Effects of Discrete Fracture Network Modeling Choices on Repository Performance Characteristics

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INTRODUCTION

There must be post-closure performance assessments to provide reasonable assurance that a generic nuclear waste repository system will achieve sufficient safety and meet the relevant requirements for the protection of humans and the environment over a prolonged period of time [1][2][3]. It is especially important to identify the expected concentration of radionuclides in groundwater and subsurface/waste storage properties that are most important to repository performance. In order to estimate these, many factors are studied with one of the most important being subsurface multiphase flow and transport.

Discrete fracture network (DFN) modeling has become the alternative approach to continuum approaches for simulating flow and transport through sparsely fractured rocks in the subsurface [4]. In this work, DFNs are generated using dfnWorks, a parallelized computational suite developed by Los Alamos National Laboratory [4]. The DFNs are then mapped to an equivalent continuous porous medium (ECPM) using the open-source tool mapDFN, which allows for nuclear waste repository performance assessment simulations of coupled heat and fluid flow and reactive radionuclide transport in both porous media and fractured rock [5]. These simulations are performed using PFLOTRAN, a parallel multiphase flow and reactive transport code [6].

One important modeling choice that must be made for these flow and transport simulations is the fracture transmissivity used to determine the continuum permeability field of the ECPM, as described in [5]. For this study, the application problem is a crystalline repository reference case with host rock properties comparable to the Forsmark site in Sweden [7] and this case initially assumed a single "correlated" transmissivity relationship for the entire computational domain. However, new parameterizations were provided for the correlated transmissivity relationship based on depth [7] and new capabilities in dfnWorks enabled the use of the depth-dependent correlated relationship for the crystalline reference case. Both relationships are defined as:

$$T = ar^{b} \tag{1}$$

where r is the fracture radius, T is the transmissivity, and a and b are parameter values that were fit to data. The difference in parameterizations for the two transmissivity relationships is shown in Table 1.

TABLE 1. Transmissivity relationship parameterizations.

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)

To understand the effect of adding depth-dependence to the transmissivity relationship, this study compares ECPM properties and repository performance quantities of interest for each relationship. The underlying DFN is fixed so that the only difference to the system is the transmissivity relationship.

APPROACH

The work described in this paper is a continuation of work documented in a milestone report for the Geologic Disposal Safety Assessment on UQ/SA [8]. In the original study, it was found that all but one quantity of interest (QoI) showed a statistically significant difference between the two transmissivity relationships and it was therefore concluded that transmissivity relationship did not have a significant impact on repository performance characteristic for the sample of DFNs used. However, since the original study only sampled 20 DFNs in total, there was interest in if a larger sample set might yield different results. Therefore, instead of just 20 DFNs, the analyses described here utilizes a new set of 100 randomly generated DFNs.

The same modeling and data extraction process used for the previous study was used in this analysis and the same QoIs (shown below) were assessed to observe if there were any changes to the initial conclusions.

- Maximum ^{129}I concentration in the aquifer
- Repository median residence time (MdRT) in years

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- Fraction of tracer still in the repository at 1 million years
- Fractional mass flux from the repository at 3 thousand years
- Ratio between the mass flow rate from the aquifer to east boundary and the mass flow rate from the rock to east boundary
- Ratio between the mass flow rate from the rock to aquifer and the mass flow rate from the rock to east boundary

However, this study, unlike the previous one, also compares the specific QoIs above to graph metrics. Graph metrics reflect the topology of the network using a set of nodes connected by edges which can potentially be useful for a comparison such as the one completed in this study since flow and transport is strongly channeled through the fracture network. The graph metrics used in this study are constructed using dfnWork's dfnGraph utility and specific graph metrics were extracted using dfnWorks and NetworkX [9]. When constructing these graph metrics, dfnGraph can create two different types of graph representations based on user preference. The first representation, a fracture graph (which is the one used in this study), treats each fracture as a node and the intersection between them as edges. On the other hand, for intersection graphs, the intersections are treated as nodes and the fractures are the edges. Since the graph metrics just describe the network topology, they can first be used to verify that the behavior of a specific DFN is identical between the two transmissivity relationships. Once it is determined that the DFNs are showing the same behavior, the correlation between QoI and graph metric can be compared between the two transmissivity relationships. The specific graph metrics that were compared to the repository performance QoIs are shown below. These are discussed in more detail in the 2020 GDSA SA/UQ report [9].

