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Allocating Transmissivities from Constant Head Tests for the Development of DFN Models

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Abstract

Constant head tests are commonly used for field measurements of fracture transmissivity. As a bulk transmissivity is measured for each test section, it is frequently unclear how this transmissivity relates to the hydraulic properties of individual fractures. The goal of this study is to determine if constant head tests conducted at scales larger than the average fracture spacing can be used to generate discrete fracture network (DFN) models that describe transport. The methodology involved generating DFNs using measurements from constant head tests conducted at lengths both above and below the average fracture spacing at a site in Ontario, Canada. Transport predictions from DFNs produced from different scales of hydraulic tests were compared to determine if a method for proportioning larger-scale test results to obtain a DFN representative of the smaller-scale tests could be established. The results of this study indicate that the choice of method used to apportion bulk transmissivities has a significant impact on transport simulations, with a difference in mass arrival of over a factor of two at travel distances less than 50 m. While the most appropriate method is case specific, the error resulting from the choice needs to be considered when using DFN models.

Keywords

Fractures, Constant head tests, Discrete fracture networks, Solute transport

Introduction

Fractures in sedimentary and crystalline bedrock units provide the primary pathways for groundwater flow and contaminant transport. It is well recognized that fractures complicate contaminant migration by allowing for the rapid movement of groundwater through convoluted pathways (Hsieh and Shapiro, 1996; Le Borgne et al. 2006; Neuman, 2005; NASEM, 2015). To understand these pathways and in particular to successfully predict solute transport in fractured rock aquifers, a standard approach is to use numerical models based on discrete fracture frameworks (Chapman et al. 2013; Hyman et al. 2015; Lapcevic et al. 1999; McKay et al. 1993; Pierce et al. 2018; Sudicky et al. 2008). For this to be successful, however, accurate estimates of the physical attributes of a fracture network, including the hydraulic apertures (or transmissivities) of individual fractures, are required (e.g. Golder Associates Ltd., 2010; Neuman, 2005; Parker et al. 2012).

Numerous field methods, such as flow metering, constant head tests, and FLUTE liner profiling can be used for the determination of fracture properties (Price et al. 1980; Frampton and Cvetkovic, 2010; Nastev et al. 2004; Parker et al. 2012; Persaud et al. 2018; Quinn et al. 2011; Quinn et al. 2012). One of the most widely-utilized methods is constant head testing using straddle-packer systems (NASEM, 2015; Novakowski et al. 2007; Quinn et al. 2011). The method involves injecting water into a vertical section of the borehole isolated between two packers at a constant hydraulic head and measuring the resulting flow rates (Ziegler, 1976). These tests thus measure a bulk transmissivity for the entire section tested which are often 2 m or greater in length due to the difficulty and cost associated with smaller measurement scales (e.g. as in Shapiro and Hsieh (1998); Niemi et al. (2000), and Nastev et al. (2004)).

The most significant difficulty with the bulk transmissivities obtained from constant head testing is that a single, large-scale test section (i.e. a larger test interval than average fracture spacing) may include several fractures. Thus, it can be unclear how the bulk transmissivity obtained from tests conducted at scales larger than the fracture spacing relates to that of individual fractures. The bulk transmissivity is composed of the sum of the contributions from the fractures and the matrix (Snow, 1969). Individual fracture identification at < 2 m typically requires either numerous constant head tests at very small scales or the independent interpretation of open fractures from acoustic televiewer or core logs (Hess, 1985; Lemieux et al. 2006; Paillet et al. 1987; Williams and Johnson, 2004). The first method is very costly and has rarely been conducted in practice while the latter often yields uncertainty as to the number of open fractures (West et al. 2005).

The issue of assigning transmissivities from bulk tests to individual fracture features has long been recognized (Snow, 1969; Raven, 1986; Neuman, 2005). In the past, it was common practice to evenly divide a transmissivity among the observed fractures (Maini, 1971). However, it has since been reported that only a small proportion of all fractures observed in core logs will be active (Chilès and Marsily, 1993; Hitchmough et al. 2007; Quinn et al. 2011). Thus, evenly dividing the measured transmissivity is likely not appropriate in most settings.

Numerous advances in determining individual fracture transmissivities from hydraulic tests conducted in large intervals have been made in the last two decades. For example, Novakowski (2000) suggested that the assumption of one active fracture when calculating fracture aperture from bulk transmissivity may be valid. Therefore, the transmissivity of an interval could be converted to an effective single-fracture aperture using the cubic law (Snow, 1965). This would provide the most conservative estimate of contaminant transport as estimated groundwater

velocities would be conservatively high. A multitude of other methods for determining fracture transmissivity have also been proposed.

