Evaluating the Effect of Internal Aperture Variability on Transport in Kilometer Scale Discrete Fracture Networks

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Abstract

The apertures of natural fractures in fractured rock are highly heterogeneous. However, in-fracture aperture variability is often neglected in flow and transport modeling and individual fractures are assumed to have uniform aperture distribution. The relative importance of in-fracture variability in flow and transport modeling within kilometer-scale field-scale fracture networks has been under a matter of debate for a long time because the flow in each single fracture is controlled not only by in-fracture variability but also by boundary conditions. Computational limitations have previously prohibited researchers from investigating the relative importance of in-fracture variability in flow and transport modeling within large-scale fracture networks. We address this question by

incorporating internal heterogeneity of individual fractures into flow simulations within kilometer scale three-dimensional fracture networks, where fracture intensity, P_{32} (ratio between total fracture area and domain volume) is between 0.027 and 0.031 [1/m]. A recently developed discrete fracture network (DFN) simulation capability, *dfnWorks*, is used to generate DFNs that include in-fracture aperture variability represented by a stationary log-normal stochastic field with various correlation lengths and variances. The Lagrangian transport parameters, non-reacting travel time and cumulative retention, are calculated along particles streamlines. It is observed that due to local flow channeling early particle travel times are more sensitive to in-fracture variability than the tails of travel time distributions, where no significant effect of the in-fracture transmissivity variations and spatial correlation length is observed.

Key words: *Discrete Fracture Networks, Subsurface flow and transport, Heterogeneity, Advective Transport, Aperture variability, High-performance Computing, Fractured rock*

1 Introduction

Characterizing how individual fracture attributes, e.g., aperture variability and fracture network connectivity and density, influence flow and transport through low permeability rocks in the subsurface is a key question in a variety of energy, defense, and groundwater applications [Berkowitz et al., 2002; Dentz et al., 2004; Gelhar, 1986, 1987]. A variety of computational approaches have been developed to address this challenge including the discrete fracture network approach (DFN), where fractures are explicitly represented and create a network that represents fractured rock [Dershowitz, 1999; Cvetkovic and Frampton, 2012; Hartley and Joyce, 2013; Poteri, 2014]. One

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4 46 advantage of DFN models over continuum based models, such as stochastic continuum
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7 47 and dual/multi permeability models [Neuman, 2005; Lichtner and Karra, 2014; Painter et
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9 48 al., 2002], when investigating flow and transport through sparsely fractured rock is that
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11 49 they can represent a wider range of transport phenomena [Painter et al., 2002; Painter and
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14 50 Cvetkovic, 2005], which in turn can be explicitly linked to fracture network attributes
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16 51 such as densities, size, orientation, and fracture aperture.

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19 52 Various physical processes such as geological stress and strain, chemical
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24 54 fracture. The numerous computational [Tsang and Tsang, 1987; Tsang and Tsang, 1989;
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26 55 Moreno et al., 1988; Moreno and Tsang, 1994], laboratory [Moreno et al., 1985; Keller et
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28 56 al., 1999], and field studies [Neretnieks et al., 1985; Bourke, 1987] of flow in single
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31 57 fracture have demonstrated that internal fracture aperture variability results in fracture-
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33 58 scale flow channeling that impacts transport properties. Tsang and Tsang [1987]
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35 59 suggested that flow within a fracture plane could be considered as a series of parallel one-
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37 60 dimensional “flow tubes” due to flow channeling. Bourke [1987] observed similar flow
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40 61 tubes in an in situ experiment of flow through a fracture plane. Computational studies of
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42 62 channeling phenomena [Larsson et al., 2012; Larsson et al., 2013; Moreno et al., 1988;
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44 63 Tsang and Tsang, 1989] investigated how spatial correlation length and hydraulic
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46 64 conductivity effect on transport within a single fracture. Larsson et al. [2012] considered
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48 65 a spatial correlation length of applied heterogeneity in a range between 2% and 18% of
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50 66 the flow domain width and concluded that the transport behavior was independent of the
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52 67 correlation length in the considered range. It has been observed that increasing standard
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54 68 deviation of conductivity distribution the flow channeling width decreases, i.e., flow
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channel intensity increases due to conservation of mass [Larsson et al., 2012; Moreno and Tsang, 1994]. However, it is still poorly understood how the parameters, such spatial correlation length and conductivity variance, effect on transport when single fractures are incorporated into a complex interconnected fracture network. In such networks, there are multiple scales of heterogeneity, both between fractures and within a fracture, that influence transport properties.

