SAND2022-15665C

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Effects of Discrete Fracture Network Modeling Choices on Repository Performance Characteristics

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International High-Level Radioactive Waste Management Meeting

November 15th, 2022

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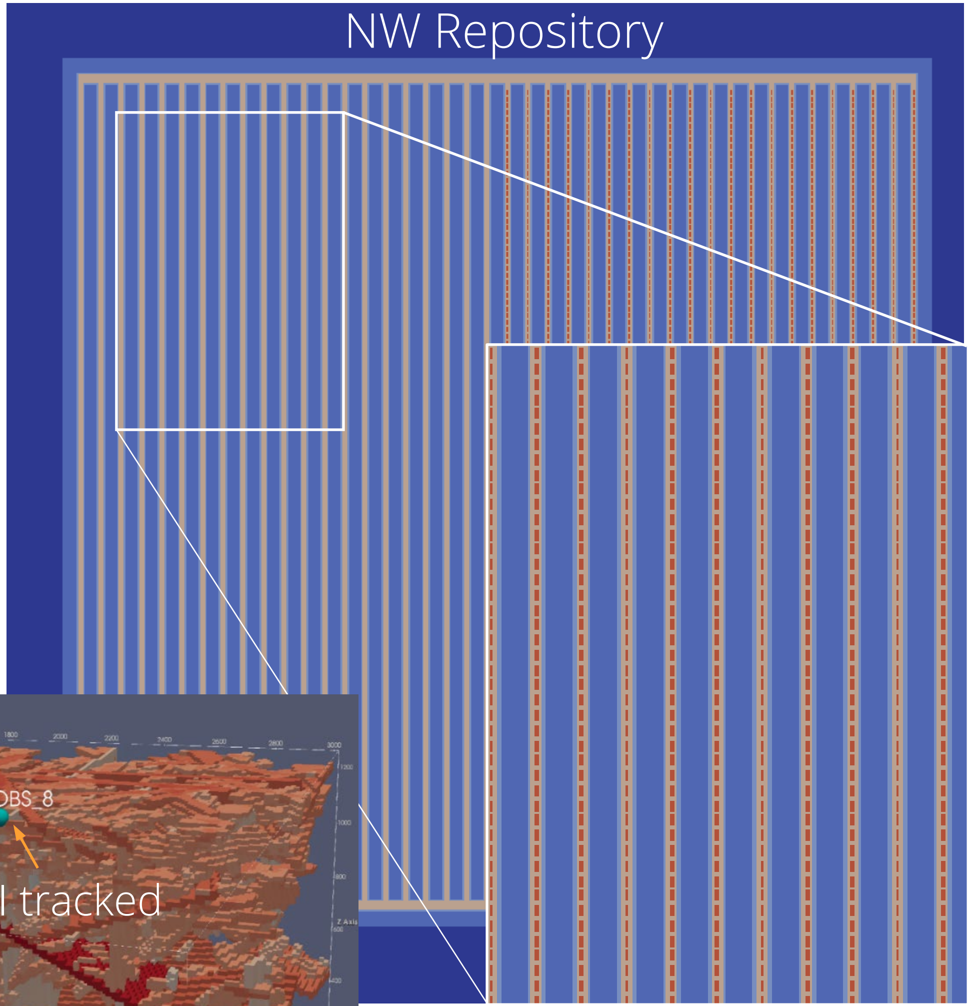
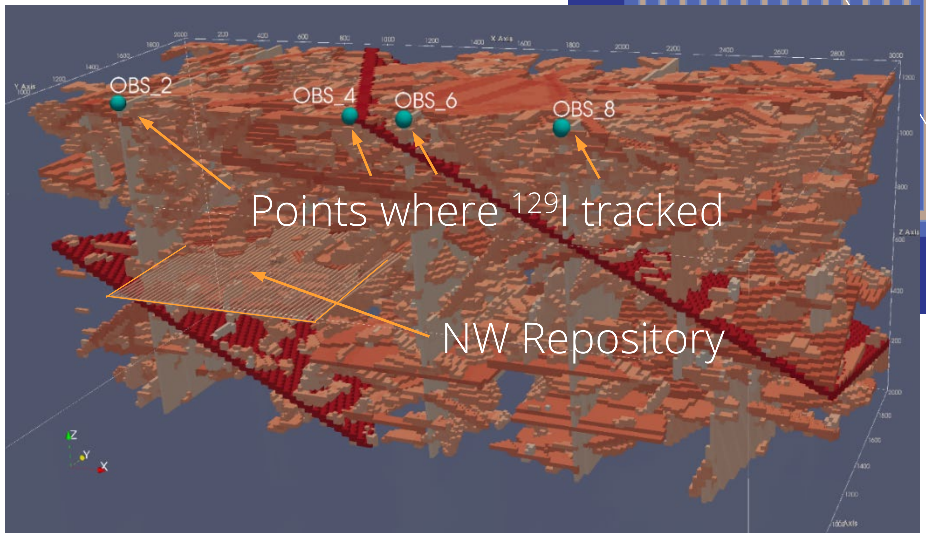
Performance assessment for nuclear waste repository site

