.038, 2.50)	0.094	$5.3 \cdot 10^{-11}$, 0.5, 1.0	$1.8 \cdot 10^{-10}$, 1.0	−8.8, 1.0
	NE	(326, 2) 14.3	(0.038, 2.70)	0.163			
	NW	(60, 6) 12.9	(0.038, 3.10)	0.098			
	EW	(15, 2) 14.0	(0.038, 3.10)	0.039			
	HZ	(5, 86) 15.2	(0.038, 2.38)	0.141			
FFM02>−200	NS	(83, 10) 16.9	(0.038, 2.75)	0.342	$9.0 \cdot 10^{-9}$, 0.7, 1.0	$5.0 \cdot 10^{-9}$, 1.2	−7.1, 1.1
	NE	(143, 9) 11.7	(0.038, 2.62)	0.752			
	NW	(51, 15) 12.1	(0.038, 3.20)	0.335			
	EW	(12, 0) 13.3	(0.038, 3.40)	0.156			
	HZ	(71, 87) 20.4	(0.038, 2.58)	1.582			
FFM03, FFM04 and FFM05>−400	NS	(292, 1) 17.8	(0.038, 2.60)	0.091	$1.3 \cdot 10^{-8}$, 0.4, 0.8	$1.4 \cdot 10^{-8}$, 0.6	−7.2, 0.8
	NE	(326, 2) 14.3	(0.038, 2.50)	0.253			
	NW	(60, 6) 12.9	(0.038, 2.55)	0.258			
	EW	(15, 2) 14.0	(0.038, 2.40)	0.097			
	HZ	(5, 86) 15.2	(0.038, 2.55)	0.397			
FFM03, FFM04 and FFM05<−400	NS	(292, 1) 17.8	(0.038, 2.60)	0.102	$1.8 \cdot 10^{-8}$, 0.3, 0.5	$7.1 \cdot 10^{-9}$, 0.6	−7.2, 0.8
	NE	(326, 2) 14.3	(0.038, 2.50)	0.247			
	NW	(60, 6) 12.9	(0.038, 2.55)	0.103			
	EW	(15, 2) 14.0	(0.038, 2.40)	0.068			
	HZ	(5, 86) 15.2	(0.038, 2.55)	0.250			

[a] Meters above sea level



Overview

Does fracture transmissivity relationship have an effect on repository performance characteristics?

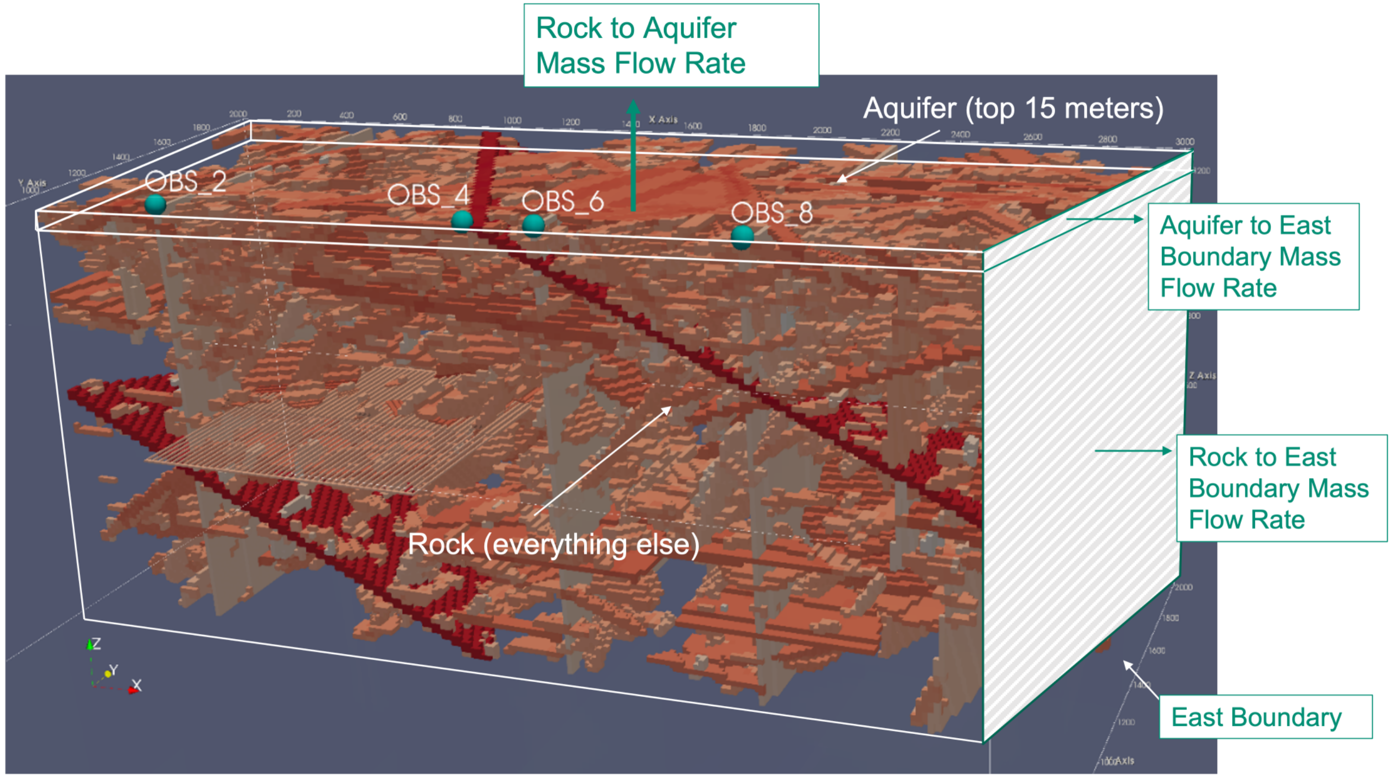
Workflow

- dfnWorks: generates three-dimensional discrete fracture networks (DFNs)
- mapDFN: meshes fracture networks and converts them to equivalent porous media (ECPMs)
- PFLOTRAN: performs flow and transport calculations for ECPMs
- Python: data extraction

Depth (meters below sea level)	Transmissivity relationship	
	Correlated, $T = ar^b$	
	Constant over domain (a, b)	Depth-dependent (a, b)
0-200	(1.6e-9, 0.8)	(6.7e-9, 1.4)
200-400		(1.6e-9, 0.8)
>400		(1.8e-10, 1.0)

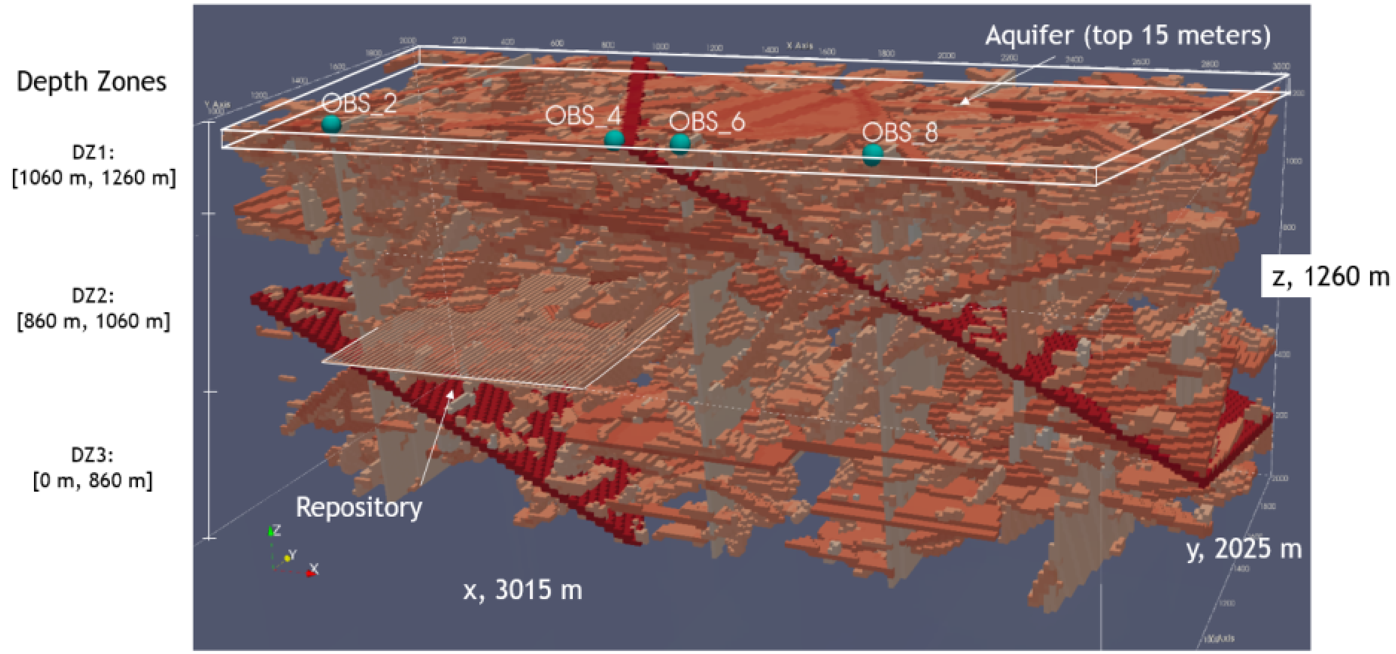
Initial Approach

- 20 DFNs generated producing a total of 40 ECPMs (20 for each transmissivity relationship)
- ECPMs used in PFLOTRAN simulations of the crystalline reference case considered 6 Quantities of Interest (QoIs) in a comparative analysis



QoIs related to dose	Maximum ^{129}I concentration in Aquifer [M]
QoIs related to repository "leakiness": functions of mass remaining in the repository of a tracer injected at time zero.	• Time when half the tracer is flushed from the repository [yr] • Fraction of the tracer left at 1 Myr • Fractional mass flux from repository at 3 kyr (mass flux from repository/mass of tracer)
Field-scale flow properties: ratios of mass flow rates at 1 million years.	• Rock to aquifer / rock to east boundary at 1 Myr • Aquifer to east boundary / rock to east boundary at 1 Myr

Data Analysis



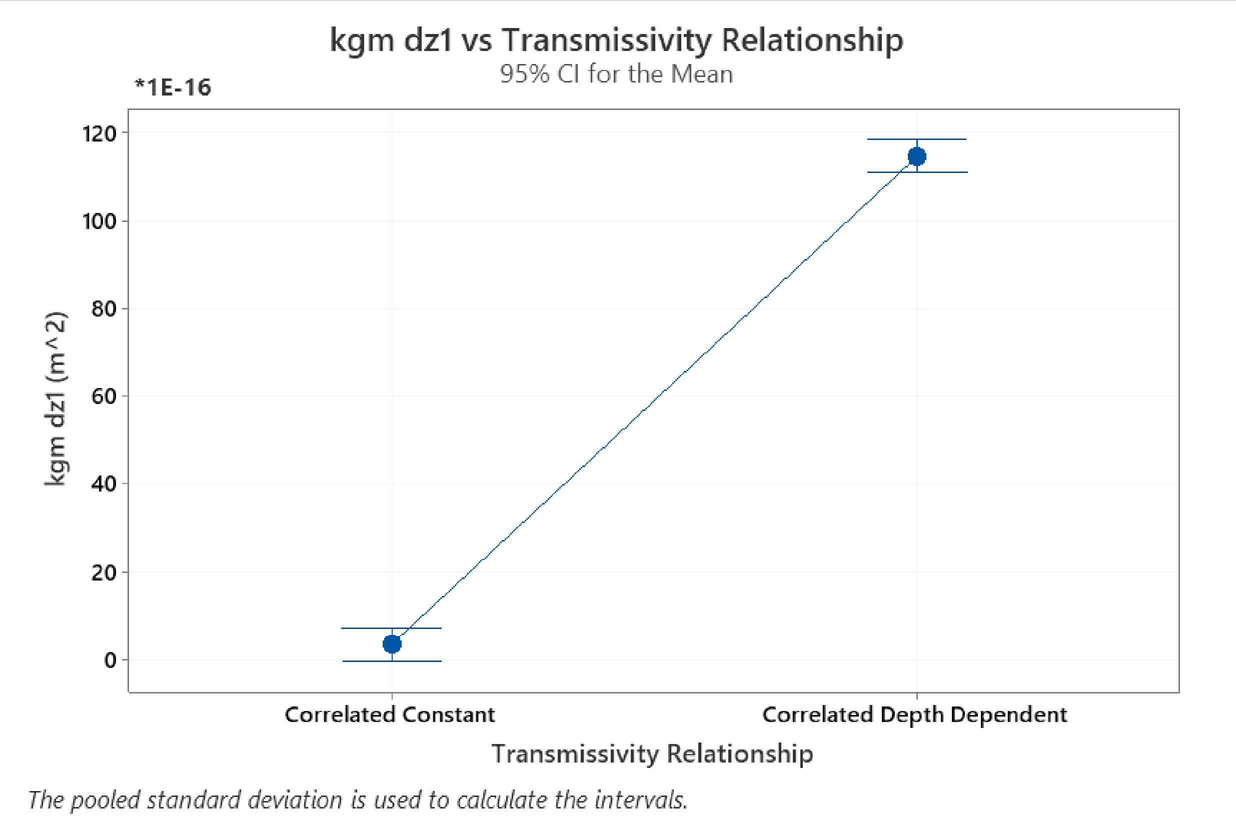
- Continuum permeability fields were summarized into domain-averaged permeability tensor components at each depth zone
  - k_{xx}= X direction
  - k_{yy}= Y direction
  - k_{zz}= Z direction
- Geometric mean permeabilities were calculated for each depth zone*