Hitchmough et al. (2007), for example, used a lognormal distribution for fracture transmissivities to estimate individual values from 3.5 m test sections. The parameters of the distribution, μ (mean), σ (standard deviation), and the proportion of non-connected discontinuities, were obtained using a maximum likelihood method. A Pareto distribution has also been suggested (Gustafson and Fransson, 2006). In this study, parameters of the distribution were determined using log-log plots and the measured transmissivity data. Random transmissivities for each fracture could then be generated using the distribution. Several more qualitative methods of estimating fracture transmissivities have also been proposed. West et al. (2005) assigned the relative probabilities of being permeable to fractures observed in core logs using physical characteristics, such as the weathering surrounding the fracture. In another study, a methodology was developed using a correlation between the critical Reynold's number and fracture aperture to estimate the number of hydraulically active fractures in a test section (Quinn et al. 2011). While each of these methods appear reasonable, there is still no clear consensus on obtaining estimates of individual fracture characteristics without the use of additional hydraulic testing (e.g. flow logs or small-scale constant head tests).

The primary objective of this study is to compare several different, quantitative methods for the use of constant head tests having a test interval of ≥ 2 m to delineate conductive fractures and generate physically representative discrete fracture networks (DFNs) for numerical modelling. The focus of this study is a dolostone unit in southern Ontario, Canada, in which constant head tests from multiple scales (0.5 m and 2 m) in the same rock unit (in the same borehole) have been conducted. By comparing simulations of the transport of a conservative tracer in DFN models

produced using the two scales of measurement, we seek to establish a method for proportioning larger-scale test results to obtain a representative DFN at a site. The simulations have been conducted using a three-dimensional control-volume finite element model which uses a discrete fracture formulation and is based on the standard advection-dispersion equation.

Methods

In this study we first used core logs and transmissivity measurements from constant head tests conducted at 0.5 m intervals in a selected borehole to generate a DFN most likely to be representative of the natural setting surrounding the test borehole. This is based on the assumption (supported by core-log data) that the average fracture spacing is greater than 0.5 m. The probability distributions necessary for this generation were selected by using Kolmogorov-Smirnov tests to evaluate the fits of established functions with established parameters to the measured data. Using the DFN produced, transport of a conservative solute was simulated over a span of 50 m. This result was assumed to be the most representative of natural conditions. The solute distributions were then compared to total mass predictions from DFN models produced using 2 m constant head tests and four distinct methods of determining individual fracture transmissivities from a bulk 2 m value. These methods include evenly apportioning the bulk transmissivity amongst available fractures, using a lognormal distribution to assign fracture transmissivities, using a Pareto distribution to assign transmissivities, and assigning the bulk transmissivity to a single fracture. Finally, to support and corroborate the observations made from the above process, the same procedure was repeated using constant head data from hypothetical boreholes generated using fracture spacing and hydraulic aperture statistics collected from the same dolostone (Novakowski et al. 1999).

Site Description

This study uses constant head test results that have been collected in a previous study at a PCB contaminated site near the town of Smithville in southern Ontario. The tests were conducted in the Eramosa member of the Lockport formation, which is a Silurian-aged fractured dolostone characterized by vuggy features and laminations (Liberty, 1981). At the study site, this unit is overlain by approximately 10 m of till. The geology of the site is described in further detail in Novakowski et al. (1999) and what follows is a short summary of the site information relevant to the present research.

Transmissivity measurements at both a 0.5 m and 2 m test interval have been collected from 11 inclined boreholes distributed within an area of 1 km² at the site. The boreholes are of 96 mm in diameter and range in length from 50-60 m. A total of 384 measurements were collected in the boreholes at the 0.5 m scale and 99 at the 2 m scale. These tests were collected contiguously and were conducted over the same sections of rock (meaning the 0.5 m tests were conducted over the same depths as the 2.0 m tests), allowing for comparison.

Figure 1 shows an example of the transmissivities measured in one borehole (Borehole 59). Contiguous measurements at a 0.1 m interval were also obtained over 4 m in one of the tested boreholes. In general, these results indicate that groundwater flow in the Upper Eramosa is controlled by a few horizontal bedding-plane fractures with large apertures (>500 μm) corresponding to transmissivities of greater than $10^{-5} \text{ m}^2/\text{s}$ (Novakowski et al. 2007; Zanini et al. 2000). Furthermore, the low (0.0001) regional gradient to the south-east, the presence of high transmissivity constant head test intervals that can be correlated over multiple boreholes, and the

appearance of tracer across >100 m distances during previously conducted tracer experiments, all indicate that these fractures may be connected laterally over hundreds of meters (Novakowski et al. 1999; Novakowski et al. 2006).

The mean transmissivity of the 2 m interval constant head tests was $4 \times 10^{-4} \text{ m}^2/\text{s}$ with a standard deviation of $1.8 \times 10^{-3} \text{ m}^2/\text{s}$. The 0.5 m interval data had a mean of $1.5 \times 10^{-4} \text{ m}^2/\text{s}$ and a standard deviation of $1.1 \times 10^{-3} \text{ m}^2/\text{s}$. Note that the difference between the two means will be further discussed later in the methodology. The range of transmissivity measurement which applies to both the 0.5 m and 2 m scales was 10^{-10} to $10^{-2} \text{ m}^2/\text{s}$ (accuracy of approximately half an order of magnitude (Elmhirst, 2011)).