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



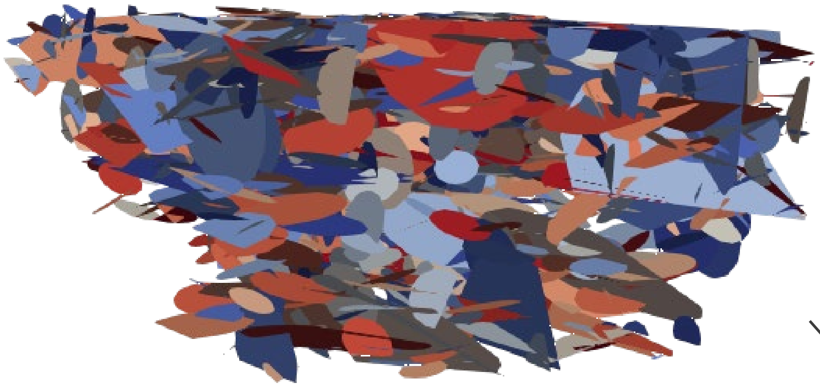
Representing Spatial Uncertainty in Fractured Crystalline Rock

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

Statistical models

DFNWorks

Los Alamos National Laboratory EST. 1943



Discrete Fracture Networks (DFNs)

mapDFN

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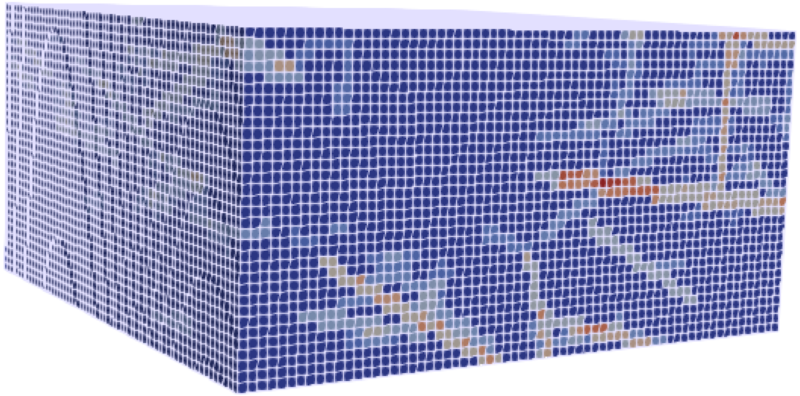
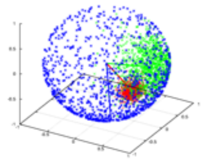


Equivalent Continuous Porous Media (ECPMs)

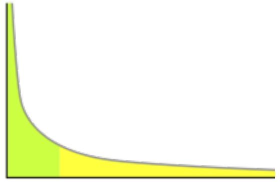
Converting to ECPM[1]

DFNWorks — Los Alamos National Laboratory, EST. 1943

- Generate DFN
  - Orientation: Fisher distribution



  - Radius: Truncated power law



- Assign $T_f = k_f b_f$

Transmissivity (T_f), Permeability (k_f), Aperture (b_f)

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!

