Journal of Hydrology 553 (2017) 59–70

Contents lists available at ScienceDirect

Journal of Hydrology

journal homepage: www.elsevier.com/locate/jhydrol

Research papers

A comparative study of discrete fracture network and equivalent continuum models for simulating flow and transport in the far field of a hypothetical nuclear waste repository in crystalline host rock

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ARTICLE INFO

Article history:
Received 8 March 2017
Received in revised form 18 July 2017
Accepted 24 July 2017
Available online 28 July 2017
This manuscript was handled by P. Kitanidis, Editor-in-Chief, with the assistance of Jean-Raynald de Dreuzy, Associate Editor

Keywords:
Fracture characterization methods
Discrete fracture network
Equivalent continuum
Nuclear waste disposal
Crystalline rock

ABSTRACT

One of the major challenges of simulating flow and transport in the far field of a geologic repository in crystalline host rock is related to reproducing the properties of the fracture network over the large volume of rock with sparse fracture characterization data. Various approaches have been developed to simulate flow and transport through the fractured rock. The approaches can be broadly divided into Discrete Fracture Network (DFN) and Equivalent Continuum Model (ECM). The DFN explicitly represents individual fractures, while the ECM uses fracture properties to determine equivalent continuum parameters. We compare DFN and ECM in terms of upscaled observed transport properties through generic fracture networks. The major effort was directed on making the DFN and ECM approaches similar in their conceptual representations. This allows for separating differences related to the interpretation of the test conditions and parameters from the differences between the DFN and ECM approaches. The two models are compared using a benchmark test problem that is constructed to represent the far field ($1 \times 1 \times 1$ km^3) of a hypothetical repository in fractured crystalline rock. The test problem setting uses generic fracture properties that can be expected in crystalline rocks. The models are compared in terms of the: 1) effective permeability of the domain, and 2) nonreactive solute breakthrough curves through the domain. The principal differences between the models are mesh size, network connectivity, matrix diffusion and anisotropy. We demonstrate how these differences affect the flow and transport. We identify the factors that should be taken in consideration when selecting an approach most suitable for the site-specific conditions.

1. Introduction

Disposal of high-level radioactive waste in a geological repository in crystalline host rock is one of the potential options under study in the United States by the Department of Energy. The disposal concept has also been studied in other countries such as Canada, Switzerland, Japan, Sweden and Finland to various degrees. Finland and Sweden currently have advanced repository implementation. A detailed review of international disposal concepts in crystalline rock is given by Rechard et al. (2011). The disposal concepts include an engineered barrier system at a nominal depth of 500 m and a natural barrier system consisting of variously fractured crystalline rock. Although the matrix rock has low permeability, the presence of fractures and faults has the potential to affect the hydrogeology of the host rock, and could result in the potential migration of radionuclides to the accessible environment. For this reason, the design of a disposal system in a crystalline rock requires a robust characterization of the fractured host rock.

Various fracture modeling approaches have been employed to represent the fractured rock. The approaches can be broadly divided into Discrete Fracture Network (DFN) and Equivalent Continuum Model (ECM) (Zhang and Sanderson, 2002). Various techniques are also used within the broad categories to characterize fractured rock.

The DFN approach is widely used in various applications, including nuclear waste disposal (Uchida et al., 1994; Dershowitz

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http://dx.doi.org/10.1016/j.jhydrol.2017.07.046
0022-1694/

et al., 1998, 1999). In DFN approach interconnected networks for fractures are explicitly represented. Most DFN models (conventional DFN) assume that flow and transport only occur through the network with no participation of the rock matrix. In the model each fracture is a two-dimensional planar object with specific shape and size and object-specific hydraulic properties such as transmissivity and aperture. If the location of a fracture is known, then the fracture can be deterministically included in the model. Otherwise, fractures are generated stochastically based on the probability distributions of fracture orientation and size derived from field observations. The fracture generation also requires the knowledge of the fracture intensity expressed either in terms of fracture area per unit volume or number of fractures in the modeling domain. Small fractures, whose radius is smaller than a cutoff value, are usually excluded from the fracture network. The fracture transmissivity and aperture are often assumed to be positively correlated with the fracture size – larger fractures generally have higher transmissivity and aperture (Dershowitz et al., 1999). Recently, discrete fracture matrix models where fractures and matrix are coupled directly have been developed (Ahmed et al., 2015a,b). However, this formulation is complex and computationally intense. Therefore, simplified matrix representations (Hao et al., 2013; Karra et al., 2015) are usually used instead.