Core logs with detailed descriptions of fracture depths were also collected in each borehole. From the core logs, it was determined that the average vertical spacing of the horizontal fractures is between 0.39 and 0.53 m and can be fit by a power law with $R^2=0.90$ (Novakowski et al. 2000; West et al. 2005). This is shown in Equation (1), where frequency is the proportion of values corresponding to a spacing measured in metres:

$$\text{Frequency} = 8.1123 * (\text{Spacing})^{-1.7695} \quad (1)$$

Because of this spacing, we define the 2 m constant head tests as large-scale (above the fracture spacing) and the 0.5 m tests as small-scale (at or below the fracture spacing). Vertical fractures are also present in the unit. From core logs in the several boreholes that were drilled in the inclined orientation, the average horizontal spacing is 0.77 m and can also be fit using a power law with $R^2=0.75$ (Novakowski et al. 1999). Based on fracture height data collected from a nearby quarry face, the vertical fractures are mostly less than 1m in length, with a mean of 0.68 m and a standard deviation of 0.89 m (Gartner Lee Ltd., 1996). The transmissivities of the vertical fractures

were obtained from 39 constant head tests of 0.5 m length in which only vertical fractures were recorded in the corresponding core log. Most values are between 10^{-6} to 10^{-9} m²/s. There are, however, six values of transmissivity between 10^{-5} - 10^{-4} m²/s, which could represent important, connecting features. With all values included, the mean of the vertical fracture transmissivity was 1.9×10^{-5} m²/s, the standard deviation 0.47 m²/s, and the minimum and maximum were 2.0×10^{-9} and 1.9×10^{-4} m²/s, respectively.

Figure 1: Constant head tests at two scales for the chosen section of Borehole 59. A 10-meter section from elevations of 174.61 m to 182.90 m, which represents 22 m and 12 m depth along the borehole, respectively, was selected for further analysis in this study.

Other relevant site properties include the hydraulic conductivity of the matrix, which has been measured to be between 10^{-9} m/s and a maximum of 10^{-6} m/s using constant head tests conducted at 0.1 m spacing. From 47 measurements at this spacing where no fractures were observed in the core log, the mean K was 10^{-7} m/s and standard deviation was 1.9×10^{-7} m²/s. As

these values are orders of magnitude lower than that of the conductive horizontal fractures, flow in the matrix is considered negligible in this study. Thus, the matrix can be ignored when apportioning transmissivity from constant head tests. The porosity of the matrix was reported to have a mean value of 6.5 % (Novakowski et al. 1999) and does play a role in transport through the fractures via matrix diffusion.

Generation of DFNs from small-scale constant head tests

In order to develop a methodology to determine individual fracture transmissivities from large-scale constant head tests, a ten-meter section from one of the boreholes was first chosen (Figure 1). The segment was selected in such a way that the error in total transmissivity between the different scales of measurement was minimized. This criterion was necessary as amongst much of the data, there were large (>50%) discrepancies between the sum of the 2 m interval tests and the sum of the corresponding 0.5 m interval tests, thus making comparison difficult. This discrepancy arises due to slight errors (± 0.02 m) in positioning of the packers in contiguous tests for both scales of measurement. Even in the selected section, which had the lowest error amongst all of the comparative data, there was a 16% difference in the sum of measured transmissivities between the two scales of measurement. For this section, the error mostly resulted from one 2 m interval in which two adjacent 0.5 m interval tests had equal transmissivities which were also individually equivalent to the corresponding 2 m test. Thus, the cause of this error was likely a slight overlap between test sections at the lower scale, which caused one or more fractures to be measured twice. By eliminating one of the two 0.5 m tests, the error between the two scales is reduced to ~1%.

Core logs and the transmissivity measurements from 0.5 m intervals were next used to generate a simple DFN considered to best represent the hydraulically active fractures in the vicinity of the borehole (Figure 2). The process to do this is summarized in a flow chart shown in Figure 3. This will be referred to as the 0.5-m DFN. Using intervals with measured hydraulic conductivity (transmissivity divided by test section length) greater than that of the largest matrix value (10^{-6} m/s), active horizontal fractures were generated at elevations indicated by the core log. These were assigned apertures calculated using the cubic law and the measured transmissivity. Where the core log indicated that more than one fracture was present in a conductive interval, two end-member scenarios were tested; the first involved assigning all the transmissivity to a single fracture whereas the second allocated it evenly between all observed fractures. For the 10 m interval selected, this only occurred in the 1m span where the overlap error occurred. Four fractures were recorded here.

Figure 2: A DFN generated using transmissivity data from 0.5 m constant head tests. Vertical exaggeration is 5×

Thus, two DFNs were generated, one in which the transmissivity was assigned to just one of the four fractures and another in which the total transmissivity of that 1 m section was evenly divided amongst all four.