[1]Stein, E., J. M. Frederick, G. E. Hammond, K. L. Kuhlman, P. Mariner, and S. D. Sevougian (2017). "Modeling Coupled Reactive Flow Processes in Fractured Crystalline Rock." In Proceedings of the 16th International High-Level Radioactive Waste Management Conference. Charlotte, North Carolina. https://www.osti.gov/servlets/purl/1417242

Overview

- Does fracture transmissivity relationship have a significant effect on repository performance characteristics?
- Two transmissivity relationships
  - Correlated Constant
  - Correlated Depth-Dependent
- Utilizes a crystalline repository reference case that relies on Forsmark data[2]
- Original study was completed last year using a sample set of 20 DFNs[3]
- New study is a continuation of the original with a larger sample set (100 DFNs)

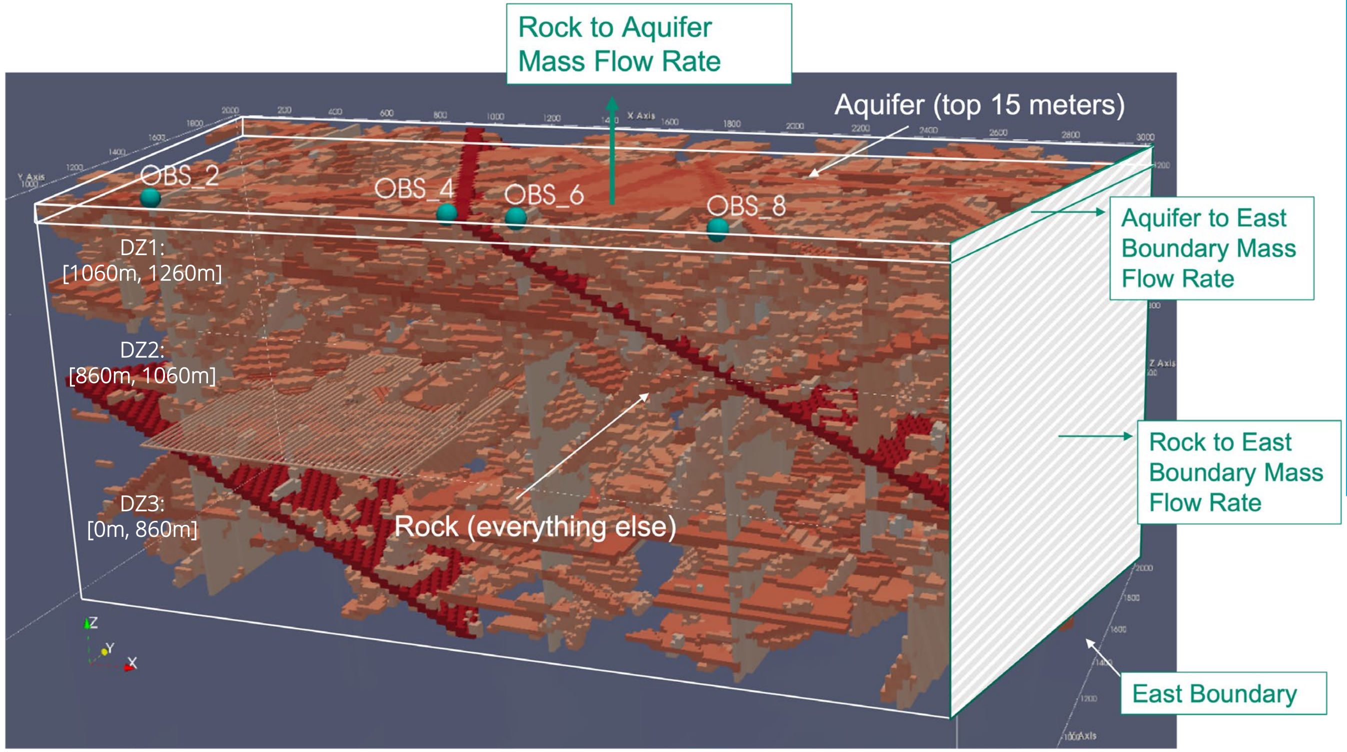
Depth (meters below sea level)	Transmissivity relationship[2]	
	Correlated, $T = ar^b$	
	Constant over domain (a, b)	Depth-dependent (a, b)
0-200	(1.6e-9, 0.8)	(6.7e-9, 1.4)
200-400		(1.6e-9, 0.8)
>400		(1.8e-10, 1.0)