- Average degree (average number of intersections a fracture is part of)
- Density
- Length of shortest path
- Number of intersections with repository
- Number of edges (intersections)
- Number of nodes (fractures)
- Shortest travel time

RESULTS

The information shown in the subsequent tables and plots is representative of all 200 cases, 100 for the correlated constant (CC) relationship and 100 for the correlated depth dependent (CDD) relationship: outliers were not removed. Interval plots were used to examine the mean values for each type of data and the associated 95% confidence interval on the means computed over the 100 samples for each relationship. Lack of overlap in the confidence intervals indicates the CDD transmissivity relationship influenced the results significantly.

To compare the correlation between QoI and graph metric, scatterplots and a Pearson correlation was used to compare the level of correlation between a specific QoI and graph metric for the both the CC and CDD cases. The Pearson correlation is simply a measure of linear correlation between two sets of data and the higher the r value to the stronger the correlation. An r value of 1 or -1 means the two data sets of perfectly correlated (whether it is in the positive direction or negative direction) and a r value of 0 means no correlation. In practice, it is generally assumed that a correlation of0.1 to 0.3 (both positive or negative) is considered small, a correlation of 0.30 to 0.50 considered medium, and a correlation of >0.50 to be large.

QoI Comparison

In the previous study, the only QoI to show a statistically significant difference between the two transmissivity relationships was the ratio between the mass flow rate from the aquifer to east boundary and the mass flow rate from the rock to east boundary. As can be seen in Figure 1, it is still not accurate to say the transmissivity relationship is statistically significant for the maximum ^{129}I concentration in the aquifer due to the large and overlapping intervals. However, as can be seen in Figures 2, 3, 4, and 5, there is quite a large difference between the two transmissivity relationships. The repository median residence time, fraction of tracer still in the repository, fractional mass flux from the repository and the ratio between the mass flowrate from the rock to aquifer and the mass flow rate from the rock to east boundary all now show a statistically significant difference between the CC and CDD transmissivity relationship. Based on this, it can be assumed the original set of DFNs (which was a total of 20) was too small to draw concrete conclusions about statistical significance. However, the maximum ^{129}I concentration, which is perhaps the most important QoI, still shows no difference.

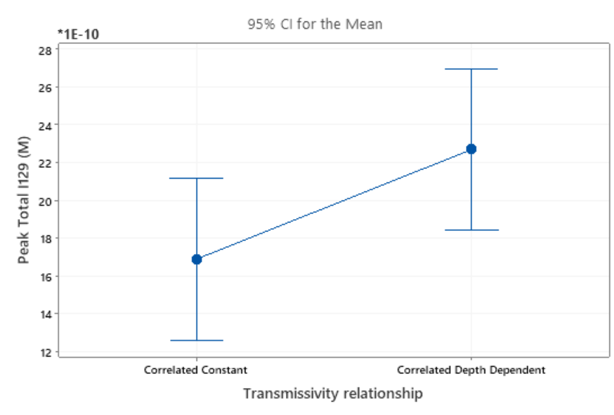

Figure 1. Interval plot for the scaler maximum ^{129}I concentration [M] in the aquifer after 1 million years versus transmissivity relationship.

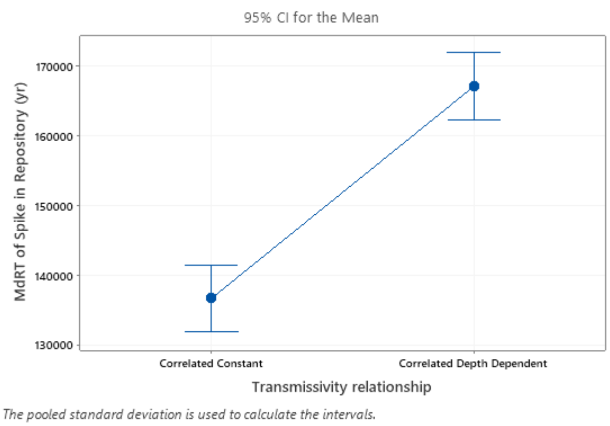

Figure 2. Interval plot for the time when half the tracer is gone from the repository in years versus transmissivity relationship.