Another concern in studies of in-fracture variability within an individual fracture is the application of the unrealistic boundary conditions for flow, which limit the usefulness of the results in field-scale applications. Specifically, flow in an individual fracture is not controlled solely by aperture variability. It is also determined by the fracture's position within the network; fluid may only enter and exit a fracture where it intersects with other fractures in the network. This limited connectivity has been shown to result in network-scale flow channeling within fractures even if the parallel plate approximation is used, e.g., [Aldrich et al., 2015; Hyman et al., 2015c]. Proper characterization of the relative importance of these two types of channeling mechanisms – internal aperture heterogeneity-induced or network geometry-induced – in transport processes requires a DFN simulator that can include heterogeneous fractures embedded within a kilometer-scale three-dimensional DFN, where network geometry is strongly pronounced. There have been previous attempts to study the influence of in-fracture variability on transport [Painter, 2006; Nordqvist et al., 1992], but they were limited by a lack of reliable numerical tools for modeling particle transport in large-scale fracture networks. While the one-dimensional pipe-network approximation for transport modeling [Cacas et al., 1990; Dershowitz and Fidelibus, 1999] is computationally efficient, its

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4 92 application to three-dimensional fracture network is limited because it disregards explicit
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6 93 details of three-dimensional particle transport. Recently, de Dreuzy et al. [2012] studied
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9 94 the effect of internal aperture heterogeneity on the effective permeability of a large DFN,
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12 95 but they did not consider transport. The authors found that there are couplings between
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14 96 flow heterogeneities at the fracture scale and flow heterogeneities at the network scales.
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16 97 A consequence of these couplings is that for a given network topology the DFN's
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21 99 fracture is modeled as a parallel plate with a given permeability [de Dreuzy et al., 2012].
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24 100 Painter and Cvetkovic [2005] proposed an approach for direct upscaling of
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26 101 discrete fracture network simulations, where transport trajectories, extracted from
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29 102 relatively small scale DFNs, are used in a Monte Carlo calculation to obtain transport
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31 103 results at field scale. [Cvetkovic et al., 2010; Cvetkovic and Frampton, 2010] analyzed
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33 104 transport behavior in small scale DFN with and without in-fracture variability. They
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36 105 observed an increase in travel time when internal fracture variability was included. By
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38 106 accounting for reactive transport and comparing results against the in situ TRUE tracer
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41 107 experiments, they conclude that internal variability effects transport times, however it is
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43 108 not a dominating factor for reactive transport [Cvetkovic et al., 2010; Cvetkovic and
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48 110 The effect of fracture aperture heterogeneity on transport through fracture
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51 111 networks can be studied by considering the non-reacting travel time τ_{nr} [T] and
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53 112 cumulative reactivity parameter β_{nr} [T/L] (also referred as transport resistance) of a
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56 113 plume of particles advecting through the flow field [Cvetkovic et al., 1999; Cheng et al.,
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58 114 2003; Painter, 2006; Cvetkovic et al., 2010; Cvetkovic and Frampton, 2010; Cvetkovic
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and Frampton, 2012; Larsson et al., 2013]. These Lagrangian random variables are key parameters that control advection, diffusive mass transfer and surface sorption of dissolved solutes [Cvetkovic et al., 1999]. The importance of τ and β , as a pair of correlated parameters, for the predictive modeling of transport and retention in heterogeneous fractures and fracture networks, including DFNs, was previously established by [e.g. Cvetkovic et al., 1999; Cheng et al., 2003; Painter, 2006; Cvetkovic et al., 2010; Cvetkovic and Frampton, 2010; Cvetkovic and Frampton, 2012], where the correlation between $\log(\beta)$ and $\log(\tau)$ has been suggested to be linear. Previous analyses [Painter et al., 2002; Cvetkovic et al., 2004] of comprehensive DFN simulations using the FracMan platform [Outters, 2003] demonstrated that the distributions of τ and β are non-Gaussian. Once the probability distributions for these parameters are known, probabilistic simulations of transport can be performed with relatively little effort [Cvetkovic et al., 1999; Painter, 2006; Frampton and Cvetkovic, 2007a, 2007b; Cvetkovic and Frampton, 2012]. Although these studies advanced our understanding of contaminant transport in fractured rock, further quantification of tracer transport and retention in fractured rock modeling requires a transition from a single fracture or small DFNs to large-scale fracture networks where heterogeneity in at least two scales is accounted with varying range of boundary conditions [e.g. Cheng et al., 2003].

Using a recently developed DFN computational suite capable of such simulations, *dfnWorks* [Hyman et al., 2015b], where each fracture is assigned a shape, location, and orientation based on a geological fracture characterization of natural sites, we investigate how in-fracture aperture variability influences transport properties in kilometer-scale fracture networks. We have extended *dfnWorks* to incorporate both

fracture-to-fracture and in-fracture variability, thus allowing the importance of single-fracture aperture variability embedded within a fracture network to be reliably assessed at field scale. The spatially variable aperture values on each fracture are stationary, isotropic, correlated random fields of values drawn from a log-normal distribution in accordance with geological data [Gale et al., 2005]. The mean aperture value is determined using a correlated power-law relationship based on the fracture length. In order to be consistent with a real fractured rock system, the simulated networks are loosely based on the sparsely fractured granite in Forsmark, Sweden [SKB, 2011], which potential repository site for spent nuclear fuel. Fracture networks are generated within a one-kilometer cubic domain. Each DFN is composed of several thousand fractures and has fracture intensity, P_{32} , between 0.027 and 0.031 [1/m]. Two numerical experiments are conducted: 1. Multiple in-fracture variability fields are generated on the same DFN realization while keeping fixed fracture geometry and 2. Ten independent DFN realizations with different geometries and in-fracture aperture variability distributions are generated, and three variances of aperture distributions are produced in every realization. For each DFN, a steady state flow solution is obtained and non-reactive solute transport is simulated using a Lagrangian particle tracking method [Makedonska et al., 2015]. We focus on advection-dominated flows because advection in fractures is a principal mechanism for contaminant transport. Local groundwater velocity is a fundamental control for mass exchange between mobile water in fractures and immobile zones in the rock matrix and controls retention as well as transport [Cvetkovic et al., 1999]. Therefore, understanding the spatial structure of particle trajectories and Lagrangian velocities for advecting solutes is foundational for understanding contaminant transport with and