[2] *Joyce, S., L. Hartley, D. Applegate, J. Hoek, and P. Jackson (2014). "Multi-scale groundwater flow modeling during temperate climate conditions for the safety assessment of the proposed high-level nuclear waste repository site at Forsmark, Sweden." Hydrogeology Journal, 22(6):1233–1249.*

[3] *Smith, M., T. Portone and L.P. Swiler (2022). "Effects of Fracture Transmissivity Relationship on Repository Performance Characteristics." In Proceedings of the 3rd International Discrete Fracture Network Engineering Conference. Santa Fe, New Mexico.*

Quantities of Interest

- Compares Quantities of Interest (QoIs) for the two transmissivity relationships to the results of the original study
- New study also compares the correlation between QoIs and various graph metrics



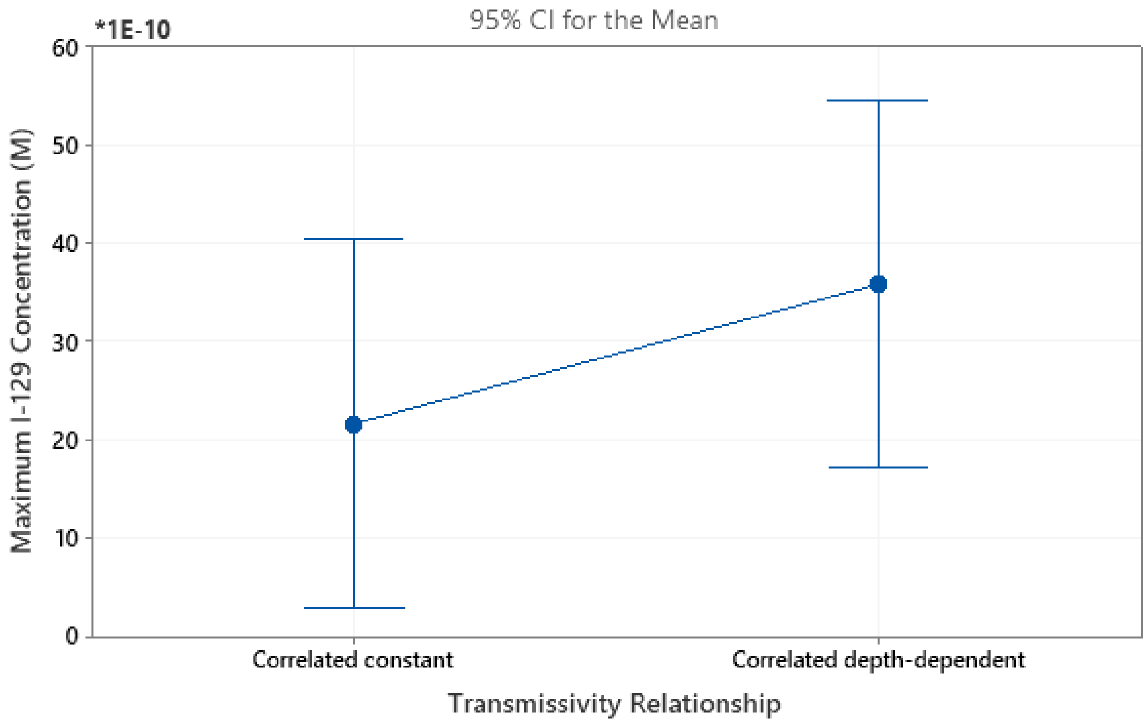
QoIs related to dose	Maximum ^{129}I concentration in Aquifer [M]
QoIs related to repository "leakiness": functions of mass remaining in the repository of a tracer injected at time zero.	• Time when half the tracer is flushed from the repository [yr] • Fraction of the tracer left at 1 Myr • Fractional 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