In ECM individual fracture properties are translated into the properties of an equivalent porous medium. Different techniques have been proposed, but the main goal remains the same – reproduce the behavior (e.g. flow and transport) of the corresponding fracture network. The ECM is commonly used when the number of fractures in the model domain is large and/or the interaction between the matrix and fractures is an important factor. Examples of the ECM approach are found in Hsieh et al., (1985), Neuman and Depner (1988), Carrera et al. (1990), Tsang et al. (1996), Altman et al. (1996), Jackson et al. (2000), Hartley and Joyce (2013). One of the main challenges with the ECM approach is that anisotropic permeability needs to be adequately represented to capture the preferential flow pathways in fractures. Jackson et al. (2000) provided a method of self-consistency that checks whether the ECM adequately represents the actual fracture system represented by a DFN method. They utilized the self-consistency method to demonstrate that the effective permeability of the ECM represents the fracture network.

Both DFN and ECM are useful tools for fracture modeling and for predictions of flow and transport. A number of studies compared DFN and ECM approaches, e.g. Selroos et al. (2002) and Leung et al. (2011). The common approach used in these studies is to specify the test/experiment conditions and let DFN and ECM modelers to develop their corresponding models. The modeling results are compared in terms of key upscaled observables, e.g., effective permeability and solute transport. However, details of the conceptual models and corresponding parameters were seldom provided. As a result, it is not possible to separate differences related to the interpretation of the test conditions and parameters from the differences between the DFN and ECM approaches.

This paper addresses this problem by developing an ECM approach that matches as closely as possible the DFN model in the conceptual representation and parameters. The same numerical code PFLOTRAN is used to simulate flow and transport to ensure that a fair comparison is possible. Under this formulation we can determine the advantages and disadvantages of the two approaches with regard to simulating flow and transport in fractured crystalline rock. The goals of this study are:

(1) To identify the differences between the predictions of flow and transport with DFN and ECM approaches in the far field of a hypothetical nuclear waste repository located in crystalline host rocks.
(2) To separate the differences related to the discrete versus continuum approach from the differences in the conceptual representation.
(3) To provide robust fracture characterization tools for use in flow and transport modeling of generic deep geologic disposal of nuclear waste in crystalline rocks. The tools would also be utilized in other simulation processes such as thermal analysis.

An outline of DFN and ECM approaches is provided in Section 2. The benchmark problem used for the comparison is described in Section 3. Section 4 describes modeling of flow and transport together with effective permeability estimation and observation of breakthrough curves for the different fracture network realizations. The major findings of this analysis are described in Section 5.

2. Modeling approach

The DFN and ECM approaches used in this study are described in Sections 2.1 and 2.2, respectively. Both models use the same numerical solver for flow, PFLOTRAN. PFLOTRAN (Lichtner et al., 2015) is an open source, state-of-the-art massively parallel subsurface flow and reactive transport code that solves mass balance with Darcy's law invoked for flow. The advection-diffusion equation (ADE) in PFLOTRAN is used for transport simulations in both models. Transport within the DFN is also simulated using a Lagrangian particle tracking code (Makedonska et al., 2015). Breakthrough curves from all transport models, ADE-ECM; ADE-DFN; and particle tracking-DFN, are compared.

2.1. The DFN approach

Using DFN to model flow and transport through fractured media is an alternative to traditional continuum approaches where effective parameters are used to include the influence of the fractures on the transport properties through a porous medium. In the DFN approach, networks of fractures are created where the geometry and properties of individual fractures are explicitly represented. These networks are meshed for computation and the governing equations are numerically integrated to simulate flow. The choice to include the detailed geometry of the fractures and the connectivity of the fracture network allows for a more accurate representation of physical phenomenon and robust predictive simulation of flow and transport through fractured rocks compared to continuum approaches (Painter and Cvetkovic, 2005).

In this study, we use the computational suite dfnWorks (Hyman et al., 2015a) to generate a discrete fracture network representation of the fracture network and to solve the flow equations therein. dfnWorks combines the feature rejection algorithm for meshing (FRAM) (Hyman et al., 2014), the LaGriT meshing toolbox (LaGriT, 2013), the parallelized subsurface flow and reactive transport code PFLOTRAN (Lichtner et al., 2015), and a Lagrangian particle tracking method (Makedonska et al., 2015; Painter et al., 2012). FRAM is used to generate three-dimensional fracture networks and LaGriT is used to create a computational mesh representation of the network for computation. PFLOTRAN is used to numerically integrate the governing flow equations. dfnWorks has been used in a variety of studies including hydraulic fracturing (O'Malley et al., 2015; Hyman et al., 2016a; Karra et al., 2015) and parameter assessment for subsurface flow and transport in large fracture networks (Hyman et al., 2015b; Makedonska et al., 2016; Hyman et al., 2016b). Details of the suite, its abilities, applications, and references are provided in Hyman et al., 2015a.

Fig. 1 outlines the dfnWorks Workflow. Network generation is performed using DFNGEN (top row). The feature rejection algo-