without retention in the rock matrix. We impose no-flow boundary conditions along the fractures. Particles do not interact with the fracture walls or the surrounding matrix, thereby omitting processes such as diffusion, adsorption or precipitation. While these processes are important, we focus on non-reactive advective transport as a first step to identify the influence of internal aperture variability on transport through field-scale fracture networks without additional complications.

We begin with a brief overview of *dfnWorks* and our adopted discrete fracture network characteristics (Section 2.1), followed by a description of computational mesh characteristics (Section 2.2) and the methodology of incorporating in-fracture variability (Section 2.2). Theoretical formulations of Lagrangian variables, τ and β , are shown in Section 2.3. The configuration of conducted numerical experiments is given in Section 3, obtained results and their discussion are presented in Section 4.

2 Methodology

2.1 Discrete Fracture Network Model

The computational suite for subsurface flow and transport simulation based on DFN modeling, *dfnWorks* software [Hyman et al., 2015b], is used to generate fracture networks and then simulate steady state flow and particle tracking. In the model, fractures are represented by intersecting planar polygons randomly placed within a three-dimensional domain. Fractures are assigned a size, shape, location, orientation, and aperture based on statistical distributions. In the model used here, fractures are circular and we use the term size and radius interchangeably.

The adopted semi-generic fracture networks are loosely based on the well-

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4 184 characterized fractured granite site in Forsmark, Sweden. The Forsmark area is located in
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6 185 northern Uppland within the municipality of Östhammar, about 120 km north of
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11 187 and brittle deformation. The ductile deformation has resulted in large-scale, ductile high-
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16 189 fractured but less affected by ductile deformation, are enclosed between the ductile high
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21 191 We adopt a subset of the fracture sets identified at Forsmark. The statistical
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25 193 200 and 400 meters below ground level and are provided in Table 1; fractures with a
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27 194 radius larger than 560 meters are considered deterministic and are not included. Three
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$$f(\theta) = \frac{\kappa \cdot \sin\theta \cdot e^{\kappa \cdot \cos\theta}}{e^{\kappa} - e^{-\kappa}}, \quad (1)$$

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39 198 where θ is the deviation of the fracture pole orientation from the mean orientation and the
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51 203 The fracture radii at Forsmark obey a truncated power-law distribution [SKB,
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53 204 2011] with lower and upper cut-off radii of circular fractures, R_0 and R_u , respectively.
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55 205 The power-law distribution is sampled by first generating uniformly a random number u
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58 206 over the interval $[0.0, 1.0]$. The fracture radius, R , is then calculated as
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$$R = R_0 \cdot \left[1 - u + u \cdot \left(\frac{R_0}{R_u} \right)^\alpha \right]^{-1/\alpha} . \quad (2)$$

We only consider clusters of fractures that connect between domain faces. Isolated clusters do not participate in the fluid flow in the model because pressure boundary conditions only apply to clusters that intersect a boundary. Thus, isolated fractures are removed after the fracture generation process is complete.

Although the DFN is loosely based on natural fracture characteristics of Forsmark site, the presented results are not intended to reproduce the processes of subsurface flow and transport at the Forsmark site. The main goal of the study is to show how incorporating internal heterogeneity into a large-scale DFN model influences upscaled transport properties in a more generic setting.

2.2 Mesh Generation

The generation of the fracture network is performed using FRAM algorithm (Feature Rejection Algorithm for Meshing strategy), described in detail in [Hyman et al., 2014]. The computational mesh produced on each fracture in the network allows us to resolve internal fracture aperture heterogeneity directly. During the fracture generation process, we require that the DFN never keeps a fracture that produces a feature of size less than h with other intersecting fractures or domain boundaries; a feature of size less than h provides a firm lower bound on the required resolution of the mesh. When the resulting network is meshed, all features can be resolved by generating triangular cell edges with a minimum length slightly less than h . By constraining the network so that all features in the network are greater than h , FRAM ensures that pathological cases, which degrade mesh quality, are not present in the network. Under these conditions, a conforming Delaunay triangulation algorithm can be used to ensure that the line of

intersection between any two fractures is preserved in the mesh as long as the lines of intersections are discretized in steps less than h . Details of the conforming Delaunay triangulation algorithm are provided in Murphy and Gable [1998]. The mesh cells meet stringent criteria on the cell shape and overall mesh quality to ensure stability and accuracy of the physical solution and enables accurate particle tracking [Hyman et al., 2014; Hyman et al., 2015b]. We further select h so that correlations in the in-fracture aperture field are resolved. Once the network generation is complete a Delaunay triangulation is produced using the Los Alamos Gridding Toolbox *LaGriT* [LaGriT, 2013]. Additional information about the FRAM methodology and its implementation are provided in Hyman et al. [2014].