For simplicity, all the transmissivity in the selected constant head tests was assumed to belong to horizontal fractures. While this is unlikely the reality, the site has been shown to be dominated by horizontal fractures (see the site description). Additionally, while there is some evidence of a small number of highly transmissive vertical fractures at the site, those represent a small proportion of the measurements. Overall, there wasn't a strong overlap observed between vertical fractures and transmissive intervals across the site. As an example, of the 20 selected constant head test intervals, only 8 had core log evidence of vertical fractures (10 fractures observed). Of these, only one interval with a transmissivity higher than that of the matrix had vertical fractures present. This was the interval with multiple fractures discussed above. These arguments indicate that the error created through this assumption is likely minimal. Furthermore, as this assumption was consistent between the 0.5 m and 2 m scales, the impact on the conclusions is negligible.

Vertical fractures were initially added to the DFN to connect the horizontal fractures using statistics from Novakowski et al. (1999) and Gartner Lee (1996) discussed above. It was found, however, that changes to the vertical fracture properties (length, spacing, transmissivity) had little impact on transport at distances relevant to this study, as a result of the dominant horizontal flow gradients. Even removing the vertical fractures did not have a significant impact on the breakthrough at either observed distance. Because of this, it was concluded vertical fractures had little impact in this study and did not need to be considered further.

Using the DFNs generated above, flow and transport simulations were conducted in a $500 \times 500 \times 10.3$ m domain using a control-volume finite element model (Therrien and Sudicky, 1996). This model was selected for this study because it uses measurable physical properties for the matrix and fractures and can represent the complex geology at the Smithville site. The domain size was chosen to prevent the solute from interacting with the boundaries. For flow, constant head boundaries were used at two edges of the domain (left and right) to maintain the measured regional hydraulic gradient of 0.0001. The other sides were set as no flow boundaries. To simulate tracer migration, a tracer with properties like that of an inert dye was added at a constant concentration of 1 g/L to the entire upstream boundary of the domain. Again, the other boundaries were set as no flux. The initial concentration in the domain was 0 g/L. In order to achieve appropriate discretization for accurate simulation of matrix diffusion around the fracture, the block dimensions

Figure 3: A flowchart of the process involved in creating DFNs from the 0.5 m interval transmissivity data and core logs.

(element sizes) were optimized by reducing the minimum and maximum block sizes until the transport solution did not vary visually. This resulted in vertical discretization having blocks that were 700 μm in thickness adjacent to the horizontal fractures and coarsening outwards to 0.5 m by a factor of 2 following the methods suggested by Kozuskanich et al. (2012), and Weatherill et al. (2008). Horizontally, blocks of 0.7 x 0.7 m were used. At the three edges of the domain where solute was not inserted, the horizontal discretization was coarsened to larger (5 m) elements for computational efficiency. This coarsening did not have any visual impact on transport at relevant distances to this study, likely due to the distance between the observation points and the edges of the domain.

The mass of tracer in each fracture at 20 m and 50 m distance from the injection boundary was recorded for each simulation using inspection points located centrally (i.e. at 250 m) along an axis transverse to flow. The masses in the fractures at each distance were then summed vertically to obtain a total mass as a function of time. The masses in the rock matrix were negligible. The distances were chosen such that sufficiently developed breakthrough curves could be observed without the need for hydraulic gradients higher than what was observed at the site. Horizontal fractures are assumed to be continuous over distances of >50 m in this study, as previously discussed. The total simulation time was 115 days. The free-water diffusion coefficient was chosen to agree with what was used by Novakowski et al. (2004). The dispersivity was chosen to agree with values reported by Gelhar (1992) and Zhou et al (2007) for this scale. Other relevant parameters for the simulation (Table 1), such as matrix porosity, are arithmetic averages from field and lab measurements obtained at the site (Novakowski et al. 1999).

Generation of DFNs from large-scale constant head tests

DFNs comparable to those generated from the 0.5 m interval test data were developed using the constant head tests conducted with 2 m packer intervals in the same 10-m section (Figure 4). These will be referred to as 2-m DFNs. In the creation of these DFNs, the vertical spacing of the horizontal fractures was determined through random generation from the measured distribution reported previously. The horizontal lengths and matrix properties were identical to those of the 0.5-m DFNs. To obtain fracture transmissivities, four different methods of dividing the 2 m test transmissivities were tested. These are listed below.

Figure 4: DFNs produced using four different methods of dividing measured 2m interval transmissivities. **a:** Transmissivity divided evenly. **b:** One fracture placed in each 2m interval. **c:** Lognormal distribution. **d:** Pareto distribution. Vertical exaggeration in the figure is $5\times$

- Bulk transmissivity was divided evenly amongst generated fractures within the interval (Figure 4a).

- Transmissivity was assigned to a single fracture placed in the center of each interval (Figure 4b). When a single fracture per interval was used, the vertical position was not found to have an impact and thus the center of the interval was chosen for simplicity.
- A lognormal distribution was used with the measured mean and variance for 2 m interval constant head tests (see site description) to randomly generate transmissivity values for fractures (Figure 4c). The random generation was repeated in a loop for each 2 m test section until the sum of the generated fracture transmissivities was within a 10% error margin of the measured transmissivity.
- Apportioned measured transmissivities with a Pareto distribution (Figure 4d). The parameters of the Pareto distribution were determined from a log-log plot as described by Gustafson and Fransson (2006). Random generation from this distribution was repeated using the same methodology as for the lognormal distribution.