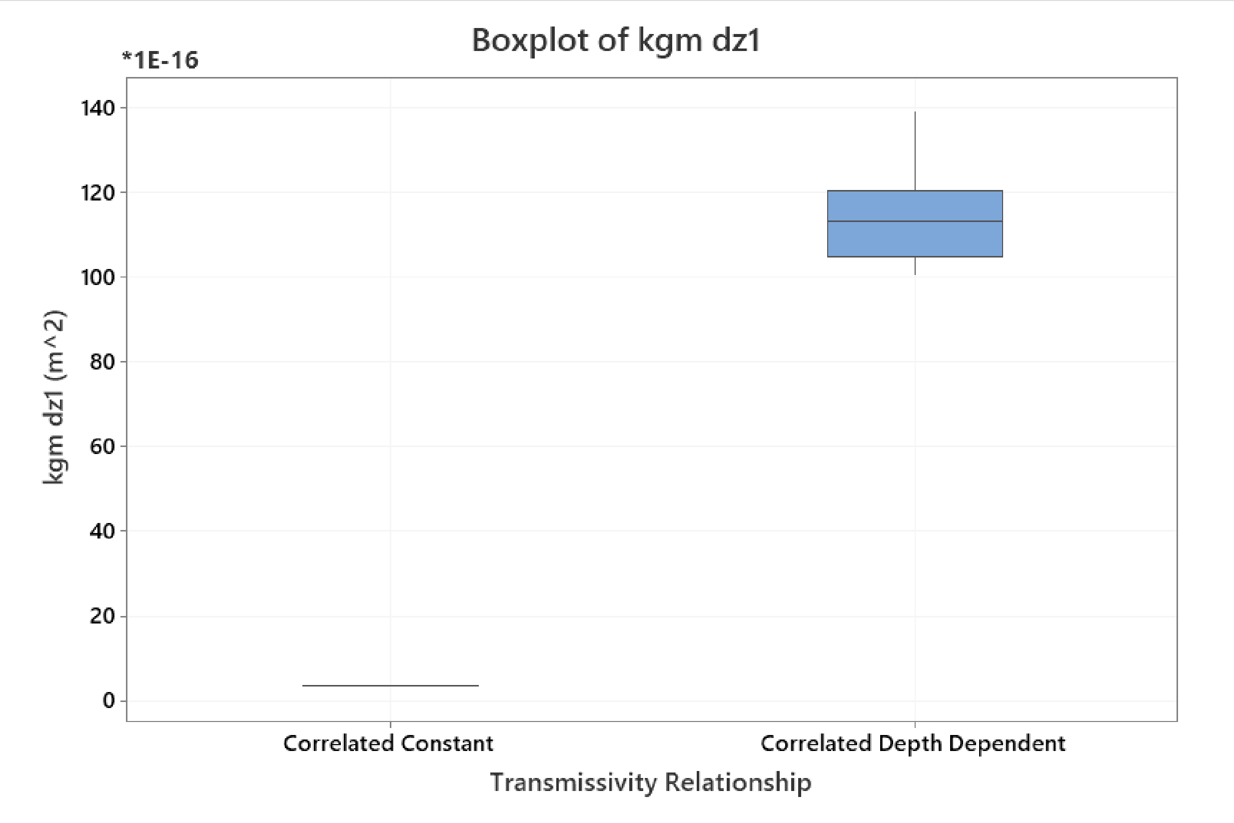
$$k_{gm} = \sqrt[3]{k_{xx}k_{yy}k_{zz}}$$

- Statistical analyses used
  - Main Effects Plots
  - Box Plots
  - Scatter Plots

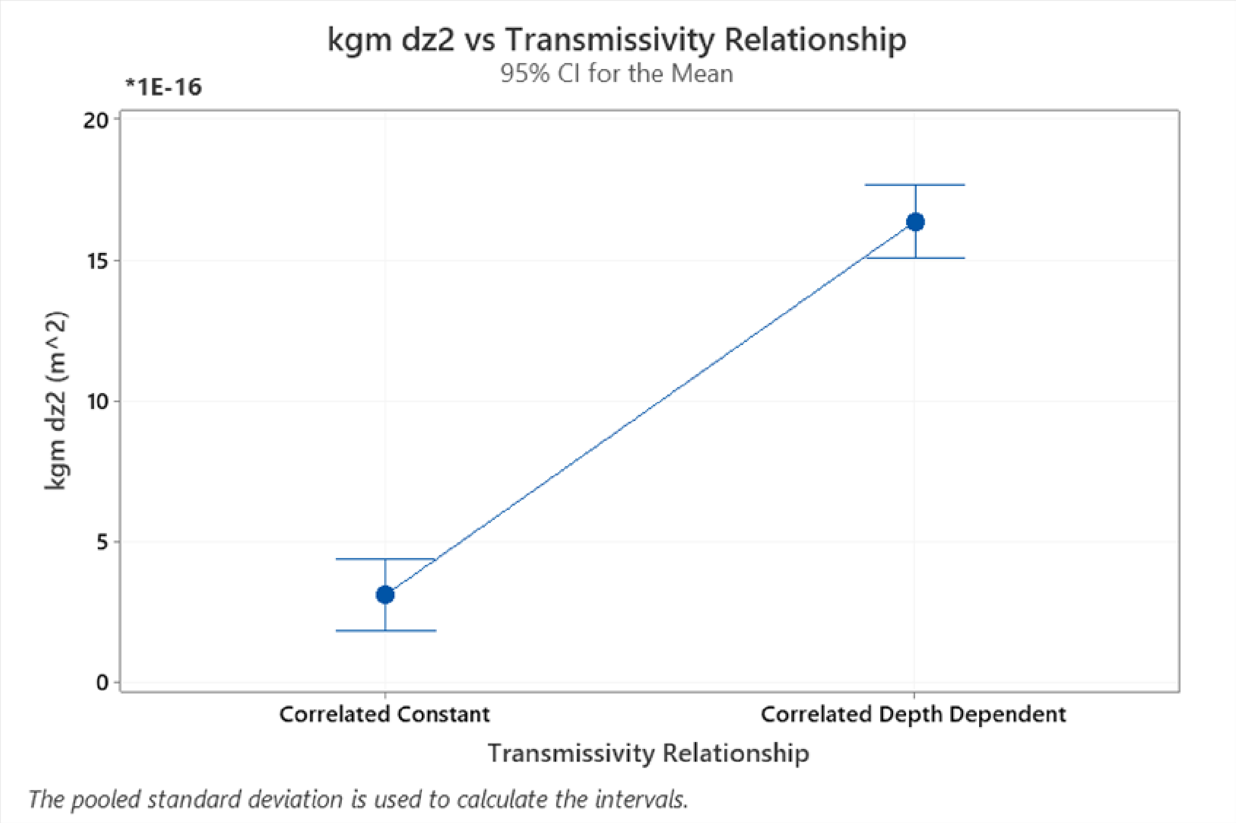
*Note: This is a geometric mean of the domain-averaged permeability tensor components.