Figure 1 shows a close-up view of several fractures of different size intersecting each other. The mesh is refined near fracture intersections and slightly coarsened (up to certain limit) away from fracture intersections. This spatial variability of the mesh reduces the mesh size (total number of vertices and cells) and in turn reduces computational cost. This approach of fracture discretization is suitable for modeling flow and transport on large-scale fracture networks with in-fracture variability in reasonable computational times; each flow simulation takes around one hour on sixteen cores.

2.3 Simulation of in-fracture variability

Once a DFN is generated and the computational mesh is produced, the value of aperture and transmissivity of each individual fracture is calculated independent of the fracture network. Fracture transmissivity, σ , is estimated using a power-law relationship of a correlated transmissivity model [SKB, 2011]

$$\log(\sigma) = \log(\gamma \cdot R^\omega), \quad (3)$$

with parameters $\gamma=1.6 \times 10^{-9}$, $\omega=0.8$. The fracture aperture, b , is correlated to fracture radius and calculated using the cubic law [e.g. Adler, 2012]

$$\sigma = \frac{b^3}{12} \cdot \frac{\rho g}{\mu}. \quad (4)$$

In Eq. 4 ρ is a water density, g is gravity acceleration and μ is a water viscosity. In the current study, a perfectly correlated relationship between fracture radii and transmissivity in Eq. 3 is used. Other possibilities of semi-correlated and uncorrelated fracture size-transmissivity relationships have been suggested as well [SKB, 2011].

The geostatistical toolkit *gstat* [Pebesma, 1998; Pebesma, 2004] is used to generate a correlated random field of apertures for each fracture in the network and each computational grid cell is assigned a unique value of aperture. Sequential unconditional Gaussian simulation is used to generate each random field of apertures constrained by a simple kriging variogram. The classical simple kriging method assumes that the arithmetic mean value of the random field along each fracture is known; in our case the mean fracture aperture, b , is known for every polygon (Eq. 4). On each fracture several locations are chosen randomly and given the known mean value of aperture. Sequential Gaussian simulation is used to perform a local neighborhood selection according to given spatial correlation length, λ , and to avoid discontinuities in the simulated surfaces, which caused by changes in the local neighborhood used in kriging [Pebesma, 1998; Pebesma, 2004]. However, due to the refined resolution near the fracture intersections the number of cells on a single fracture can be prohibitively large to using sequential Gaussian simulation for the generation of the random field. Therefore, we first generate the field on a coarse mesh representation of the fracture, one that still resolves the correlation length

of the field but does not resolve intersections, and then project that random field onto the higher resolution conforming mesh using barycentric interpolation. This is similar to the methodology applied in de Dreuzy et al. [2012]. The obtained Gaussian random field of aperture in every fracture is transformed to a log-normal distribution to align with geological data [Bonnet et al., 2001; Gale et al., 2005]. For example, Gale et al. [2005] used diagenetic process to improve fracture description, which helps to increase realism in subsurface flow and transport simulations and suggest log-normal distribution of aperture along fractures. In our model, a log-normal distribution of aperture implies a log-normal distribution of transmissivity because we link aperture and transmissivity via cubic law, albeit with different distribution parameters. There are other studies that suggest that the distribution could be a truncated Gaussian distribution, [de Dreuzy et al. 2012], but we do not consider that here.

Our two control parameters are the spatial correlation length, λ , and the variance of transmissivity field on each fracture. The applied spatial correlation length, λ , is defined as a function of fracture radius, R , as $\lambda=c \times R$. The following values of coefficient c are considered in the current study: $c=0.1, 0.3, 0.5$, and 0.7 . Figure 2 shows an example with one circular fracture containing distributed aperture values according to different spatial correlation lengths. In case of relatively small correlation length (Fig. 2a) aperture distribution along the fracture appears to be noisy, while increasing λ (Fig. 2c-d) creates clear low and high transmissivity zones along the fracture. Figure 3 shows aperture distributions for the entire DFN corresponding to three considered cases of distribution variance: $\text{Var}(\ln(b))=0.6$, $\text{Var}(\ln(b))=1.0$, and $\text{Var}(\ln(b))=2.3$.

When the aperture and transmissivity are defined on each computational cell on

every fracture in the network according to applied spatial correlation length, λ , and a variance, a steady state flow solution is obtained and the Lagrangian transport is simulated.