Note that for each case listed, fractures with apertures below approximately 100 μm were removed in post-processing because of their minimal impact on transport and to increase the computational speed. This threshold was selected as it corresponds to a hydraulic conductivity of $1 \times 10^{-6} \text{ m/s}$.

Mass transport was then simulated through the DFNs and the total mass crossing a point at the 20 m and 50 m thresholds in the fractures was calculated in the same way as previously discussed. The discretization, boundary conditions, and matrix properties of the domain were identical to those of the 0.5-m DFN simulations. For each method used for dividing transmissivity, the DFN creation and transport simulation procedure were repeated in a Monte Carlo approach until the mean and variance of the breakthrough curves stabilized ($\pm 5\%$). This resulted in

approximately 40 simulations for each method used to apportion transmissivity. Finally, the mean curve and the inter-quartile produced from the 2-m DFNs at 20 m and 50 m were compared to the breakthrough curves produced from the DFNs produced by constant head tests at 0.5 m test intervals to determine which apportionment method produced similar transport characteristics to the DFN generated from the small-scale constant head tests.

Comparison to Hypothetical Scenarios

As it is noted that the preceding exercise is based on one field example out of a virtually infinite number of examples in nature, additional exploration of both the method and other possible network arrangements is needed. To further evaluate the different methods for dividing transmissivities, additional scenarios with different hypothetical distributions of conductive fractures were used. This was also undertaken to avoid the error between scales in the constant head test data collected from the field. In this case, hypothetical core logs and 0.5 m interval tests were generated along with corresponding 2 m constant head test data derived from these tests. This was completed by first using random spacing and fracture aperture distributions to generate a hypothetical 2-D DFN with a 10 m height and 50 m length (Table 2). The power law in Equation (1) was used for spacing. Fracture aperture statistics were obtained by isolating 0.5m interval constant head tests with 1 fracture recorded and using the cubic law to calculate apertures. A Kolmogorov-Smirnov test was used to evaluate the fit of the resulting data to a lognormal distribution. A fit was not rejected at 95 % confidence, and the calculated p-value was 0.15. Thus, a lognormal distribution with a mean transmissivity of $4.9 \times 10^{-4} \text{ m}^2/\text{s}$ and a standard deviation of $2.1 \times 10^{-3} \text{ m}^2/\text{s}$ was used to generate transmissivities for each fracture.

Each hypothetical DFN was then used to generate constant head test results by vertically summing the transmissivities of the 0.5 m and 2 m intervals. The hydraulic conductivity of the matrix was simply assumed to be 1×10^{-8} m/s for this. The positions of each fracture were also recorded. Finally, the methodology described in the previous two sections was then repeated to compare the transport properties of a DFN produced using small-scale tests to those of DFNs produced using 2 m interval tests. For this study, three hypothetical DFNs were generated, which are listed below.

- One (Case #1) was selected because of its similarity to the measured section examined in this study (Figure 5). In particular, most highly conductive fractures were situated in different 2 m intervals for both the measured data in BH59 and the first hypothetical case.
- The other two DFNs (Cases #2 and #3) were chosen to have more closely spaced fractures (i.e. multiple conductive fractures in each 2 m interval). This allowed for the comparison between different methods of dividing transmissivities for cases where there was more than one conductive fracture in each 2 m test interval.

Each case was selected to avoid containing multiple fractures in any one 0.5 m length interval of high transmissivity ($>1 \times 10^{-4}$ m²/s) in order to prevent the associated uncertainty in the 0.5 m DFN.

Figure 5: Transmissivities produced from the hypothetical constant head test generation. In Case #1, the spacing of the fractures considered to be highly conductive is sparse, with an average spacing of less than one per 2 m interval. Case #3 represents a more closely spaced generation, with multiple fractures in each 2 m interval.

Results

Comparison of Simulated Transport from 0.5m and 2m Measurements at BH59

Results from the simulation of mass transport through generated 0.5-m DFNs at two selected times are shown in Figure 6. This figure displays the full simulation domain of 500 m and includes the inspection distances of 20 m and 50 m. Little to no interaction of the solute with the domain boundaries was observed. Note that variation of the horizontal fracture positions also had negligible impact on the breakthrough curves.

Figure 6: Cross-sectional view of the HydroGeoSphere transport simulation results at two different times. The 20 m and 50 m observation planes are shown as red lines. Vertical exaggeration is approximately 25×

Figure 7 shows the mass breakthrough curves for transport through the 0.5-m DFNs and the 2-m DFNs produced by the various methods of apportioning the constant head test results. Each curve represents the cumulative total tracer mass crossing the observation planes with changing

time. The results at both 20 m distance and 50 m distance from the source are shown. As discussed in the section above describing the generation of fracture networks from the small-scale measurements, there was uncertainty regarding the number of conductive fractures in one of the 0.5 m intervals. Therefore, two curves are presented for the 0.5-m DFN to represent the end-member cases. The simulation in which transmissivity was assigned to one of the four fractures in the uncertain interval is referred to as the upper bound as it represents the upper limit on transmissivity for a single fracture in the relevant interval. The other, in which transmissivity was evenly divided amongst the four fractures, is referred to as the lower bound.