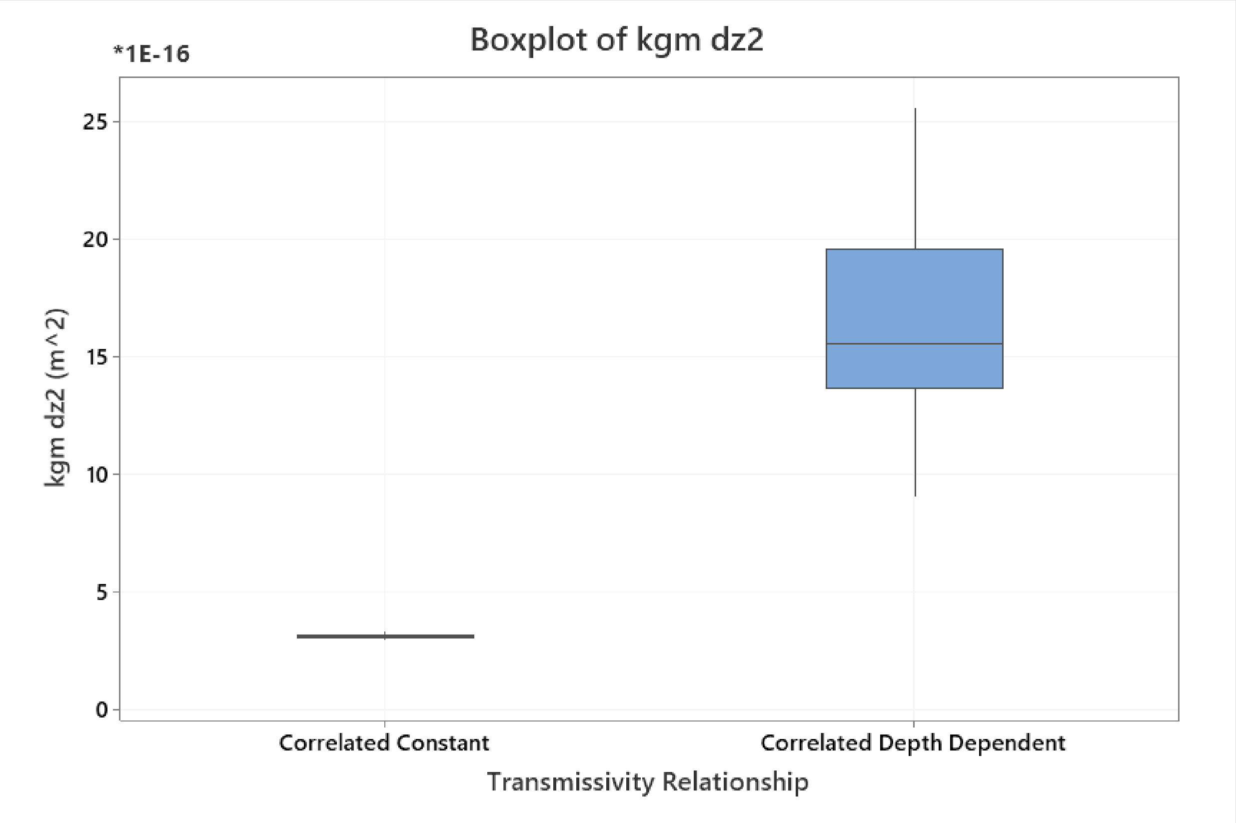
Geometric Mean Permeability – dz1



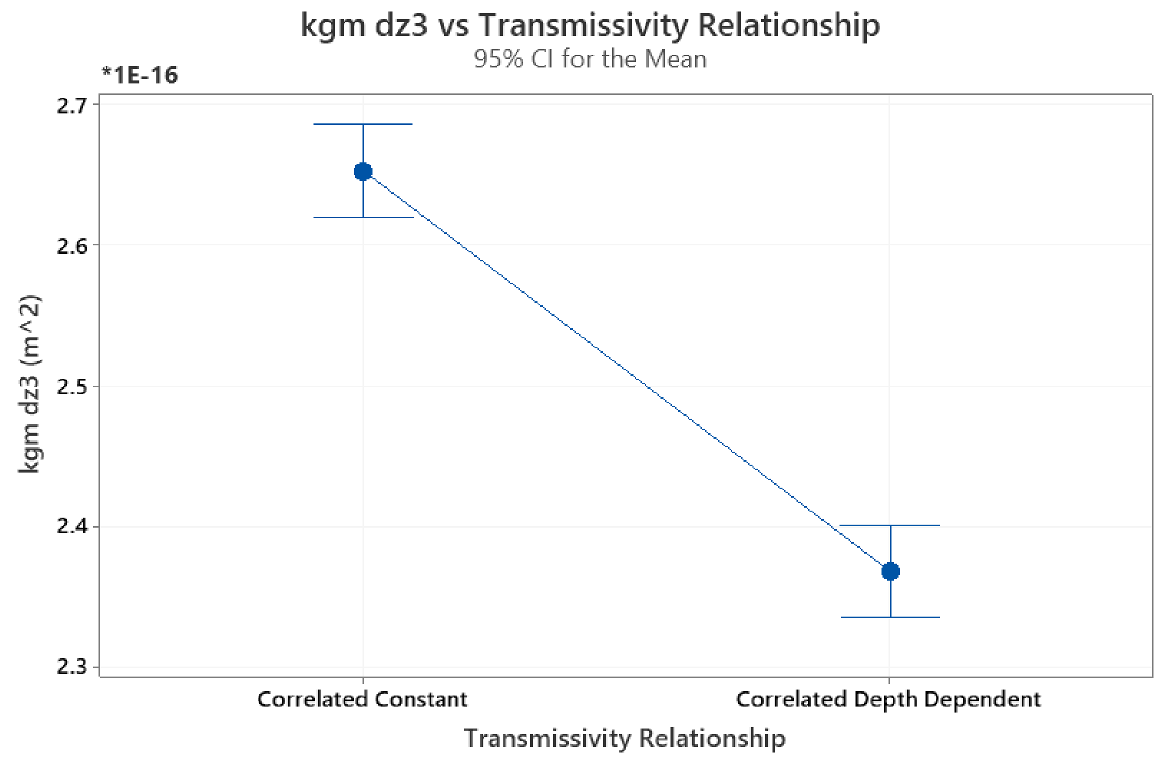


Geometric Mean Permeability – dz2

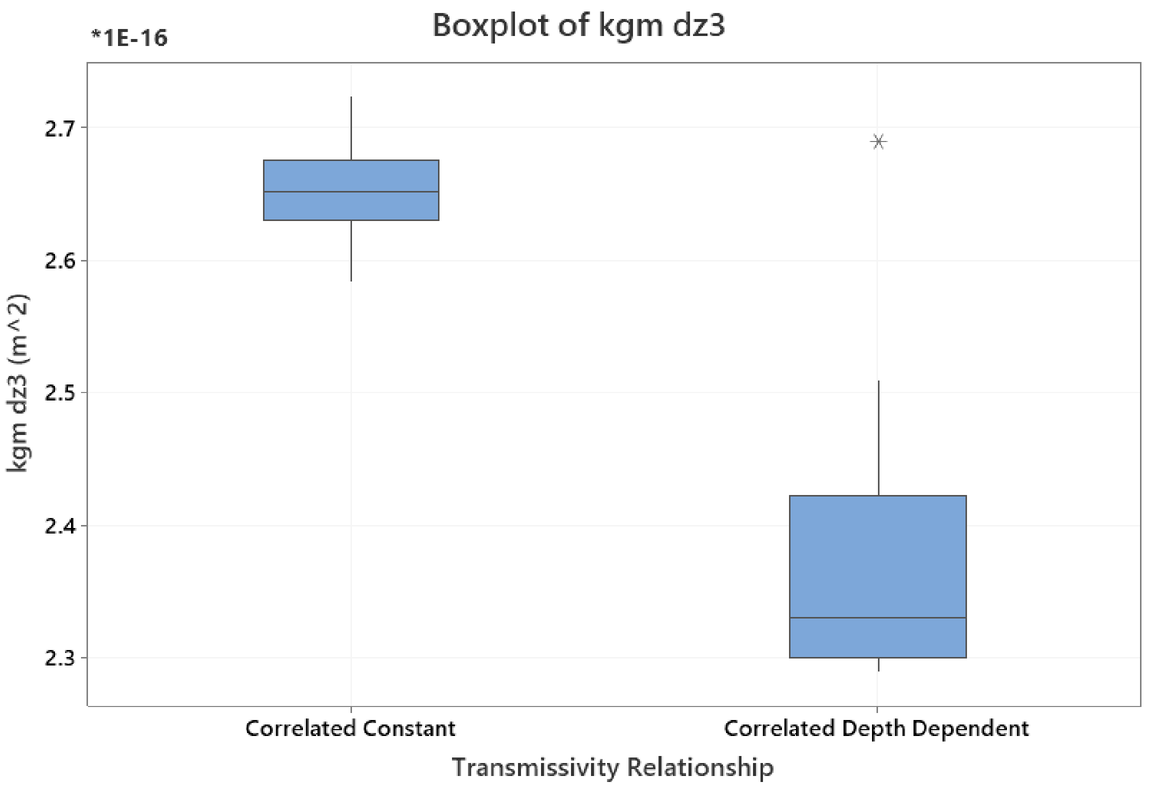




Geometric Mean Permeability – dz3



The pooled standard deviation is used to calculate the intervals.

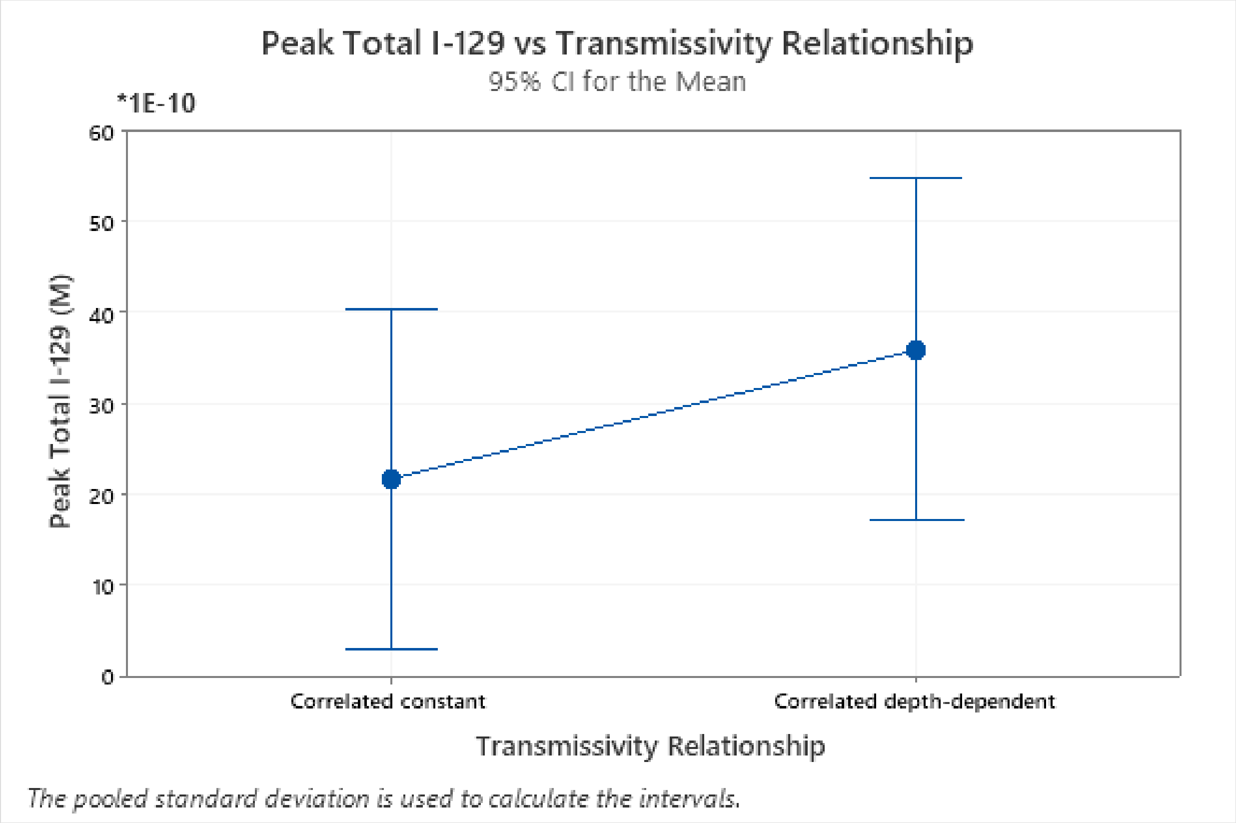


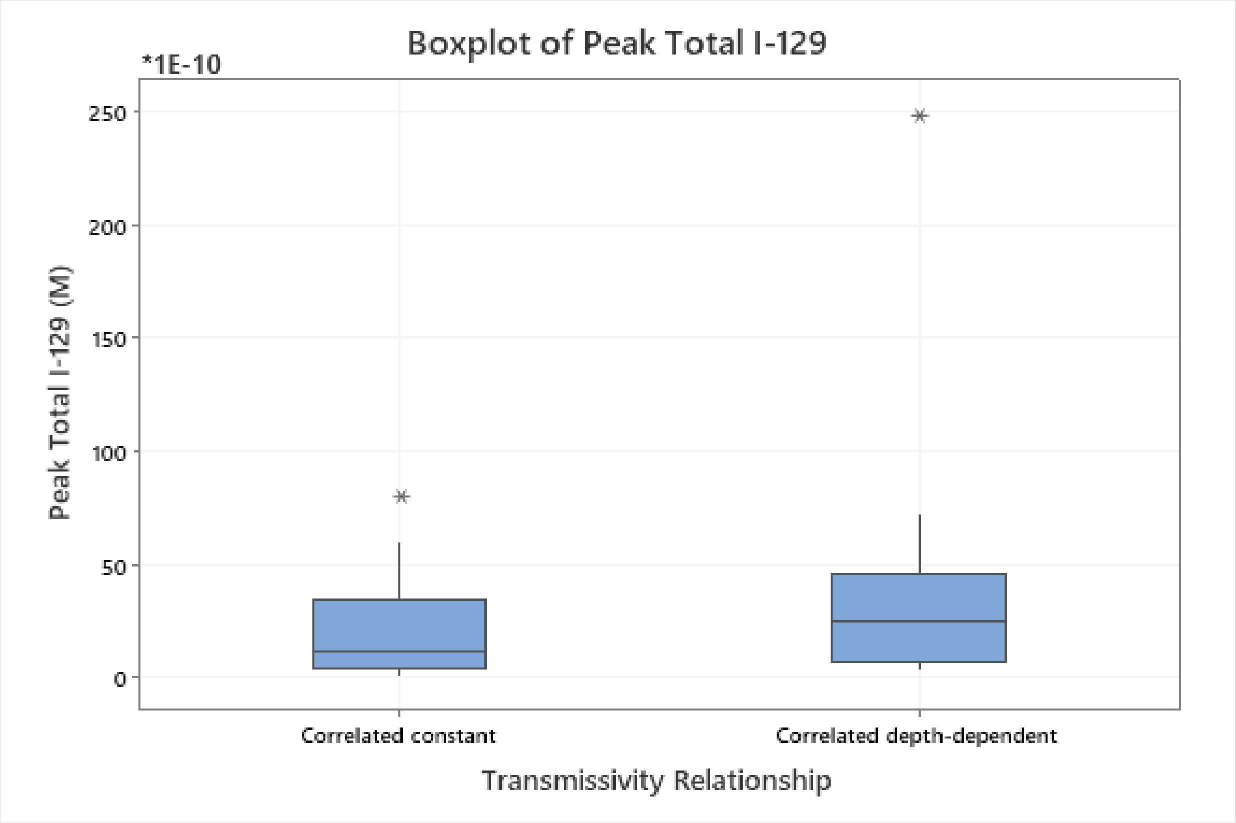
Permeability Differences

Depth Zone	Transmissivity Relationship							
	Correlated Constant $[m^2]$				Correlated Depth-Dependent $[m^2]$			
	k_{gm}	k_{xx}	k_{yy}	k_{zz}	k_{gm}	k_{xx}	k_{yy}	k_{zz}
dz1	3.47E-16	3.52E-16	5.28E-16	2.25E-16	1.15E-14	2.02E-14	2.11E-14	3.55E-15
dz2	3.12E-16	2.87E-16	4.70E-16	2.25E-16	1.64E-15	2.09E-15	2.53E-15	8.57E-16
dz3	2.65E-16	2.20E-16	4.01E-16	2.12E-16	2.36E-16	1.82E-16	3.60E-16	2.03E-16