2.4 Calculation of Lagrangian variables

In terms of particle transport modeling, one of the main interests is the time required for a particle to be transported by advection from the in-flow to the out-flow boundary of the domain. Transport through a network is controlled by two Lagrangian variables: τ , the travel time for a particle moving with water from in-flow to out-flow boundary, and β , a retention parameter related to the normalized surface area available for diffusional transfer to the rock matrix. These observables are defined [Cvetkovic et al., 1999] via integrals along the trajectory x'

$$\tau = \int_0^x \frac{1}{v(x')} dx' \cong \sum_{i=1}^n \frac{l_i}{v_i}, \quad (5)$$

$$\beta = \int_0^x \frac{1}{v(x')\hat{b}(x')} dx' \cong \sum_{i=1}^n \frac{l_i}{\hat{b}_i v_i}, \quad (6)$$

where the particle trajectory is a path through the network, passing through a series of n control volume cells with its instantaneous velocity and aperture in each cell i . Here $\hat{b}_i = b_i/2$ is the half-aperture of the current cell, v_i is a particle velocity in the cell, and l_i is a length of the i -th cell in the pathway, x is the total travel distance through the fracture network from in-flow to out-flow boundary.

3. Configuration of Numerical Experiments

The simulation workflow starts from DFN generation and production the computational mesh on generated polygons in three-dimensional domain of size 1000 m $\times$ 1000 m $\times$ 1000 m. After fracture network generation is complete, the connectivity test

is performed, and all isolated fractures or fracture clusters that do not connect inflow-outflow boundaries of the domain are removed because they do not participate in the flow. The final fracture network consists of ~5000 fractures and ~4 million computational cells; fracture intensity, P_{32} , is between 0.027 and 0.031 [1/m]. Then in-fracture variability is included. We begin by analyzing transport in a single DFN realization with 10 different realizations of in-fracture variability for each correlation length and variance. In this case the fracture geometry is fixed and multiple independent realizations of the internal aperture distributions are considered. Next, we construct 10 independent DFN realizations with different geometries based on the same fracture distributions. In this numerical experiment every DFN realization has only one in-fracture variability case for each considered correlation length, λ , and variance.

The parallel subsurface flow and transport code, PFLOTTRAN [Lichtner et al., 2015], is used to obtain the steady state flow solution within the network, using aperture and transmissivity field defined for every fracture in fracture networks. Constant pressure boundary conditions are applied to the top (1 MPa) and the bottom (2 MPa) sides of the domain, what corresponds to hydraulic gradient of 0.1 [m/m], and assumes fluid flow along Z direction, from the bottom to the top boundary. The effects of gravity and hydrostatic conditions are not included in the simulations. An example of the steady state pressure solution in one of the DFN realizations is shown in Fig. 4a. Figure 4b-c show the transmissivity distribution over the entire DFN. The constant transmissivity along each fracture is shown in Fig. 4b; we refer to this case as the *reference case*. Transmissivity varies between fractures in accordance with Eq. 3. Figures 4c-d show transmissivity distribution with $\text{Var}(\ln(\sigma))=0.6$

and $\text{Var}(\ln(\sigma))=2.3$, respectively. The actual minimum and maximum of transmissivity values are listed below the color legends, however colors are scaled according to the reference case (Fig. 4b). The smooth transition of transmissivity from cell to cell can be observed in the case of low variance (Fig. 4c) and more abrupt changes in the transmissivity field are observed at high variance of transmissivity (Fig. 4d).

The particle tracking method of [Makedonska et al., 2015; Painter et al, 2012] is used to simulate non-reactive advective transport through the networks to calculate τ and β . Particles are placed equidistant on each fracture edge that crosses the in-flow boundary of the domain. 10^6 particles are released from in-flow boundary in each DFN and followed to the out-flow boundary integrating τ and β (Eqs. 5, 6) in each computational cell along the way. The aggregate values of τ and β from the multiple simulations are considered to create the distributions. We focus on the empirical distributions of τ and β ; both, the cumulative (CDF) and complementary cumulative (CCDF), are considered. The CDF is used to study early breakthrough times and the tail of the CCDF is used to investigate the longest travel times [Cvetkovic et al., 2010; Cvetkovic and Frampton, 2010; Cvetkovic and Frampton, 2012]. In the distributions, particles are weighted by their initial flow fluxes at the in-flow boundary, which correspond to constant concentration of input contaminated mass. The influence of injection modes, flux-weighted or resident, on travel time distributions in three dimensional DFN was studied by [Frampton and Cvetkovic, 2009; Hyman et al., 2015c]. Both groups of authors found that flux-weighting provides more stable statistics than resident injection and is less sensitive to differences between realizations. In accordance with their findings, we use flux-weighted injection.

Figure 5 shows an example of CDF (green lines) and CCDF (pink lines)

distributions of travel time, τ , obtained by individual simulations in both numerical experiments ($\lambda=0.5R$, $\text{Var}(\ln(\sigma))=1.0$). Fig. 5a displays CDF and CCDF of travel time obtained on individual realizations together with ensemble curve (black lines); which corresponds to results of the first numerical experiment, where multiple in-fracture variability samplings are applied to the same DFN realization. Fig. 5b shows travel time results of the second experiment. Here each CDF and CCDF distribution belongs to an individual DFN realization with a unique geometry and in-fracture variability representation. Black lines in Fig.5 show the total CDF, determined using all particles. The general behavior of individual simulations is close to each other. The low variances indicate that the considered number of independent realizations is reasonable for the purpose of the study. In the next section, for the discussion of the behavior of τ and β CDF and CCDF distributions, we show the ensemble results for clarity.