Quantities of Interest Comparison

Quantity of Interest		Original Study (20 DFNs)	New Study (100 DFNs)
QoIs related to dose	Maximum ^{129}I concentration in Aquifer [M]	No significant difference	No significant difference
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]	No significant difference	Significant difference
	Fraction of the tracer left at 1 Myr	No significant difference	Significant difference
	Fractional mass flux from repository at 3 kyr (mass flux from repository/mass of tracer)	No significant difference	Significant difference
Field-scale flow properties: ratios of mass flow rates at 1 million years.	Rock to aquifer / rock to east boundary at 1 Myr	No significant difference	Significant difference
	Aquifer to east boundary / rock to east boundary at 1 Myr	Significant difference	Significant difference

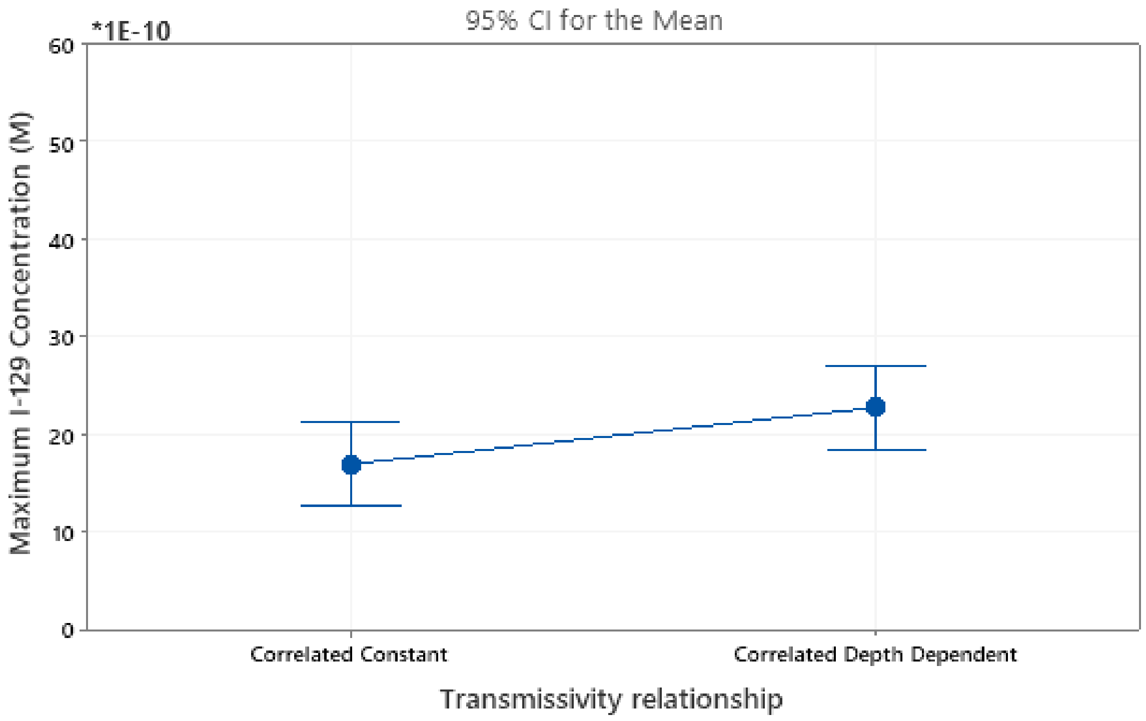
Maximum ^{129}I Concentration in the Aquifer

