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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.

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 advantage of DFN models over continuum based models, such as stochastic continuum and dual/multi permeability models (Neuman, 2005; Lichtner and Karra, 2014; Painter et al., 2002), when investigating flow and transport through sparsely fractured rock is that they can represent a wider range of transport phenomena (Painter et al., 2002; Painter and Cvetkovic, 2005), which in turn can be explicitly linked to fracture network attributes such as densities, size, orientation, and fracture aperture.

Various physical processes such as geological stress and strain, chemical dissolution, precipitation and erosion, result in apertures that vary within an individual fracture. The numerous computational (Tsang and Tsang, 1987; Tsang and Tsang, 1989; Moreno et al., 1988; Moreno and Tsang, 1994), laboratory (Moreno et al., 1985; Keller et al., 1999), and field studies (Neretnieks et al., 1985; Bourke, 1987) of flow in single fracture have demonstrated that internal fracture aperture variability results in fracture-scale flow channeling that impacts transport properties. Tsang and Tsang (1987) suggested that flow within a fracture plane could be considered as a series of parallel one-dimensional “flow tubes” due to flow channeling. Bourke (1987) observed similar flow tubes in an in situ experiment of flow through a fracture plane. Computational studies of channeling phenomena (Larsson et al., 2012;

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Larsson et al., 2013; Moreno et al., 1988; Tsang and Tsang, 1989) investigated how spatial correlation length and hydraulic conductivity effect on transport within a single fracture. Larsson et al. (2012) considered a spatial correlation length of applied heterogeneity in a range between 2% and 18% of the flow domain width and concluded that the transport behavior was independent of the correlation length in the considered range. It has been observed that increasing standard deviation of conductivity distribution the flow channeling width decreases, i.e., flow 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., 2016; Hyman et al., 2015b). 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 application to three-dimensional fracture network is limited because it disregards explicit details of three-dimensional particle transport. Recently, de Dreuzy et al. (2012) studied the effect of internal aperture heterogeneity on the effective permeability of a large DFN, but they did not consider transport. The authors found that there are couplings between flow heterogeneities at the fracture scale and flow heterogeneities at the network scales. A consequence of these couplings is that for a given network topology the DFN's equivalent permeability will not be properly predicted by a simulation where each fracture is modeled as a parallel plate with a given permeability (de Dreuzy et al., 2012).

Painter and Cvetkovic (2005) proposed an approach for direct upscaling of discrete fracture network simulations, where transport trajectories, extracted from relatively small scale DFNs, are used in a Monte Carlo calculation to obtain transport results at field scale. (Cvetkovic et al., 2010; Cvetkovic and Frampton, 2010) analyzed transport behavior in small scale DFN with and without in-fracture variability. They observed an increase in travel time when internal fracture variability was included. By accounting for reactive transport and comparing results against the in situ TRUE tracer experiments, they conclude that internal variability effects transport times, however it is not a dominating factor for reactive transport (Cvetkovic et al., 2010; Cvetkovic and Frampton, 2010).

The effect of fracture aperture heterogeneity on transport through fracture networks can be studied by considering the non-reacting travel time τ [T] and cumulative reactivity parameter β [T/L] (also referred as transport resistance) of a plume of particles advecting through the flow field (Cvetkovic et al., 1999; Painter et al., 1998; Cheng et al., 2003; Painter and Cvetkovic, 2001; Painter, 2006; Cvetkovic et al., 2010; Cvetkovic and Frampton, 2010; Cvetkovic 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., 2015a), 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 ma-