4. Results and Discussions

In the first numerical experiment one DFN realization is considered with 10 different samplings of in-fracture variability for each of the considered correlation length and transmissivity distribution variance. In this experiment the geometry of fracture network is fixed, while the fracture heterogeneity is sampled multiple times. It allows us to study the effect of variations in the in-fracture variability field transport without the influence of network variability. The cumulative and complementary cumulative distributions of ensemble τ and β are shown in Fig. 6, where each subplot corresponds to certain spatial correlation length and compares results of different variances. Left column shows τ results, right column demonstrates β distributions. Black lines show the

distributions of τ and β calculated in reference case, where no in-fracture variability is implied. For all considered spatial correlation lengths, λ , no significant divergence from reference case is observed at probability higher than 10^{-1} ($P > 10^{-1}$), which corresponds to 90% of injected mass. However, as λ and variances are increased, the deviation from the reference case is observed at $P < 10^{-2}$. Fig. 7 shows comparison of CDF and CCDF of retention parameter β between spatial correlation lengths for the same transmissivity variance. At low variance, $\text{Var}(\ln(\sigma)) = 0.6$, no significant differentiation is observed between distributions of spatial correlation lengths, while at high variance, $\text{Var}(\ln(\sigma)) = 2.3$, remarkable divergence from reference case at $P < 10^{-1}$ is seen, especially at early breakthrough curves.

Similar behavior is detected in the second numerical experiment, where 10 independent DFNs represent their individual geometry of fracture network, as well as in-fracture heterogeneity. Figure 8 shows the CDF and CCDF of travel time τ (left column) and retention parameter β (right column) comparing the results of simulations with different variances for the same spatial correlation length, λ . Figure 9 shows CDF and CCDF of β distributions comparing results of different spatial correlation lengths at the same transmissivity variance. The higher variance has a more significant effect on transport. However, this effect is noticeable at low probability only ($P < 10^{-1}$) and it mostly impacts earlier travel times.

The obtained results show that with probability $P > 10^{-1}$ in-fracture variability has no significant effect on transport within the fracture network; the particles total travel time is mostly driven by network geometry. The correlation between $\log(\tau)$ and $\log(\beta)$ is found to be linear, as suggested earlier using small fracture network simulations by

[Cvetkovich and Frampton, 2010]. At lower probability, $P < 10^{-1}$, what corresponds to less than 10% of injected mass, spatial correlation length has less influence than transmissivity variance. High variance of in-fracture variability causes local channeling of transport along fracture leading to the observed differences.

A visual demonstration of flow channeling along a fracture between two intersection lines is shown on a single fracture example, Fig. 10. The fracture is a rectangular polygon (20 [m] x 30 [m]), representing an area between two intersections in a fracture in fracture network. Color pattern shows the transmissivity distribution with spatial correlation length $\lambda = 0.1R_a$, where R_a is the average length of the rectangular sides. Three cases are shown for different variances of transmissivity (from left to right): $\text{Var}(\ln(\sigma)) = 0.6$, $\text{Var}(\ln(\sigma)) = 1.0$, and $\text{Var}(\ln(\sigma)) = 2.3$. Pressure boundary conditions are applied on the bottom (high pressure) and the top (low pressure) boundary of the fracture. Particles are placed equidistant from each other at the bottom boundary of the fracture and moving forward to the top boundary, demonstrating similarity with particles motion from one intersection line to another in any fracture in fracture network. Note that since this fracture was generated and meshed separately from DFN its resolution is slightly higher (10731 control volume cells) than a typical fracture in DFN. In the case of low variance (Fig. 10a), the trajectories are relatively straight and no flow channeling is observed. As the variance increases (Figs. 10b-c), flow channeling becomes more pronounced. Particles avoid zones with low transmissivity and move towards higher transmissivity regions. Within a connected fracture network, the similar particle behavior observed in Figure 10 occurs on every fracture as particles move from intersection to intersection between

fractures.

We observe that flow channeling affects total travel distance of particles. Figure 11 shows statistical distributions of particles tortuosity, calculated using the first numerical experiment data, where only DFN geometry is considered. Tortuosity is calculated as the ratio of the length of a trajectory, l , over the distance from in-flow to out-flow boundary, d ($d=1000$ [m]), $T=l/d$, and estimates the deviation of a particle trajectory from a straight-line path. The statistics of a particle's tortuosity does not significantly change with different spatial correlation lengths for a fixed variance. However, particle travel distance increases with increasing variance. This is likely linked to increased levels of flow channeling.