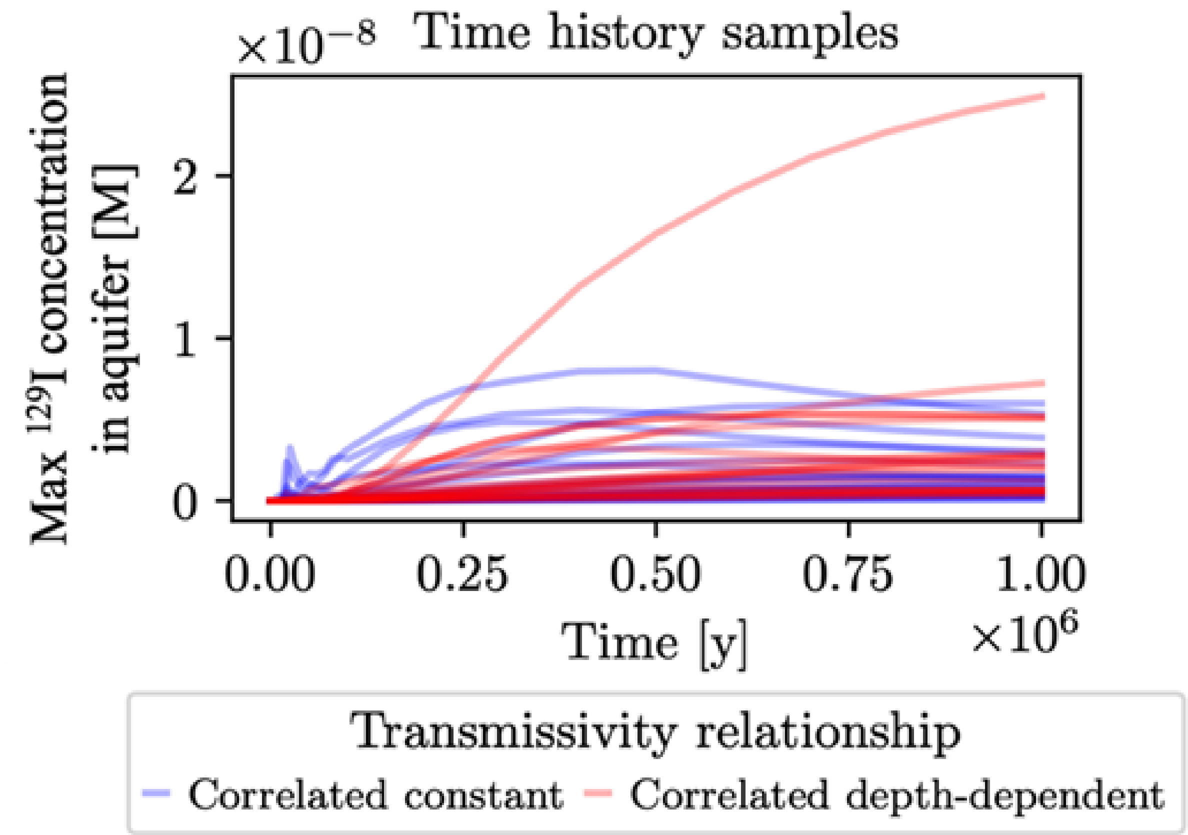
- Correlated constant transmissivity relationship had a much lower geometric mean permeability for dz1 and dz2
- Large differences in the permeability tensor components at dz1 and dz2 for the depth-dependent relationship
- Expected increase in downstream flow and little increase in vertical flow towards the aquifer for the depth-dependent relationship

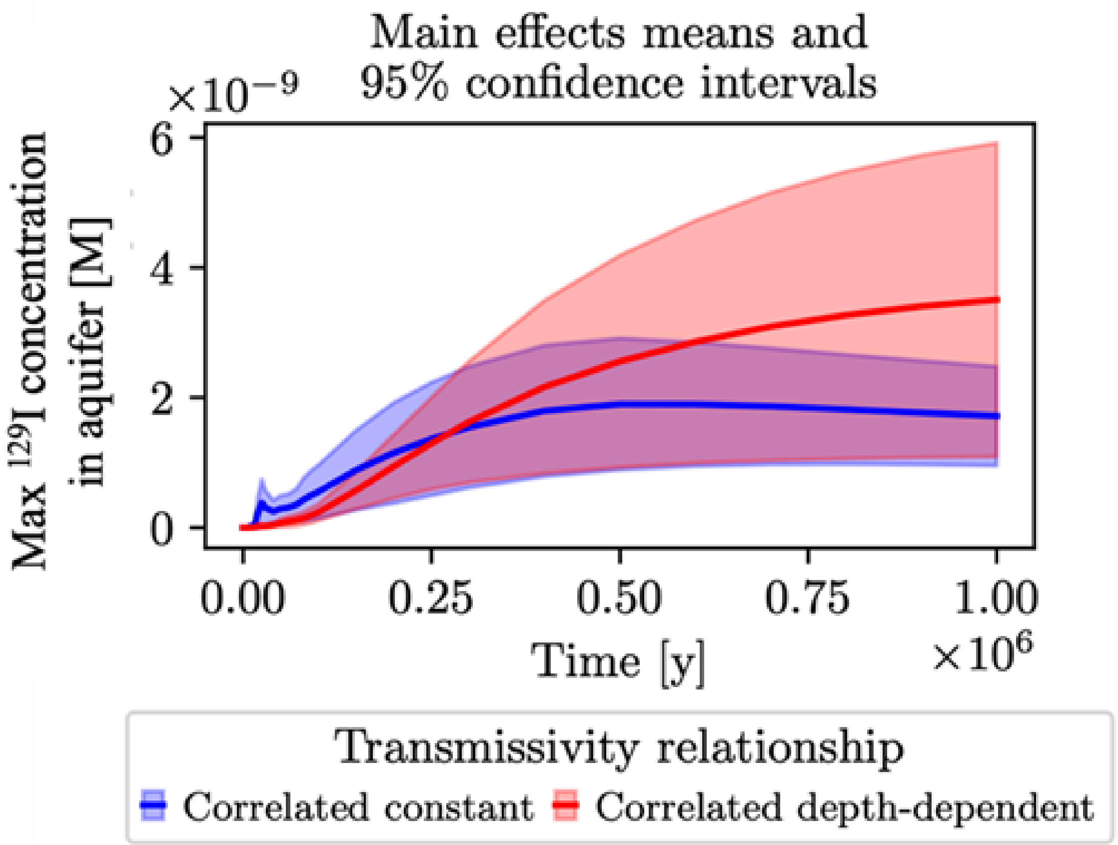
Maximum ^{129}I Concentration in the Aquifer