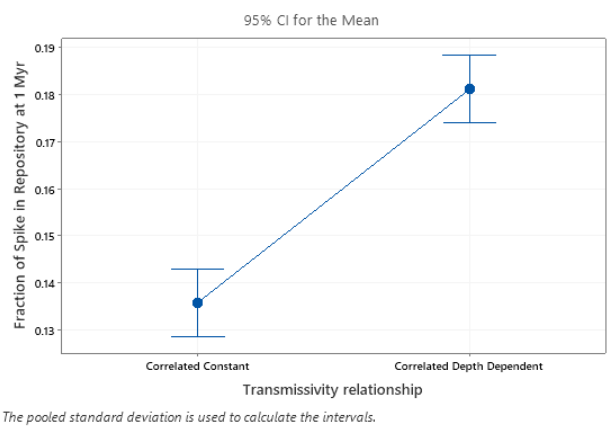

Figure 3. Interval plot for the fraction of tracer still in the repository at 1 million years versus transmissivity relationship.

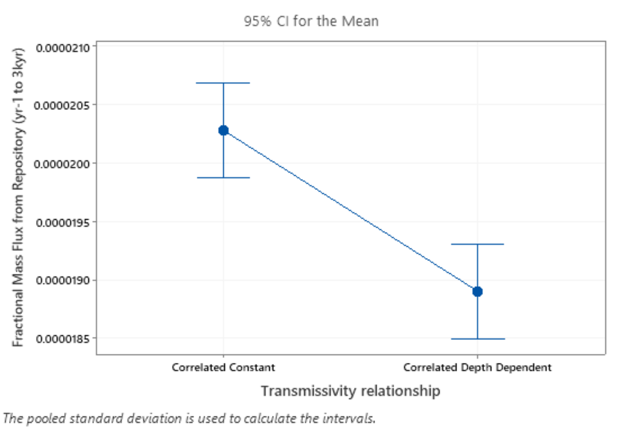

Figure 4. Interval plot for the fractional mass flux from the repository at 3 thousand years versus transmissivity relationship.

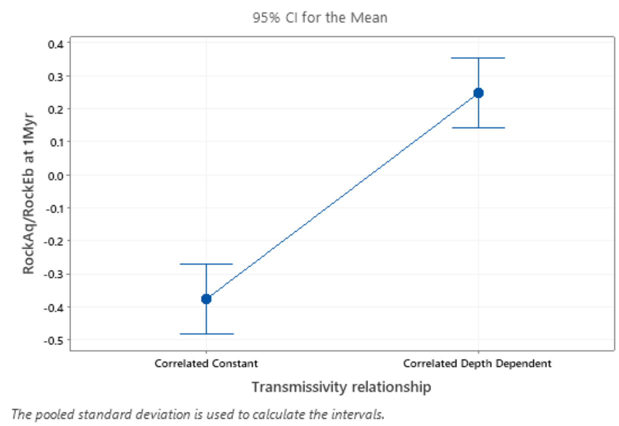

Figure 5. Interval plot for the ratio of the mass flow rates for the rock to the aquifer and the rock to the east boundary at 1 million years versus transmissivity relationship.

Correlation to Graph Metrics

Table 2 below shows the Pearson correlation between the maximum ^{129}I in the aquifer and each graph metric for both transmissivity relationships. There are multiple correlations greater than 0.30 which we deem significant, however no correlation above 0.5 was observed. Additionally, it is interesting to note that the highest correlation for the CC relationship is with the number of intersections with the repository, while the highest correlation for the CDD relationship is the number of edges (intersections).