Early breakthrough times are more sensitive to local flow channeling caused by internal heterogeneity than longer travel times. Particles that leave simulation domain first visit smaller number of fractures than those that exit at later times. Figure 12 shows an averaged number of fractures per time interval of particles travel time, τ . The data presented here is obtained in the second numerical simulation, where multiple DFN realizations are used and shows the visited number of fractures for the particles that exited the simulation domain in first five years. The particles that contribute to earlier breakthrough statistics of τ and β in the travel times less than one year visit only a few fractures and their travels can be compared to transport in a single fracture, where internal heterogeneity plays crucial role. Moreover, a small number of visited fractures means that at least some of them are big and exhibit higher transmissivity, which speeds up the transport. At longer correlation lengths, which lead to wider low and high transmissivity zones, small fractures can contribute to both, earlier and longer travel

times. The long tails of τ and β distributions are likely the results of particles that pass through many small fractures with low-transmissivity regions.

5. Conclusion

We investigated the effect of in-fracture variability on advective transport in three-dimensional kilometer scale DFNs with thousands of intersecting fractures. A Lagrangian approach is used to simulate advective transport through the fully saturated steady-state flow field within the fracture networks. The effect of the variations of spatial correlation length and transmissivity variance is investigated by considering the distributions of Lagrangian parameters, τ and β , particle travel time and retention, respectively.

The main findings are summarized as follows:

- In-fracture variability does not significantly affect the bulk of transport, e.g., the 50% breakthrough time, through large-fracture networks with complex geometry. No major difference in breakthrough times and retention distributions are observed over the range of parameters considered. In contrast, variations in transport properties seem to be dominated by network geometry.
- Deviations of statistical distributions of travel time and retention parameter from the reference case (where no in-fracture variability is included) are minor for the low values of spatial correlation length and transmissivity variance.
- The variance of the transmissivity fields affects travel distance of particles due to local flow channeling and the particles tortuosity increases with increasing transmissivity variance.
- With probability $P < 10^{-1}$, early breakthrough times and retention are sensitive to

both, the spatial correlation length and the high variance of the transmissivity field. As the transmissivity variance increases, the flow channeling occurs, which results in early breakthrough for particles that visit less number of fractures in their movement from in-flow to out-flow boundary of simulation domain.

- With probability $P < 10^{-2}$, the tails of τ and β CCDF distributions, which correspond to long travel time, are also influenced by in-fracture variability. However, the divergence from reference case is less noticeable than for early breakthrough times. In the case of low variance of transmissivity, the divergence begins at $P < 10^{-4}$ and at $P < 10^{-2}$ for high variance. The low probabilities indicate the in-fracture variability and flow channeling of individual fractures has little effect on late travel times. These results suggest that the geometry of the fracture network dominates over in-fracture variability when considering later travel times. No significant effect of spatial correlation length on late breakthrough times and retention is observed.

In this study, fracture transmissivity is positively correlated with fracture radius, and this correlation along with network topology provides sufficient means for global flow channeling to occur [Hyman et al. 2015c]. In contrast, in-fracture variability is a local driving force for flow channeling. Even within a three-dimensional kilometer-scale DFN this local mechanism appears to result in earlier breakthrough than when in-fracture variability is not included, but only if the correlation length and variance of the transmissivity field are sufficiently large. These results suggest that if the correlation length and variance of the transmissivity field are relatively small, then the geometry of

fracture network dominates transport properties over in-fracture variability. Under such circumstances, adopting a DFN model where in-fracture variability is omitted should not lead to systematic errors. However, if the correlation length and variance of the transmissivity field are sufficiently large, then using a model where in-fracture variability is not included will lead to underestimation of early breakthrough times.

In the current study the DFN parameters are loosely based on those obtained from the granite at Forsmark, Sweden. Given the number of variables and parameters available in a DFN model it is hard to isolate responses to multiple changes in the same simulations. We focus this study on a fixed set of generator parameters, such as spatial correlation lengths of aperture/transmissivity distributions along each fracture of the DFN and different variances of transmissivity distributions. We speculate that variety of fractures shape (circular, rectangular, elliptical) and fracture orientations would not significantly change the obtained results, since the particles are moving from intersection to intersection and driven by boundary conditions. However, the observed behavior of τ and β could be different if fracture densities or if a different range of length scales are considered. For example, at the core scale the length of the correlation in aperture fields would be much closer the domain size than in a kilometer DFN and would likely be more significant. The possibility of correlated sensitivity between the generator parameters, domain size, and in-fracture correlation length / variance is certainly possible and will be pursued in later work.

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4 527 **Acknowledgment**
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6
7 528 The authors thank the U.S. Department of Energy (DOE) Used Fuel Disposition
8
9 529 Campaign and DOE Fossil Energy's Strategic Center for Natural Gas and Oil for
10
11 530 financial support of the work. JDH gratefully acknowledges the support of a LANL
12
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14 531 Director's Postdoctoral Fellowship and the Center for Nonlinear studies.
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19 533 **References**
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Table 1. Statistical parameters used in simulations of the DFNs, based on fracture characteristics from Forsmark repository site, Sweden [SKB, 2011].