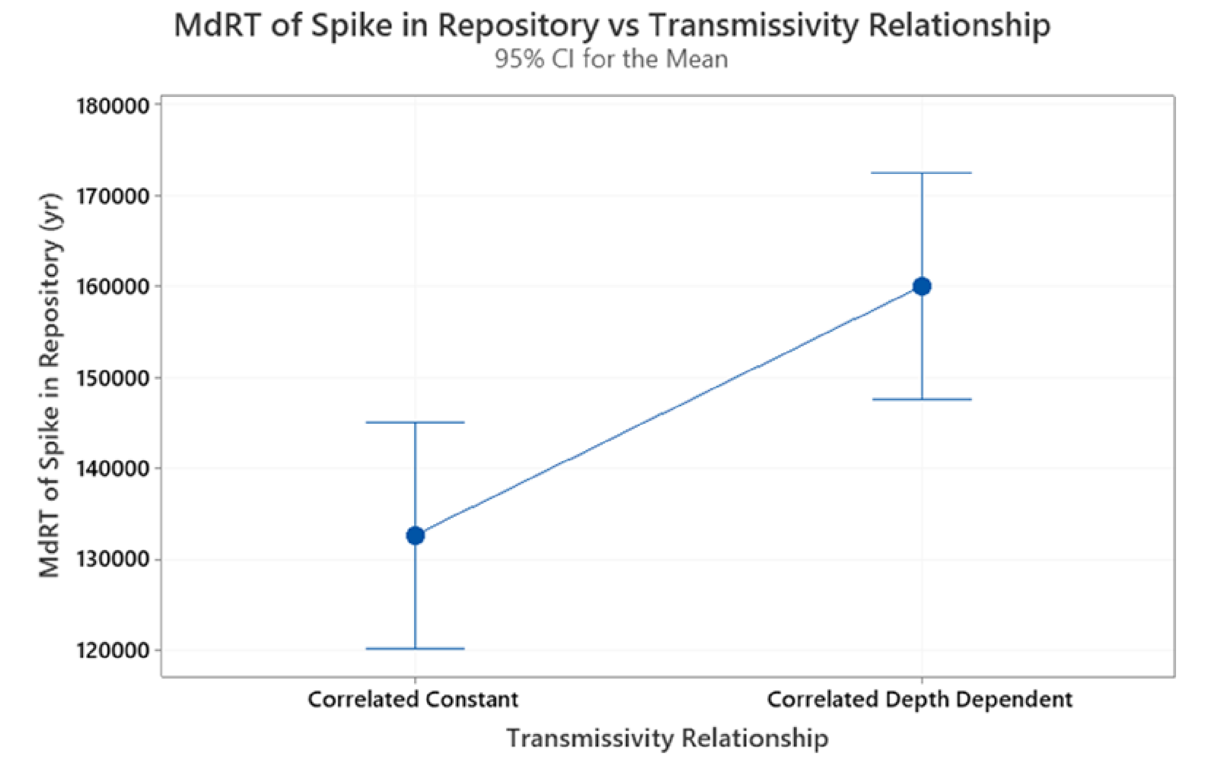


Maximum ^{129}I Concentration in the Aquifer Time History Data

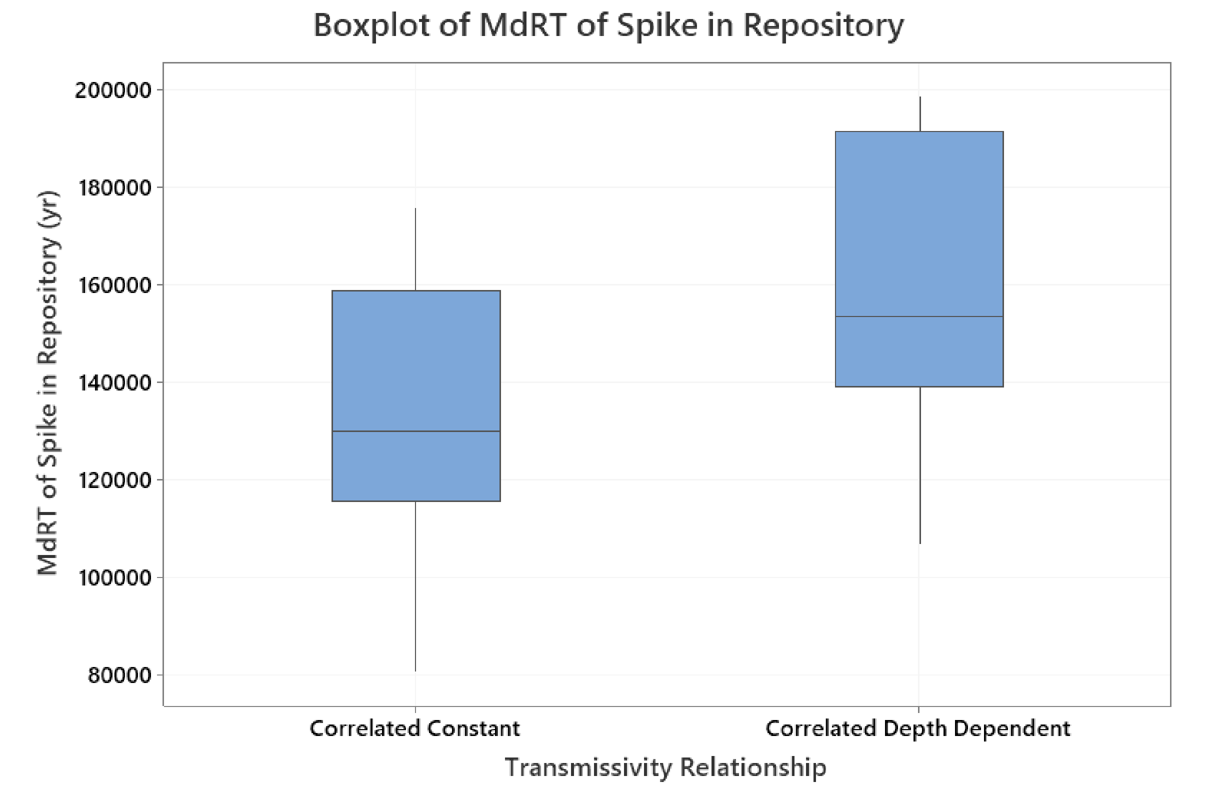




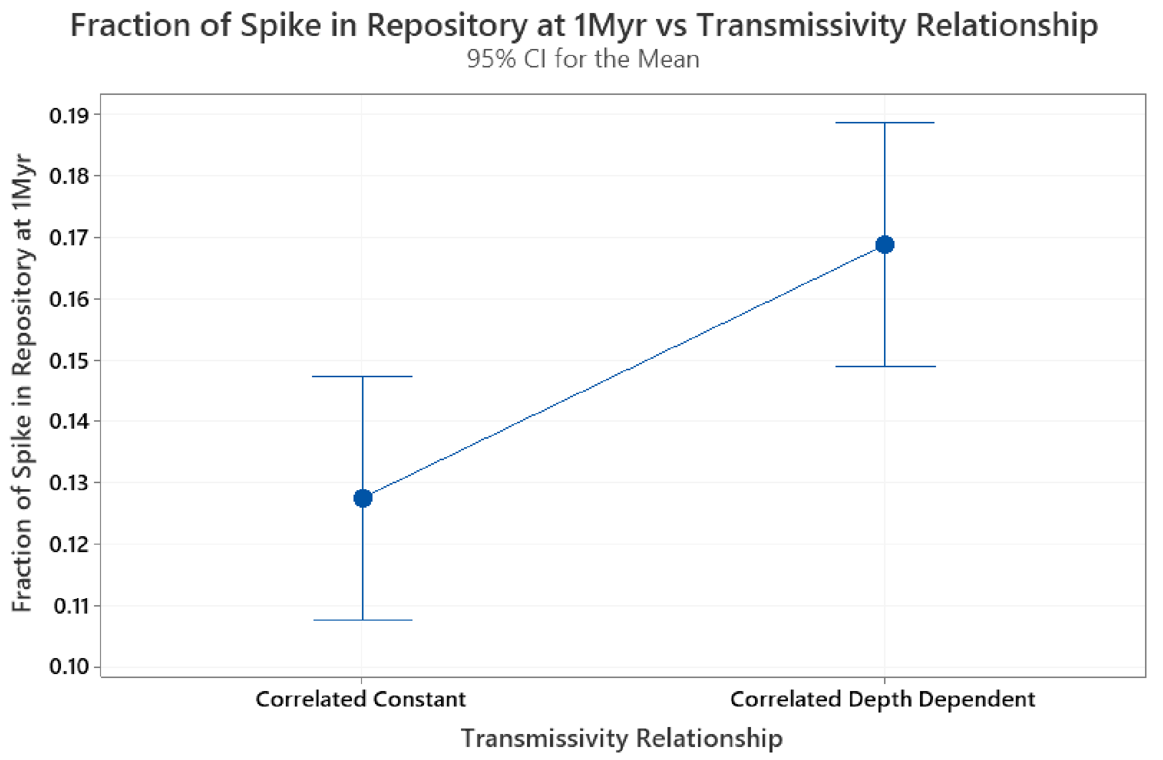
Time When Half the Mass Is Gone From the Repository



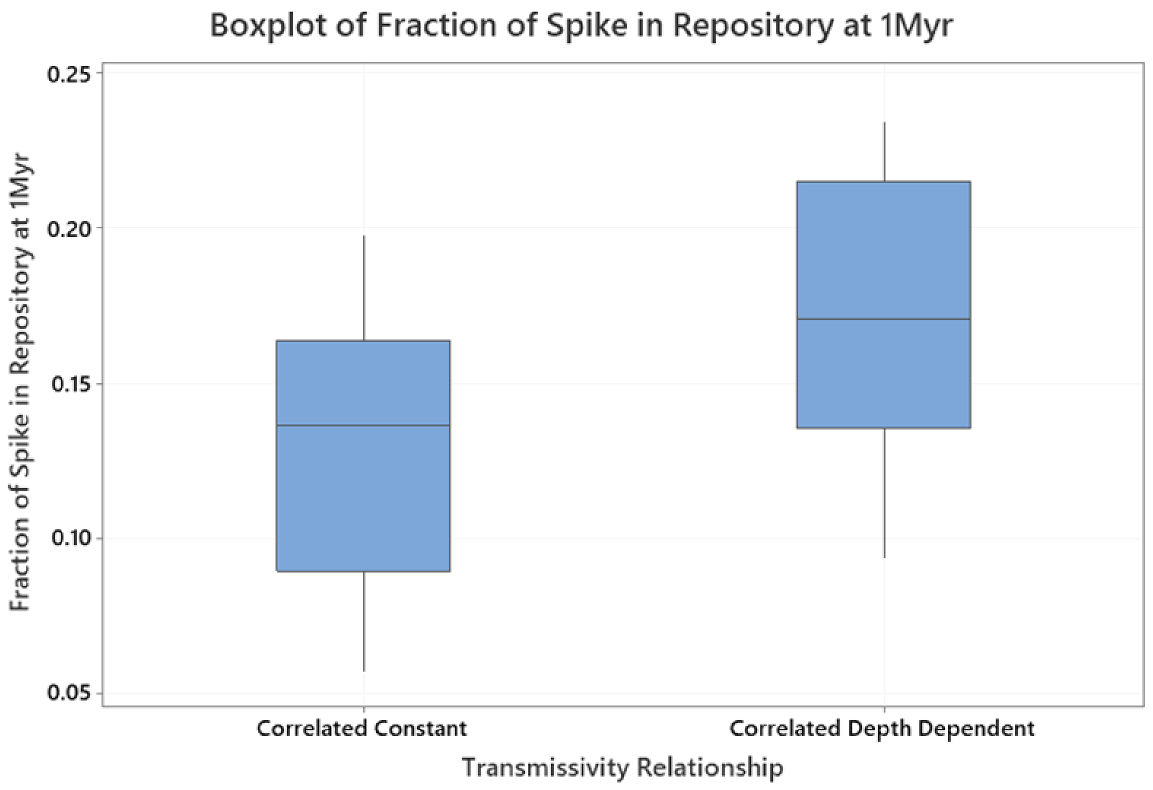
The pooled standard deviation is used to calculate the intervals.



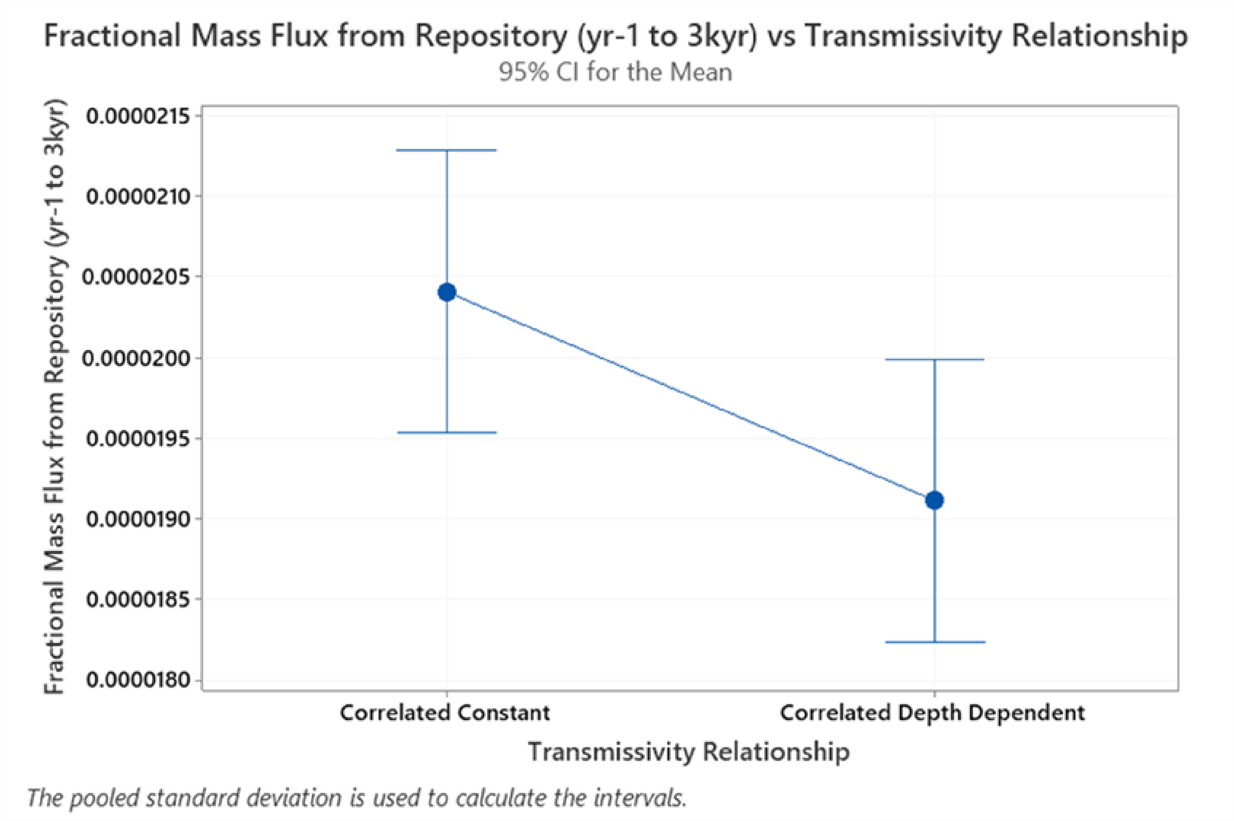
Fraction of Passive Tracer Still in the Repository at 1 million Years