20 DFN Sample Set



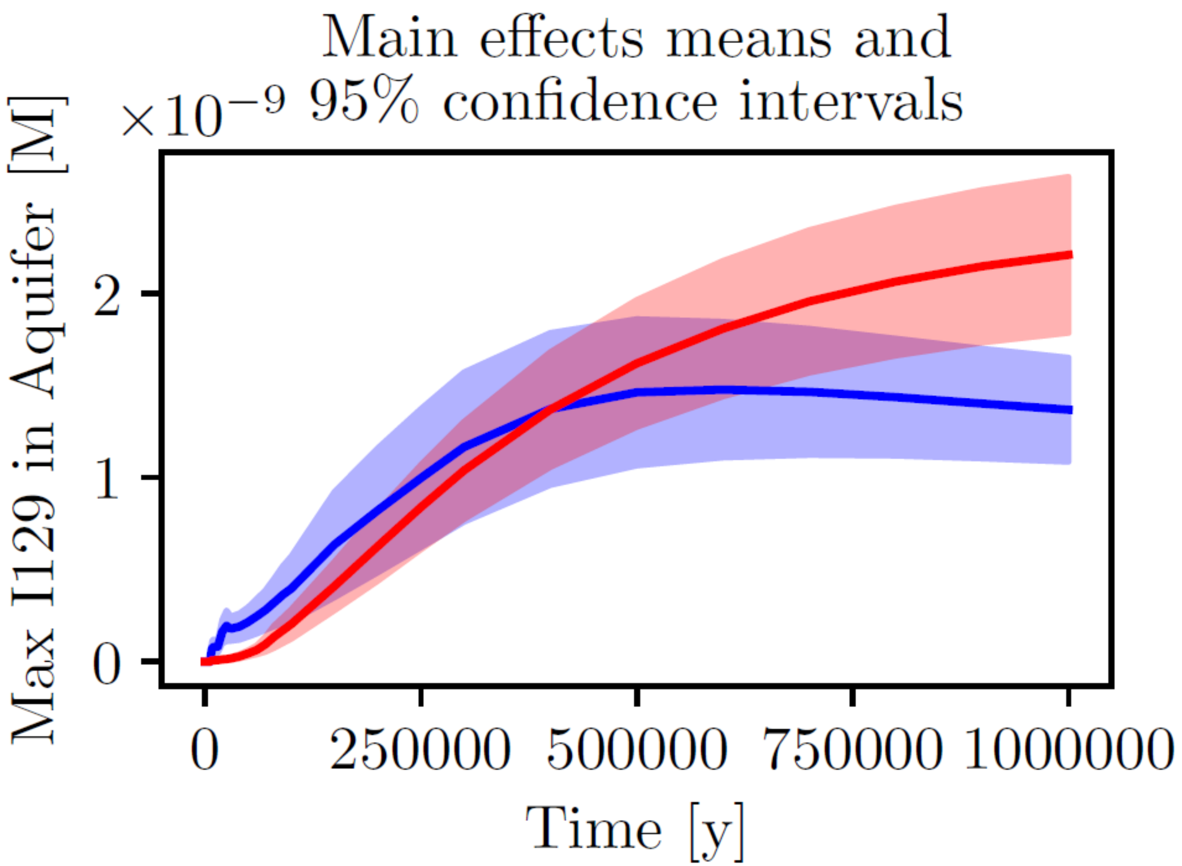
The pooled standard deviation is used to calculate the intervals.

100 DFN Sample Set



The pooled standard deviation is used to calculate the intervals.

Investigating Time History Data



- Peak concentration occurs at:
  - 400,000 years for the correlated constant relationship
  - 1,000,000 years for the correlated depth dependent relationship
- Large overlap of confidence intervals
- Correlated depth dependent continues to rise in concentration over time

Comparison to Graph Metrics

- Graphs constructed using dfnWorks dfnGraph utility and post processing to obtain specific graph metrics were obtained using dfnWorks and NetworkX
  - Average degree (number of intersections a fracture is part of)
  - Number of intersections with repository
  - Number of edges (intersections)
  - Number of nodes (fractures)

- Information related to travel times is calculated using dfnFlow algorithm
  - Shortest travel time
  - Length of shortest path (number of fractures involved in the path of shortest travel time)
  - Average travel time
  - Sum of all travel times