The DFN created using the 0.5 m interval constant head data from the chosen interval contained between 5 and 8 fractures conductive enough to be distinguished from the background. Of the conductive fractures, only 2-3 contributed significantly to transport. In contrast to this, 17 fractures were observed in the core log for the same interval. This supports the conclusions of previous results seen in the literature that only a small proportion of observed fractures contribute to flow (i.e. Chilès and Marsily, (1993)). Note that the fractures which controlled transport corresponded to intervals with transmissivities greater than $1 \times 10^{-4} \text{ m}^2/\text{s}$ (equivalent aperture = 550 μm), which is why intervals with transmissivities of this magnitude are referred to as highly conductive in this study.

For the 2-m DFNs, the mean curve of the Monte Carlo simulations and the inter-quartile range (IQR) are shown in Figure 7. Note that for the single fracture case, only a single curve is shown because there was no need to use a Monte Carlo approach to assign transmissivities to a single fracture.

Figure 7: Comparison of mass breakthrough curves from generated 0.5-m and 2-m DFNs. Results at 20 m distance are shown on the left and results at 50 m distance are on the right. The plot labelled as **a** is the even division of transmissivity, **b** is the single fracture, **c** is lognormal, **d** is the results using a Pareto distribution. The inter-quartile range (IQR) for the 2-m DFN simulations is also shown in grey.

Significant differences in the arrival times and late time masses were observed between the 0.5 m and 2 m scales for the even division of transmissivity (Figure 7a). At 50 m distance, the 2-m DFNs estimate arrival times more than 10 days later than that of the 0.5-m DFNs. Allocating the

transmissivity to one fracture provided a breakthrough curve that closely follows the most conservative estimates of the 0.5-m DFNs. Dividing the transmissivity according to a lognormal distribution also provided significantly improved estimates of mass relative to the even division (Figure 7c). This was anticipated as, based on the results of a Kolmogorov-Smirnov test at 95% confidence, a lognormal distribution was not rejected for the measured 2 m interval constant head test transmissivities ($p = 0.64$). A lognormal distribution also fit the 0.5 m constant head test data ($p = 0.23$). The Pareto distribution provided similar mass estimates to that from the lognormal distribution, especially at early times where the differences between the means were less than 0.01 g (Figure 7d).

While using a single fracture in each 2 m interval produced breakthrough curves similar to those from the 0.5-m network in this instance (Figure 7b), this would not necessarily be the case at locations with multiple transmissive features in each interval. Furthermore, the error between the observed 0.5 and 2 m transmissivity measurements created uncertainty in how successful the different methods of dividing transmissivity were at simulating transport. This is why additional transmissivity distributions considered possible at the site were generated using the method outlined previously.

Hypothetical Case Simulations

The first hypothetical case (Case #1) had a similar transmissivity profile to the BH59 data in that the highly conductive fractures ($>1 \times 10^{-4} \text{ m}^2/\text{s}$) were sparse ($>2 \text{ m}$ spacing). The results of transport simulations at 20 m distance in DFNs generated from the generated 0.5 m and 2 m transmissivity values are shown in Figure 8. Simulations at 50 m distance are included in an appendix (Appendix A) but are not displayed here as they show the same trends. As there was no

uncertainty in the 0.5-m DFN, it is represented by 1 curve here. Furthermore, as with Figure 7, the single fracture case only has one curve as it was not necessary to run in a Monte Carlo format.

Figure 8: Transport simulation results at 20 m distance for different methods of dividing transmissivity in Case #1. Plots a to d represent the same scenarios as in Figure 7.

The results of this case agree with what was observed with the measured data. At early times, the even division of transmissivity causes significant underestimations of masses while overestimating by approximately a factor of 2 at late times. Visually, the single fracture method matches the 0.5-m curve extremely well, which would be expected, as in this case, there was no more than one conductive fracture per 2 m interval. The right-tailed distributions provided inter-quartile ranges that were once again similar to one another and to the single fracture method. In this case, the Pareto distribution provided estimates that were a closer match to the 0.5-m results than the lognormal distribution at 20 m distance from the source. These observations were quantified using a root mean squared error (RMSE) estimate between the 2-m mean curve and the 0.5-m curve (Table 2). Agreement was observed between these results and the description above.

While the previous cases had extremely sparse fractures, Cases #2 and #3 have multiple highly conductive fractures in each 2 m interval that remain consistent with measurements of spacing and transmissivity from the site. While two cases were run, only one will be presented here as the conclusions from the results of the two sets are the same. As with the previous figure, Figure 9 displays the inter-quartile ranges and mean breakthrough curves for the transport simulations resulting from different methods of dividing the 2 m constant head tests and from the 0.5 m constant head tests.