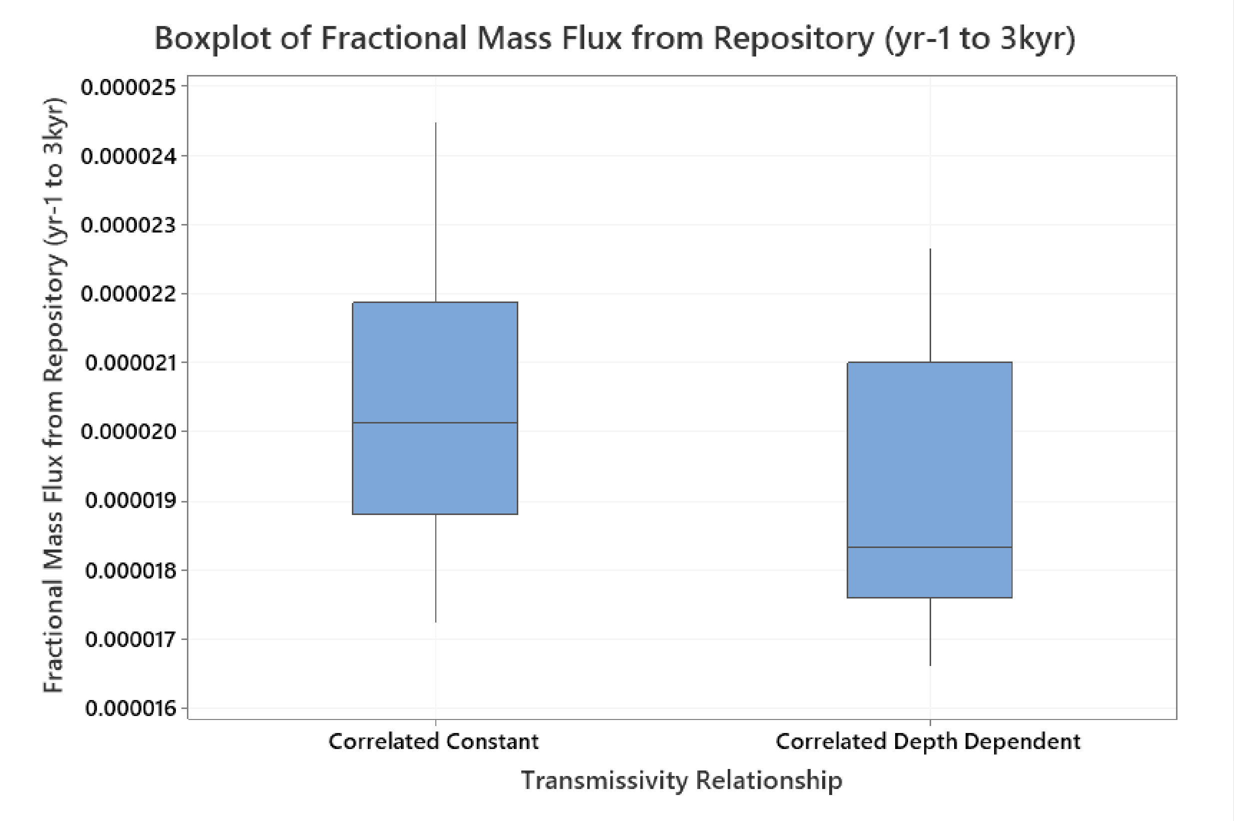


The pooled standard deviation is used to calculate the intervals.



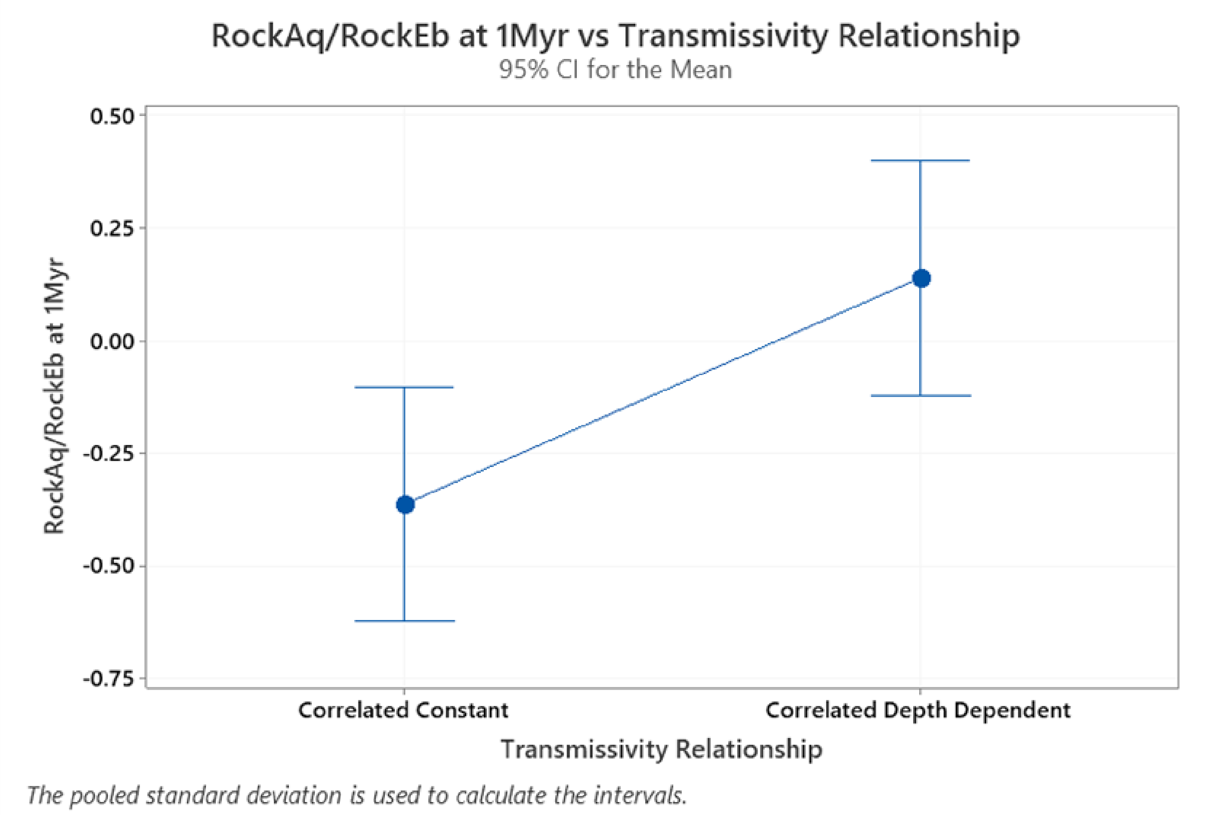
Fractional Mass Flux of Tracer Leaving the Repository After 3 Thousand Years

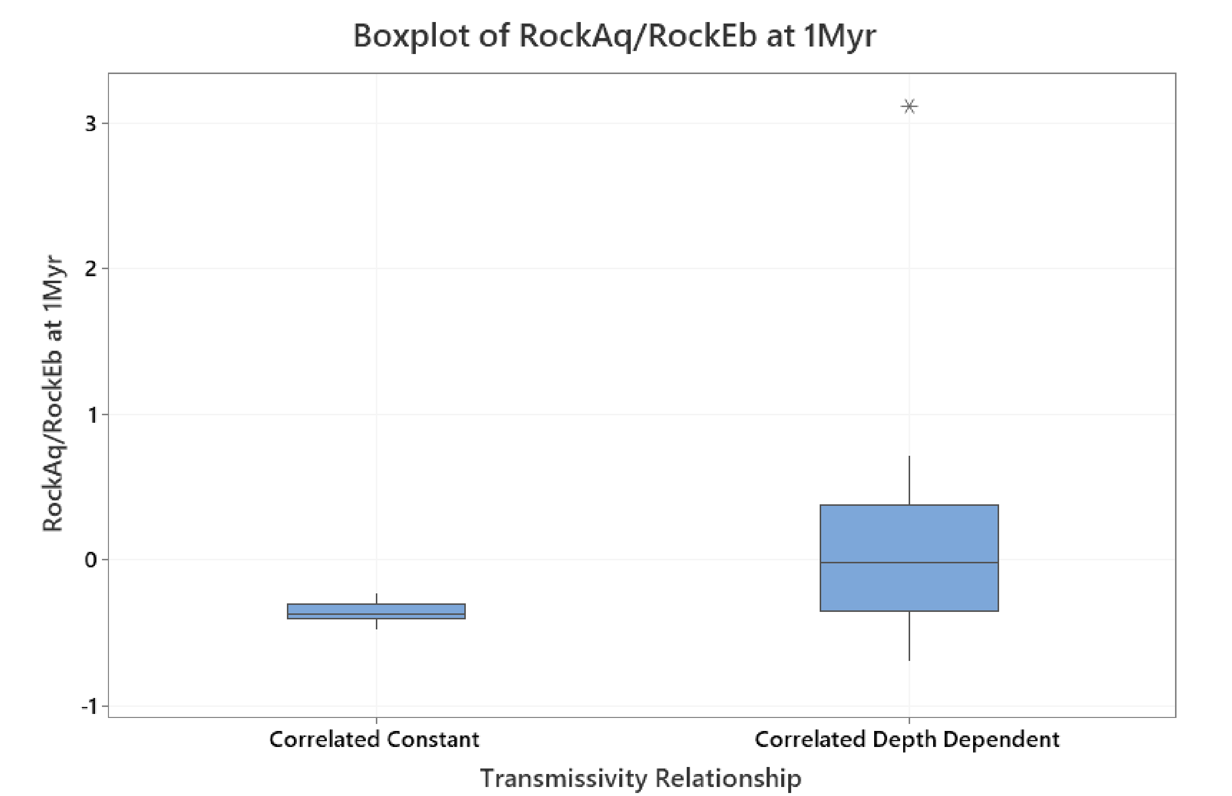




Ratio of the Mass Flow Rate From the Rock to the Aquifer to the Mass Flow Rate From the Rock to the East Boundary at 1 Million Years

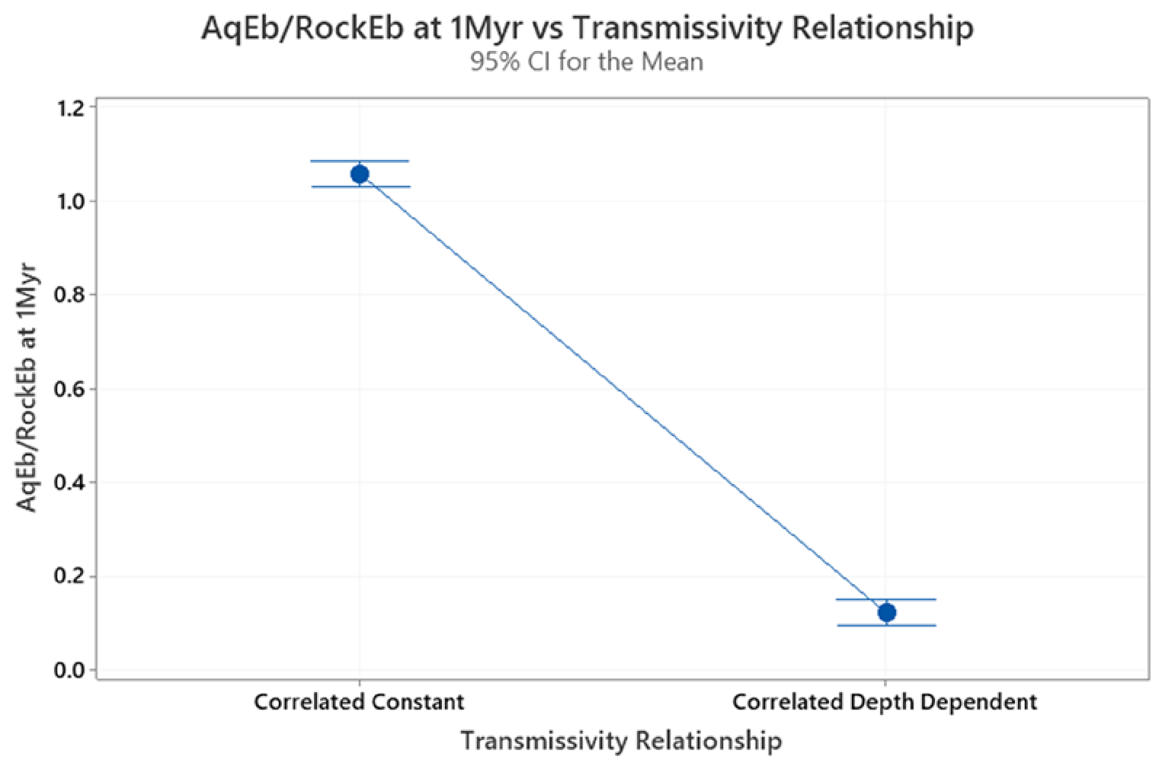
- It is expected that the mass flow from the rock to the east boundary increased for the depth-dependent relationship
- This implies that the flow from the rock to the aquifer increased as well