Travel Time Metric Computation

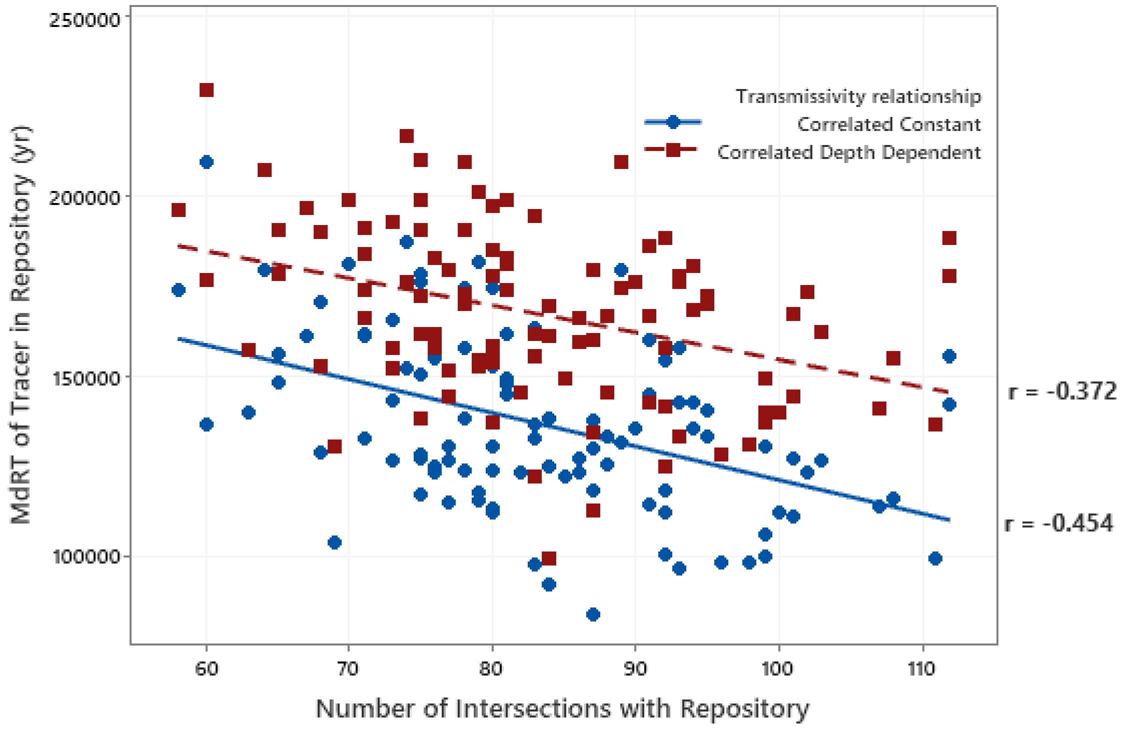
- dfnGraph's flow functionality uses an intersection graph representation
- Weights are assigned to edges (fractures) based on area and permeability of each fracture
- Weights are then used to estimate a flow time between input and output nodes in the graph
- Expectation is for travel time to provide a general ranking of speed with which the fluid can move from the repository to the aquifer

No Significant Correlation Between Graph Metrics and Maximum I-129 in the Aquifer

Graph Metric	Correlated Constant	Correlated Depth Dependent
Average Degree	-0.023	0.104
Density	0.087	0.274
Length of Shortest Path	-0.016	-0.098
Number of Intersections with Repository	0.382	0.116
Number of Edges	-0.163	-0.325
Number of Nodes	-0.125	-0.307
Shortest Travel Time	0.007	0.003
Average Travel Time	-0.065	0.091
Sum of Travel Times	-0.078	0.085

Graph Metric Correlations – General Observations

- Strongest correlations are with respect to number of intersections with repository and sum of travel times but nothing larger than r = 0.45
- Correlated constant relationship had the stronger correlation to number of intersections with repository
- Correlated depth dependent relationship had the stronger correlated to sum of travel times
- QoIs with the highest correlation are:
  - MdRT of spike in repository
  - Fraction of spike in repository at 3 thousand years and 1 million years
  - Fractional mass flux from repository
  - Rock to aquifer/rock to east boundary mass flow rate



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

- Unlike the original study, it was found that **five out of six quantities of interest assessed showed a statistically significant difference** between the two relationships

- The **maximum ^{129}I in the aquifer showed no real correlation with any graph metric** for either relationship

- The **number of intersections with repository proved to be the most useful graph metric** when considering all of the QoIs and the **strongest correlation was seen in the correlated constant relationship**

Thank You! Questions?

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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, and M. L. Smith. "Uncertainty and Sensitivity Analysis Methods and Applications in the GDSA Framework (FY2022)." SAND2022-11220R.