Figure 9: Breakthrough curve results for different methods of dividing transmissivity in Case #3 at 20m distance. Plots a to d represent the same scenarios as in Figure 7.

The results from this case are contrary to those from the measured data and Case #1 (Table 3). The use of a single fracture to divide 2 m interval transmissivities resulted in significant mass underestimates (RMSE = 0.0272 g at 20 m). This could be expected with multiple fractures in a single interval. The lognormal and Pareto methods of transmissivity assignment, however, did not

fare significantly better, with both underestimating masses even at the 75th percentile. Once again, the mean estimates provided by each right-tailed distribution were within 0.01 g of one another at early times and thus considered not significantly different. While the difference increased at later times (>70 hours), it was still small relative to the differences between the two curves and the 0.5-m breakthrough curve. With an IQR of approximately 0.075 g at late times, evenly dividing transmissivity amongst generated fractures produced the largest range of possible breakthrough curves. However, the mean curve had the lowest RMSE with the 0.5-m curve (RMSE= 0.0031 g at 20m). Thus, this was the best fit estimate in this scenario. Table 3 displays a complete set of RMSE values for the curves in Figure 9.

Discussion and Conclusions

As shown above, the choice of transmissivity allocation method has a significant impact on mass transport predictions. In this study, the mass breakthrough curves produced by evenly dividing transmissivity were more than a factor of two less than the predictions based on the use of a single fracture. At other sites with more closely spaced fractures, the observed differences in breakthrough predictions could be even larger than reported here. These cases could not be examined in this study due to a lack of necessary transmissivity or core log data needed for DFN generation.

The distances (20 and 50 m) explored in this study are short in comparison to the typical transport distances at a contaminated site (e.g., NASEM, 2015). By examining transport at larger distances (200 m) via several simulations representing different methods of dividing transmissivity from Case #1, however, it was observed that differences in predictions observed at 20 m were not eliminated with distance (Appendix B).

Note that the groundwater system at Smithville has a strong horizontal advective component, with multiple horizontal fractures having apertures over 500 μm . However, the results of this study are still applicable to geologies in which matrix diffusion plays a more important role, such as sedimentary units with smaller fractures. Matrix diffusion only retards advective mass transport and therefore the choice of method for proportioning transmissivity would still be important.

Based on our results, no method was determined to be generally more suitable than any other, notably even at a single study site. Despite using consistent fracture spacing and the same transmissivity distribution from which to generate fractures, two different cases needed different methods of dividing transmissivity to successfully match the respective 0.5-m DFNs. Where conductive fractures were spaced at intervals of greater than 2 m, a single fracture for each interval had the lowest RMSE when compared to the 0.5 m interval data. Conversely, for a spacing of less than 2 m, evenly dividing the 2 m transmissivities resulted in the lowest RMSE.

The differences between the predictions in the various cases highlight the need for considering potential error created by the method of assigning bulk transmissivities to discrete features, especially for sites where the spacing of conductive fractures is potentially less than the constant head test interval. In these scenarios, to determine if the test spacing is less than or greater than the spacing of conductive fractures and thus obtain a truly representative estimate of the transport processes, additional detailed hydraulic measurements as described above are required.

Where no further measurements are possible, the potential error could be incorporated into DFN models by using the even distribution and single fracture approaches of apportioning transmissivity as endmembers. The even division of transmissivity represents a lower bound for the maximum aperture in an interval, and thus an upper bound on the breakthrough time at an

observation borehole some distance away. Conversely, using a single fracture provides the highest aperture possible and therefore represents faster breakthrough. Note that while many cases will have a fracture spacing that is denser than the constant head test interval, at sites where the spacing is less than the constant head test interval, it is most appropriate to assign the transmissivity of the interval to a single fracture.

For every case examined, neither the use of a lognormal or a Pareto distribution produced estimates with the best match to the 0.5 m interval data (i.e. the true representation), even though the transmissivity data collected from the site best fits a lognormal distribution. Furthermore, as the methods based on the two distributions produced estimates of mass that were mostly between that for a single fracture and that for even methods of dividing transmissivity, neither distribution provided a better constraint on the possible error. Neither method was therefore determined to be useful for estimating individual fracture properties from a bulk value. Other distributions may have performed better, but as little evidence could be found in the literature for their use, they were considered outside the scope of this study.

Based on the results and the discussion above, the following conclusions are drawn from this study:

- This study highlights the difficulty in obtaining accurate estimates of transmissivity or aperture size for individual fractures from constant head tests where more than one fracture may contribute to the test.
- This research also further corroborates previous work indicating that only a small percentage of observed fractures play a role in flow and transport.
- Even when taking measurements at small scales well below the average fracture spacing (i.e. 0.1 m or 0.5 m), potential overlap in the measurement intervals can lead to significant

errors in determining the true transmissivity of a section, which further complicates any interpretation of the results.