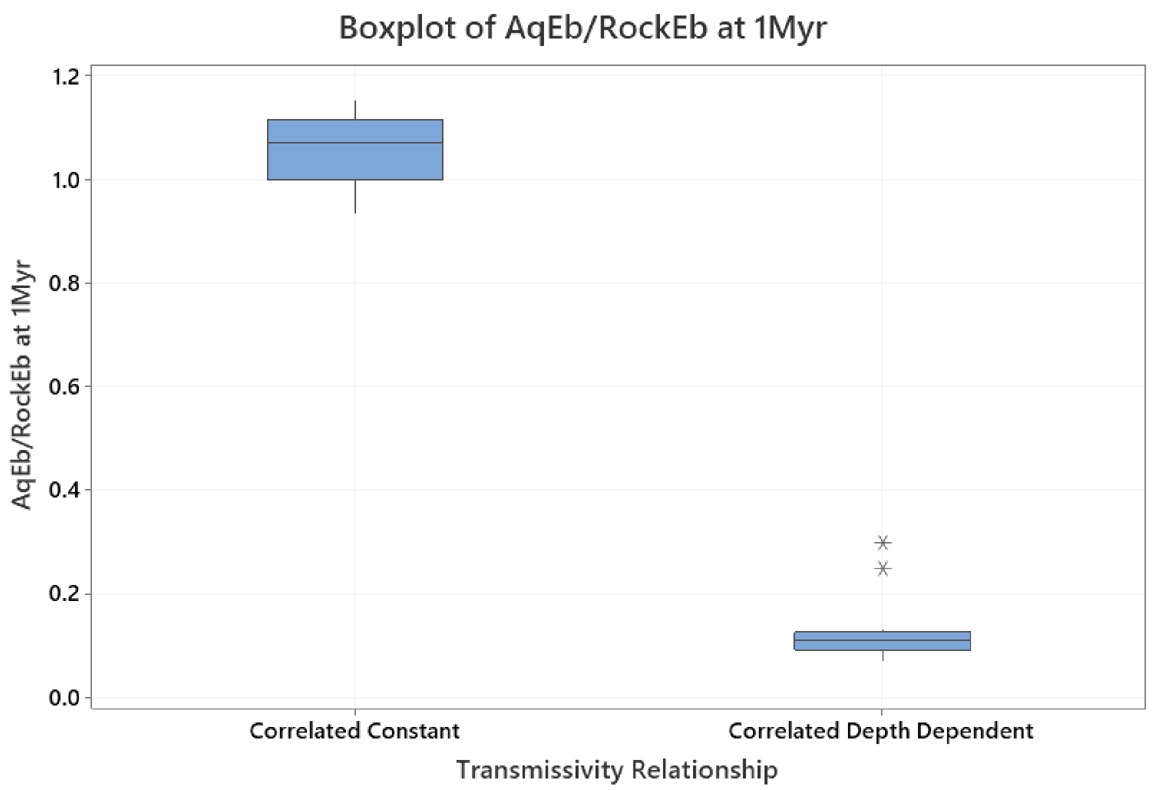


Ratio of the Mass Flow Rate From the Aquifer to the East Boundary to the Mass Flow Rate From the Rock to the East Boundary at 1 Million Years

- Mass flow rate from the aquifer to the east boundary is likely minimally affected
- Mass flow rate from the rock to the east boundary was increased significantly

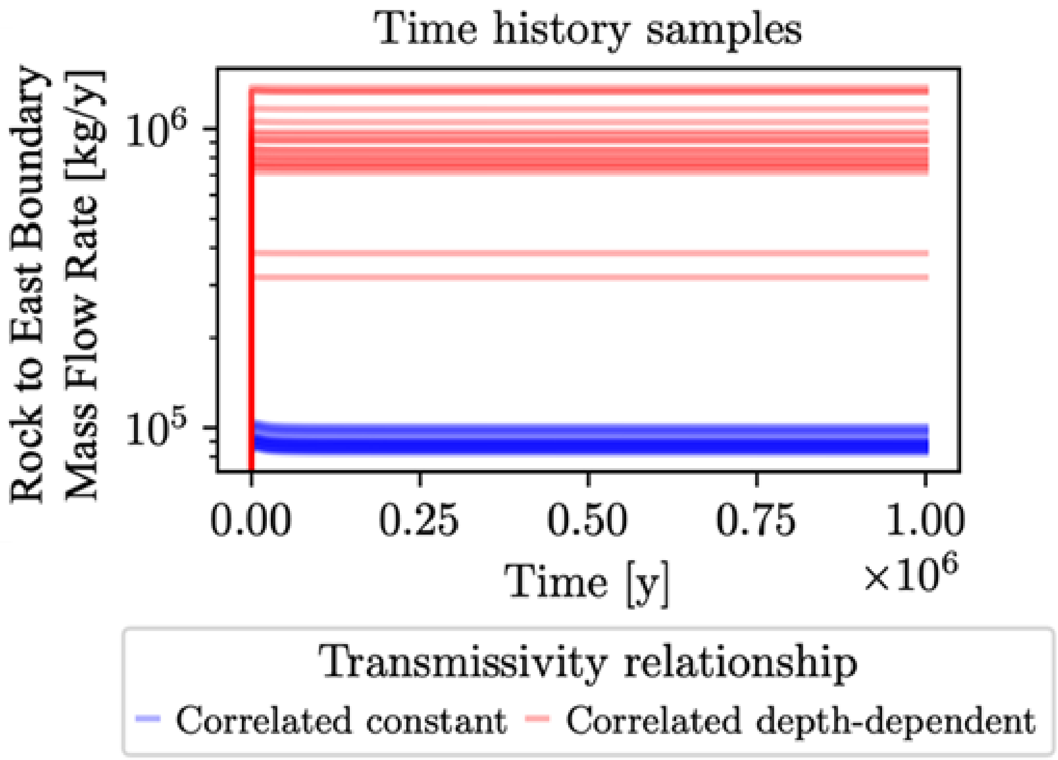


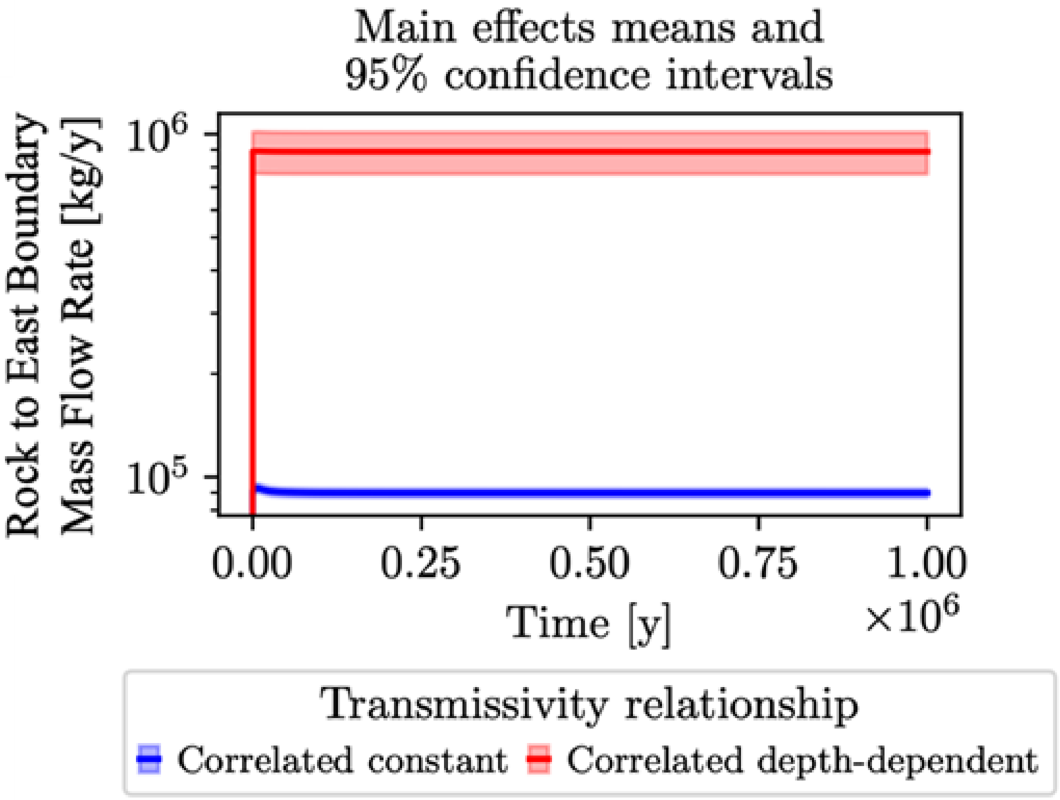
The pooled standard deviation is used to calculate the intervals.



Rock to East Boundary Mass Flow Rate

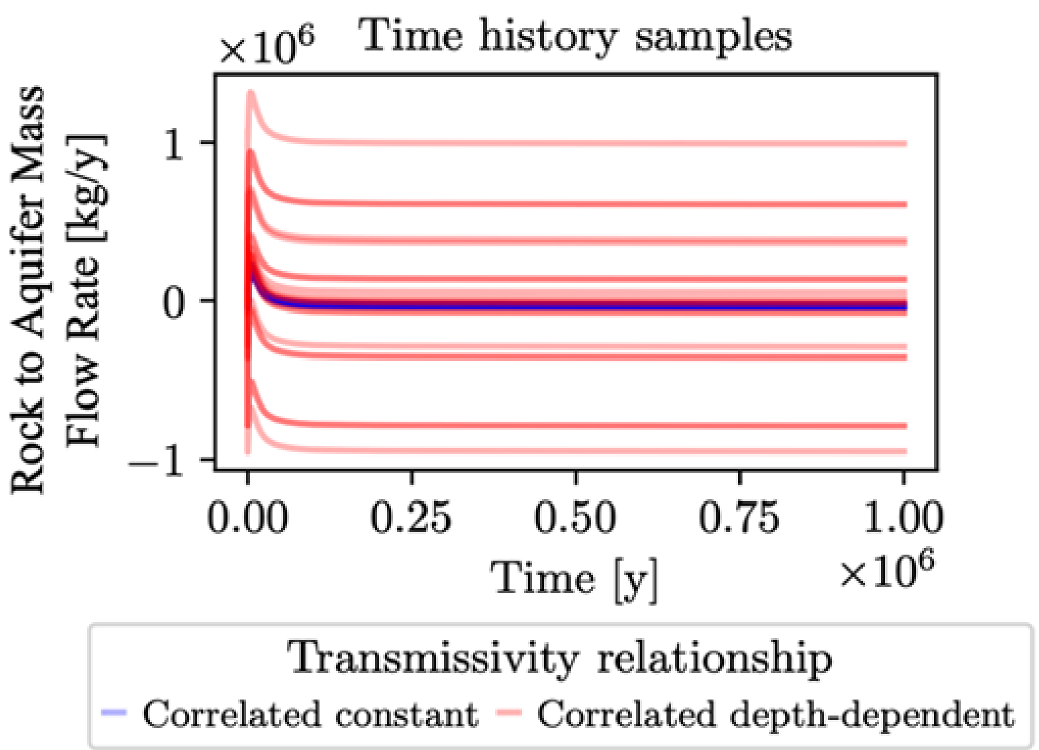
- Mean mass flow rate for the correlated constant relationship is a little less than 90,000 kg/yr while the mean mas flow rate for the correlated depth-dependent relationship is around 1,000,000 kg/yr
- Supports assumptions made earlier