TABLE 2. Maximum ^{129}I in the aquifer correlation with graph metrics

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

The number of intersections with repository graph metric seemed to have the best correlation with majority of the other QoIs as well. The strongest correlation was with the repository median residence time, fraction of tracer still in the repository at 1 million years, and fractional mass flux from the repository at 3 thousand years. This correlation is shown in Figures 6, 7, and 8 respectively as can be seen in each of the figures the Pearson correlation value is higher for the CC transmissivity relationship in every case.

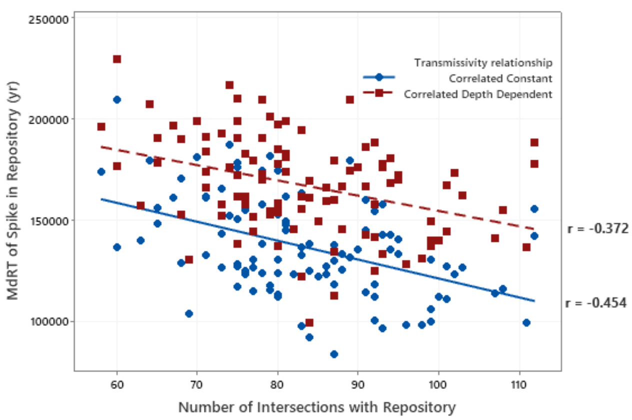

Figure 6. MdRT of spike in repository and number of intersections with repository correlation.

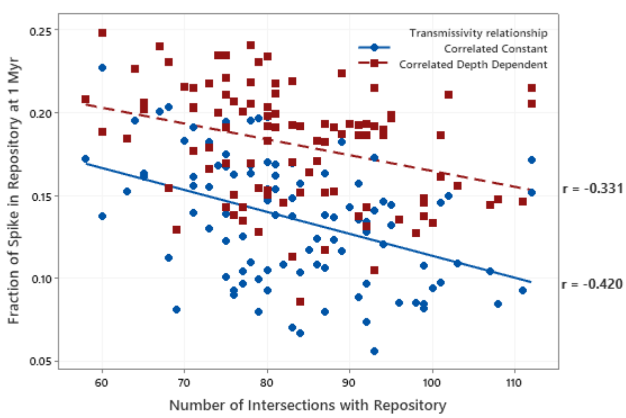

Figure 7. Fraction of spike in repository at 1 million years and number of intersections with repository correlation.

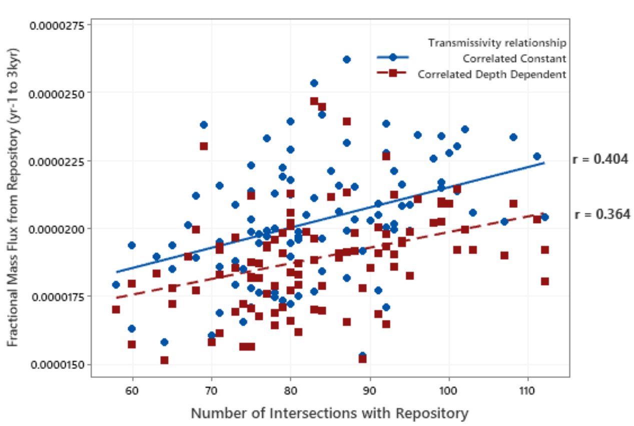

Figure 8. Fractional mass flux from repository at 3 thousand years and number of intersections with repository correlation.

DISCUSSION

In conclusion, the purpose of this study and the original 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. However, the most important QoI, the maximum ^{129}I in the aquifer, showed no real change. In addition to this the maximum ^{129}I in the aquifer showed no real correlation with any graph metric for either relationship. Although we did not see the degree of correlation we had hoped for with respect to the maximum ^{129}I in the aquifer, the number of intersections with repository proved to be the most useful graph metric when considering all of the QoIs. Interestingly enough, the strongest correlation was seen in the CC relationship as well. Additional graph metrics that are well-correlated with performance quantities of interest will be sought in future work.

ACKNOWLEDGEMENTS

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