- The choice of method used to apportion bulk transmissivities has a significant impact on mass transport results, with a factor of two or greater difference in simulated mass from different methods observed for these fracture properties over transport distances of as short as 20 m.
- None of the four distinct methods of assigning transmissivity that were examined were found to be the most suitable in every case. Where conductive fractures were spaced at intervals greater than the test spacing, assigning the transmissivity to a single fracture was the most appropriate method. Conversely, for cases in which the conductive fractures were spaced at distances less than the test spacing, evenly dividing the measured transmissivities provided the best results.
- The use of a lognormal or a Pareto distribution to generate DFNs provided mass estimates that were not the closest fit to the 0.5-m breakthrough curves in any of the tested cases. They were also unable to provide additional constraints on the range of possible breakthrough curves relative to those provided by the single fracture and even methods of transmissivity designation.
- Based on our results, error resulting from uncertainty in dividing bulk transmissivity needs to be incorporated into DFN models if they are to be used for predictive analysis or interpretation of observed transport, particularly if matrix porosity is small or if the transport time is long. More work is still required to carefully quantify the cut-offs for the transport times and matrix porosities at which the error produced becomes less significant.

- The results also emphasize the importance of additional hydraulic measurements at a site (beyond large-scale constant head tests), that can be used to identify the properties of individual fractures and to establish the spacing of conductive fractures.

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Tables

Table 1: Parameters used in the simulation of tracer migration through generated DFNs. Support for the values used is provided in the text above.

Parameter	Value
Longitudinal Dispersivity	1 m
Horizontal Transverse Dispersivity	0.1 m
Matrix Hydraulic Conductivity	1×10^{-8} m/s
Free-water Diffusion Coefficient	5.5×10^{-10} m ² /s
Porosity	7 %
Hydraulic Gradient	0.0001
Tortuosity	0.1
Bulk Density	2570 kg/m ³

Table 2: RMSE values for hypothetical Case #1. Calculated by comparing the error between the mean of the 2-m simulations for each method and the 0.5-m curve.

Method	RMSE at 20 m (g)	RMSE at 50 m (g)
Single Fracture	0.0003	0.0001
Even	0.0271	0.0133
Lognormal	0.0089	0.0051
Pareto	0.0045	0.0052

Table 3: RMSE values for hypothetical Case #3. Calculated using the same method as in Table 2.

Method	RMSE at 20 m	RMSE at 50 m
Single Fracture	0.0272	0.0111
Even	0.0031	0.0033
Lognormal	0.0220	0.0120
Pareto	0.0244	0.0112

Figure Captions

Figure 1: Constant head tests at two scales for the chosen section of Borehole 59. A 10-meter section from elevations of 174.61 m to 182.90 m, which represents 22 m and 12 m depth along the borehole, respectively, was selected for further analysis in this study.

Figure 2: A DFN generated using transmissivity data from 0.5 m constant head tests. Vertical exaggeration is 5×

Figure 3: A flowchart of the process involved in creating DFNs from the 0.5 m interval transmissivity data and core logs.

Figure 4: DFNs produced using four different methods of dividing measured 2m interval transmissivities. **a:** Transmissivity divided evenly. **b:** One fracture placed in each 2m interval. **c:** Lognormal distribution. **d:** Pareto distribution. Vertical exaggeration in the figure is 5×

Figure 5: Transmissivities produced from the hypothetical constant head test generation. In case #1, the spacing of the fractures considered to be highly conductive is sparse, with an average spacing of less than one per 2 m interval. Case #3 represents a more closely spaced generation, with multiple fractures in each 2 m interval.

Figure 6: Cross-sectional view of the HydroGeoSphere transport simulation results at two different times. The 20 m and 50 m observation points are shown as red lines. Vertical exaggeration is approximately 25×

Figure 7: Comparison of mass breakthrough curves ranges from generated 0.5-m and 2-m DFNs. Results at 20 m distance are shown on the left and results at 50 m distance are on the right. The plot labelled as **a** is the even division of transmissivity, **b** is the single fracture, **c** is lognormal, **d** is the results using a Pareto distribution. The inter-quartile range (IQR) for the 2-m DFN simulations is also shown in grey.

Figure 8: Transport simulation results at 20 m distance for different methods of dividing transmissivity in Case #1. Plots a to d represent the same scenarios as in Figure 7.

Figure 9: Breakthrough curve results for different methods of dividing transmissivity in case #3 at 20m distance. Plots a to d represent the same scenarios as in Figure 7.

Appendix A

Masses from the Different Methods of Dividing Transmissivity Observed at 50 m Distance for Cases 1 and 3

The below plots show masses at 50 m from Case #1 (Figure A1) and Case #3 (Figure A2). In the plots, A is the even division of transmissivity, B is the single fracture, C is lognormal, D is the results using a Pareto distribution.

Figure A1

Figure A2

Appendix B

Masses from Four Simulations at 200 m Distance

The plots below display four representative different simulations selected randomly from Case #1. Each represents a different method of dividing transmissivity. The first plot presents mass breakthrough with time at 20 m distance (Figure B1). At 200 m distance, the differences in arriving mass have not been eliminated and grow with time as the breakthrough profile develops (Figure B2).

Figure B1

Figure B2