Set	Orientation Distribution: Fisher			Size Distribution: Power Law			Fracture Density
	Mean Trend	Mean Plunge	Conc. k	a	R_u , m	R_o , m	Number of fractures in 1 km ³
1. (NS)	90.0°	0.0°	21.7	2.5	560	15	2093
2.(NE)	135.0°	0.0°	21.5	2.7	560	15	2000
3.(HZ)	360.0°	90.0°	8.2	2.38	560	15	7711

Figure 1. Close-up view of one of the DFN realizations; fractures of different sizes are intersecting each other. Black solid lines show the produced Delaunay triangulations. Each fracture has a unique color. Mesh coincides along intersections lines. The mesh is coarsened as the distance from intersection line increases.

Figure 2. An example of a single circular fracture with aperture variability. The applied different spatial correlation lengths are: a) $\lambda=0.1R$, b) $\lambda=0.3R$, c) $\lambda=0.5R$, d) $\lambda=0.7R$, where R is a radius of fracture, defined by Eq. 2. As the spatial correlation length increases, the areas of high and low aperture zones expand.

Figure 3. Aperture distributions of one of DFN realizations with in-fracture variability are shown, where each CDF corresponds to one of three considered cases of variances: $\text{Var}(\ln(b))=0.6$; $\text{Var}(\ln(b))=1.0$, and $\text{Var}(\ln(b))=2.3$.

Figure 4. Pressure solution and transmissivity profile of one of the DFN realizations. a) The obtained steady state pressure solution for fully saturated flow. The pressure boundary conditions are applied to the top (1 MPa) and the bottom (2 MPa) side of the domain, assuming fluid flow along Z direction. Applied boundary conditions correspond to hydraulic gradient $i=0.1$ [m/m]. b) Transmissivity profile of the DFN in the reference case, where transmissivity and aperture are constant along each fracture, but vary from fracture to fracture according to fracture radii. c) and d) show in-fracture variable transmissivity distribution with $\text{Var}(\ln(\sigma))=0.6$ and $\text{Var}(\ln(\sigma))=2.3$, respectively. The minimum and maximum values are listed below the

color legend, while the color scale is fixed for all cases according to reference case (b).

Figure 5. An example of CDF (green lines) and CCDF (pink lines) distributions of travel time, τ , obtained by individual simulations. Black lines correspond to ensemble curves. Here $\lambda=0.5R$, $\text{Var}(\ln(\sigma))=1.0$. a) CDF and CCDF of travel time obtained on single realizations in the first numerical experiment, where multiple different in-fracture variability samplings applied to the same DFN realization. b) Travel time results of the second experiment, where each CDF and CCDF distribution belongs to an individual DFN realization with a unique geometry and in-fracture variability representation.

Figure 6. CDF and CCDF distributions of the Lagrangian variable of travel time τ (right

column) and retention parameter β (left column) calculated for transport in the first numerical experiment, where multiple different in-fracture variability samplings applied to the same DFN realization. The distributions that correspond to each case of variance are compared to each other and to reference case (black lines) at the same correlation length.

Figure 7. CDF and CCDF distributions of the retention parameter β , calculated for transport in the first numerical experiment, where multiple different in-fracture variability samplings applied to the same DFN realization. The distributions that correspond to each considered correlation length are compared to each other and to the reference case (black lines) at the same variance. The difference between cases and the reference case is growing with increasing variances at Probability $<10^{-1}$.

Figure 8. CDF and CCDF distributions of the Lagrangian variable of travel time τ (right)

column) and retention parameter β (left column) calculated for transport in the second numerical experiment, where multiple DFN realizations exhibit unique geometry and in-fracture variability sampling. The distributions that correspond to each case of variance are compared to each other and to reference case (black lines) at the same correlation length.

Figure 9. CDF and CCDF distributions of the retention parameter β , calculated for transport in the second numerical experiment, where multiple DFN realizations represent a unique geometry and in-fracture variability sampling. The distributions that correspond to each considered correlation length are compared to each other and to the reference case (black lines) at the same variance. The difference between cases and the reference case is growing with increasing variances at Probability $< 10^{-1}$.

Figure 10. Single fracture configuration with simulated particle trajectories for three cases of applied variances of transmissivity distribution: a) $\text{Var}(\ln(\sigma))=0.6$; b) $\text{Var}(\ln(\sigma))=1.0$; c) $\text{Var}(\ln(\sigma))=2.3$; and spatial correlation length $\lambda=0.1R_a$, where R_a is an average length of the rectangular sides. Transmissivity distribution along the fracture is shown by color pattern, where cold colors represent low transmissivity. Solid lines show particles trajectories that are moving from bottom to top boundaries of the fracture, demonstrating similarity of particles motion from one intersection line to another in any fracture of fracture network. As the variance in transmissivity increases, flow channeling is clearly observed.

Figure 11. Statistical distributions of particles tortuosity ensemble, calculated in the first numerical experiment, where DFN geometry does not change. The CDF behavior does not change significantly with different spatial correlation length for a fixed variance; particles tortuosity increases with higher variance due to flow channeling.

Figure 12. Average number of fractures visited by particles, per a time interval of particles travel time, τ . The data presented here is calculated from the second numerical experiment, where multiple DFN realizations are used and shows the number of fractures visited by the particles that exited the simulation domain in the first five years.