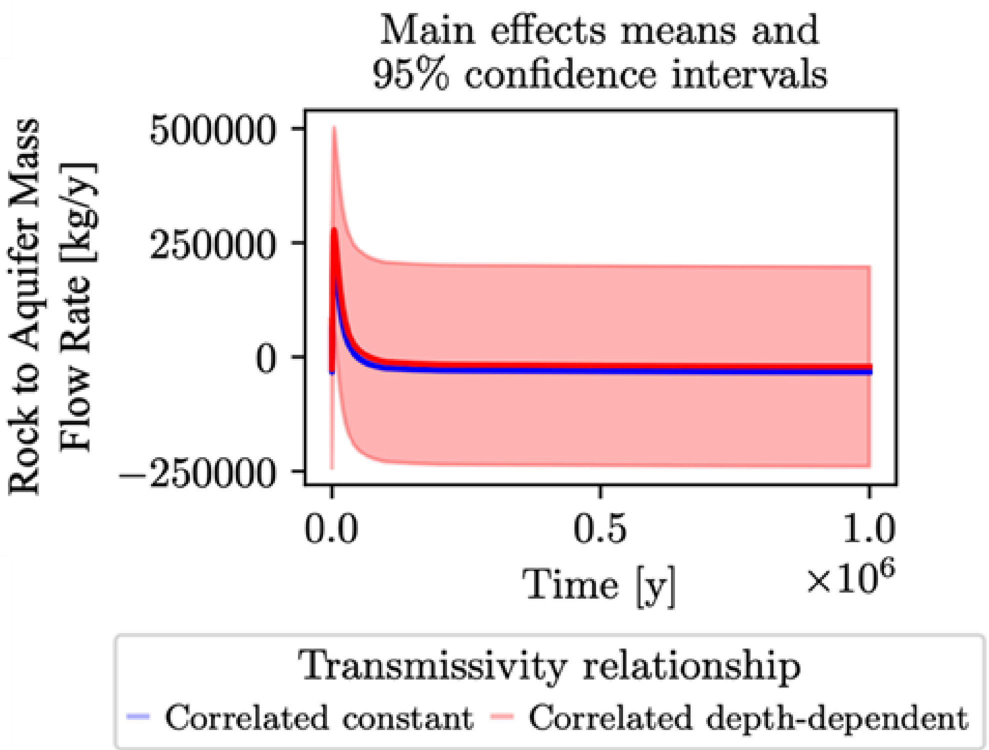




Rock to Aquifer Mass Flow Rate

- Mean mass flow rates are similar for the two relationships
- Correlated depth-dependent mass flow rate ranges from -1,000,000 kg/yr to 1,000,000 kg/yr
- Although there is a considerable range difference, mean values coincide with assumptions made earlier





Conclusions

- The purpose of this study was to determine **if a correlated depth-dependent transmissivity relationship produces a significant change** in the performance quantities for the flow and transport simulations of nuclear repositories in subsurface rock
- Results indicated a statistically significant difference for the **permeabilities of each depth zone and the mass flow rate** from the rock to the east boundary
- The **other QoIs examined showed no statistically significant difference** in means between the two transmissivity relationships **for this small sample set** of DFNS
- The large difference in flow rate from the rock to the east boundary may indicate **increased flushing for the correlated depth-dependent relationship**

Thank you! Questions?

Contact information:

Mariah L. Smith, Geosciences Engineer, Sandia National Laboratories

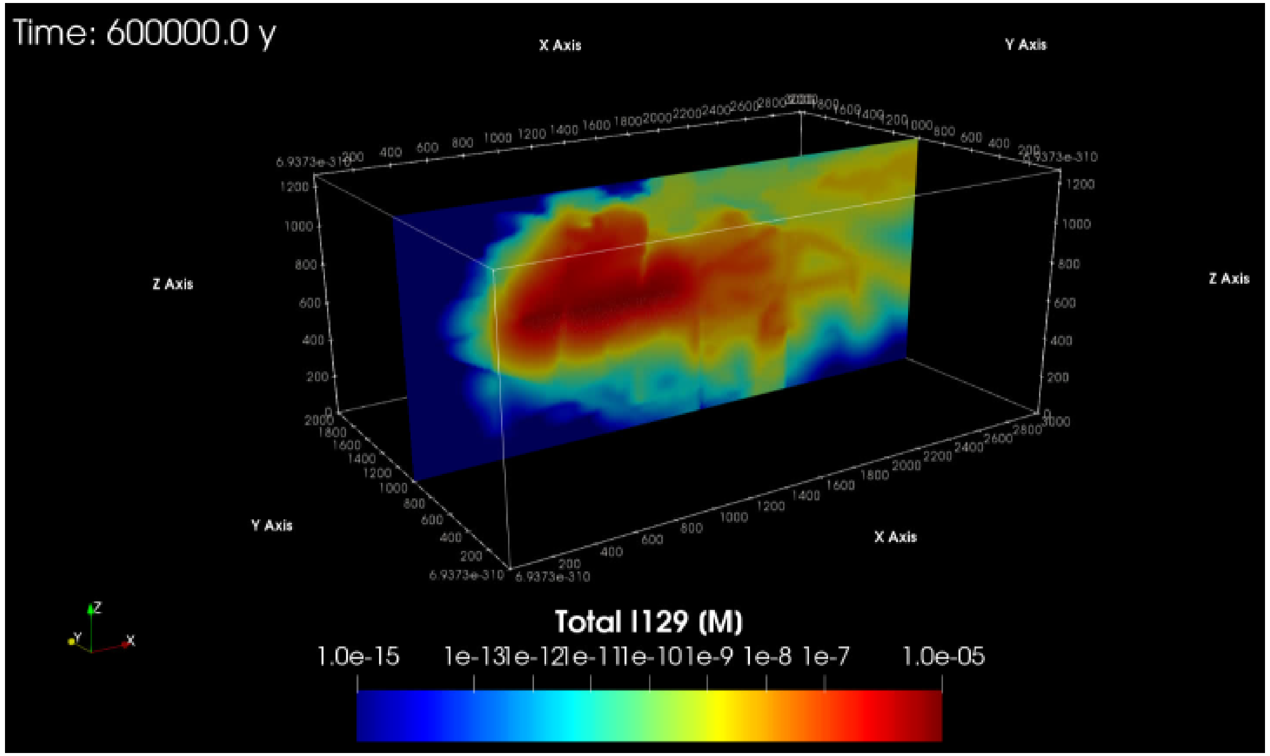
msmith7@sandia.gov

This work contributed to a chapter in a milestone report for the Geologic Disposal Safety Assessment report on UQ/SA: L.P. Swiler, E. Basurto, D.M. Brooks, A.C. Eckert, R. Leone, P.E. Mariner, T. Portone, M. L. Smith and E.R. Stein. "Uncertainty and Sensitivity Analysis Methods and Applications in the GDSA Framework (FY2021)." SAND2021-9903R.

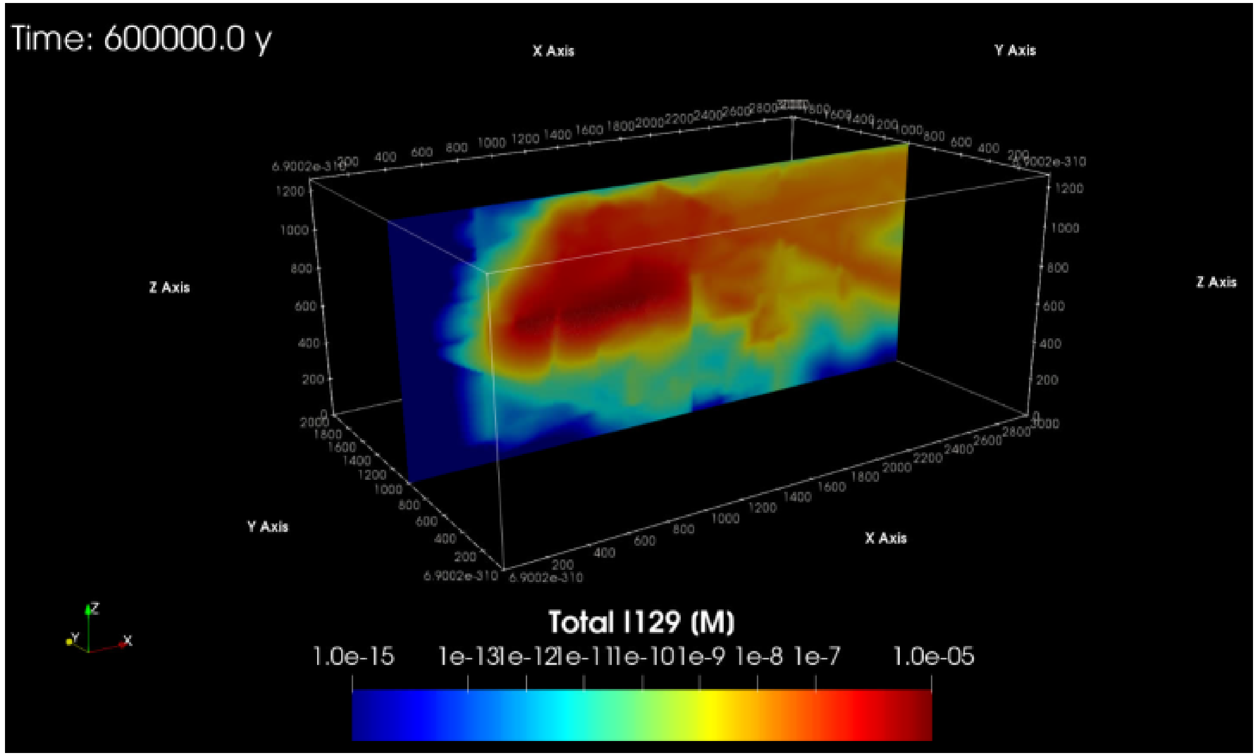
Backup Slides

ParaView Snapshots of ^{129}I movement at 600,000 years

Correlated Depth-Dependent

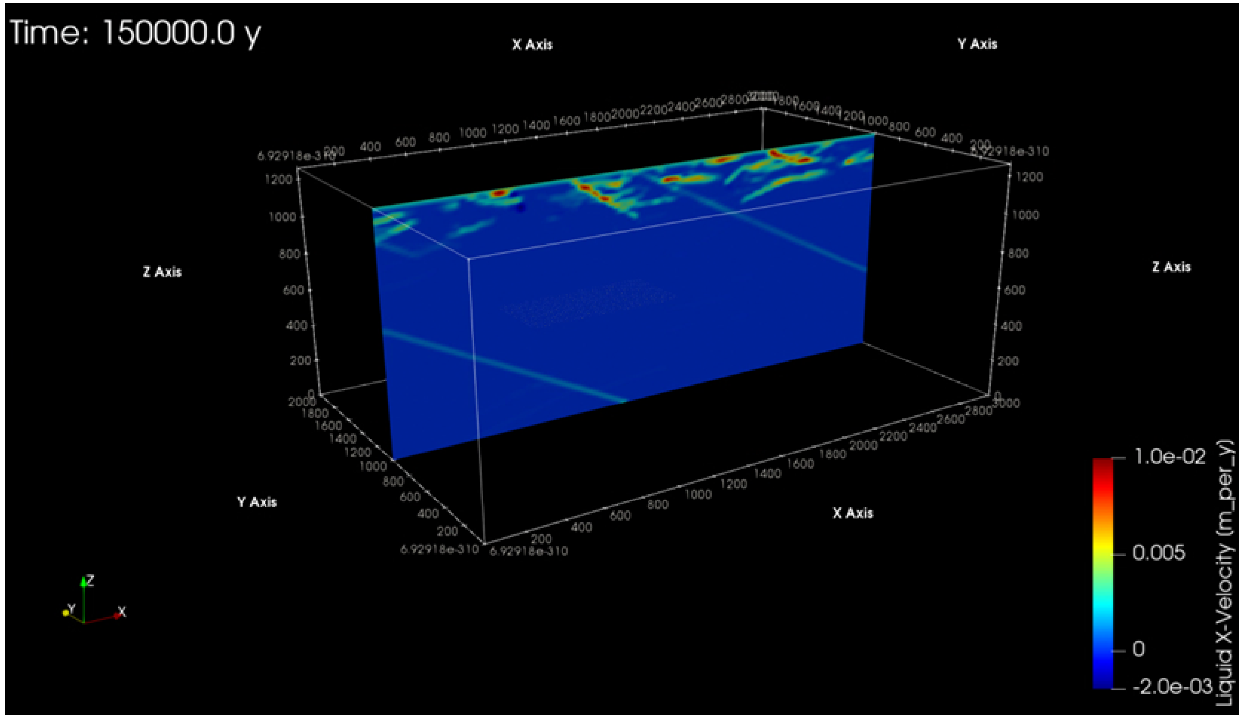


Correlated Constant



Liquid Velocity in the X Direction

Correlated Depth Dependent



Correlated Constant