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Linked multicontinuum and crack tensor approach for modeling of coupled geomechanics, fluid flow and transport in fractured rock

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ABSTRACT

In this paper, we present a linked multicontinuum and crack tensor approach for modeling of coupled geomechanics, fluid flow, and solute transport in fractured rock. We used the crack tensor approach to calculate effective block-scale properties, including anisotropic permeability and elastic tensors, as well as multicontinuum properties relevant to fracture-matrix interactions and matrix diffusion. In the modeling, we considered stress dependent properties, through stress-induced changes in fracture apertures, to update permeability and elastic tensors. We evaluated the effectiveness and accuracy of our multicontinuum approach by comparing our modeling results with that of three independent discrete-fracture-network models (DFNs). In two of the three alternative DFN models, solute transport was simulated by particle tracking, an approach very different from the standard solute transport used in our multicontinuum modeling. We compared the results for flow and solute transport through a 20 × 20 m model domain of fractured rock, including detailed comparison of total flow rate, its distribution, and solute breakthrough curves. In our modeling, we divided the 20 × 20 m model domain into regular blocks, or continuum elements. We selected a model discretization of 40 × 40 elements (having a side length of 0.5 meter) that resulted in a fluid-flow rate equivalent to that of the DFN models. Our simulation results were in reasonably good agreement with the alternative DFN models, for both advective dominated transport (under high hydraulic gradient) and matrix-diffusion retarded transport under (low hydraulic gradient). However, we found pronounced numerical dispersion when using larger grid blocks, a problem that could be remediated by the use of a finer numerical grid resolution, while maintaining a larger grid for evaluation of equivalent properties, i.e., a property grid overlapping the numerical grid. Finally, we encountered some difficulties in using our approach when element sizes were so small that only one or a few fractures intersect an element—this is an area of possible improvement that will be pursued in future research.
1 INTRODUCTION

In recent years interest in coupled fluid flow and mechanical processes in fractured rock masses, also known as coupled hydromechanical (HM) processes, has increased, along with the ever-increasing demands for energy under sound environmental considerations. The three main fields in which fractured rock coupled HM processes have been most extensively studied are nuclear waste disposal, geothermal energy (hot-dry-rock) extraction, and oil and gas extraction (Rutqvist and Stephansson, 2003). Indeed, coupled HM processes in fractured rock are central to extracting more significant amounts of geothermal energy through enhanced or engineered geothermal systems, as well as to production efforts by the surging North American shale gas industry. Hydraulic stimulation of fractured rock in such systems is used to increase permeability and energy production, but may also induce seismic events that, if felt can cause concern within the local community. The potential for induced seismicity has also been raised as a concern for deep underground injection and storage of carbon dioxide (Rutqvist, 2012). Under these circumstances, numerical modeling of coupled HM process in fractured rock can be an important tool for finding ways to optimize fluid production or injection, while minimizing the risk of inducing notable seismic events.

Coupled HM numerical models for fractured porous geological media have been available since the early 1980s, including those pioneered by Noorishad et al. (1982), who presented a coupled HM formulation and finite-element scheme that later evolved into the computer code ROCMAS. This formulation was based on an extension of Biot’s theory of consolidation (Biot, 1941) to include discrete fractures in addition to the porous matrix, and used a fully implicit solution technique. Since then, many computer codes capable of modeling coupled HM processes in fractured porous media have been developed using various numerical methods, including finite-element, distinct-element and boundary-element methods (Jing and Hudson, 2002). At the same time, more realistic constitutive models have been developed to describe coupled HM interaction in rock fractures, with the ones by Barton et al. (1985) and Walsh (1981) most commonly applied (Rutqvist and Stephansson, 2003).

Efforts have also been made to incorporate HM coupling into effective medium theories, such as the crack tensor theory—e.g., Oda (1986), Stietel et al. (1996), Kobayashi et al. (2001), Guvanasen and Chang (2004). The crack tensor is a unique measure combining four significant aspects of hydraulic and mechanical behavior in fractured rock: volume, fracture size, fracture orientation, and fracture aperture. Oda (1986) applied the crack tensor for HM modeling of rock with geological discontinuities as an anisotropic, elastic porous medium with equivalent elastic compliance and permeability tensors.
Stietel et al. (1996) used a similar approach, including 2D planar analytical treatment of cracks to calculate the equivalent anisotropic HM properties (permeability tensor, stiffness tensor, Biot’s coefficient, and Biot’s modulus) and compared their results to those from discrete fracture model simulations. Kobayashi et al. (2001) combined crack tensor theory and the Barton-Bandis model for rock joints in analyzing coupled mechanical and hydraulic processes on shaft sinking in a fractured rock mass. In that study, the elastic stiffness and hydraulic conductivity tensors were updated with resultant anisotropy and heterogeneity during a simulated shaft excavation. Guvanasen and Chan (2004) used what they characterized as a modified crack tensor theory for coupled thermohydromechanical (THM) processes, which incorporated transformation of a mechanical aperture to a deformed hydraulic aperture for upscaling the THM properties. They applied their model to simulate a large-scale DECOVALEX benchmark test in which the permeability tensor and elastic tensors were upscaled for individual fracture sets, using parameters such as mean length and spacing for each set.

A number of studies have been made in which the effective continuum HM properties have been calculated from numerical simulations using discrete fracture network models (Zhang and Sanderson, 1999; Min et al., 2004; Blum et al., 2009). For example, Zhang and Sanderson (1999) used such an approach to scale up the two-dimensional conductivity tensor for highly heterogeneous fracture networks. They scaled up local conductivity tensors, based on small sample fracture networks, to estimate the overall nature of conductivity for a relatively large region. Min et al. (2004) used distinct element modeling to calculate upscaled stress-versus-permeability properties of a fractured rock mass, and then applied it to calculate far-field radionuclide transport under thermally driven stress evolution, also associated with the abovementioned DECOVALEX benchmark test (Min et al., 2005). Blum et al. (2007) also applied their modeling approach to the same benchmark test, but used a stochastic analysis for investigating the impact of various basic HM properties on the transport simulation results. The spread of travel times in the simulation results demonstrated the significance of both HM rock properties and their spatial distribution.

For a fractured porous media, it might be useful to represent the fractures and intervening rock matrix by overlapping fracture and matrix continua, referred to as dual-continuum or dual-porosity models. This is a common approach in reservoir engineering where the storage of fluids might take place primarily in the matrix, with permeability controlled by fluid flow in fractures (e.g., Barenblatt et al., 1960, Warren and Root 1963). A generalization of this concept is realized by the multiple interacting continua or MINC model, a concept that has been extensively applied in multiphase flow and transport.
modeling (Pruess and Narasimhan, 1985). Studies incorporating both Biot’s poroelastic theory and dual-porosity concept include work on single-phase fluid flow by Berryman and Wang (1995), Chen and Teufel (1997), Bai et al. (1999), and Berryman (2002), as well as recent developments associated with multiphase fluid flow by Liu and Rutqvist (2012) and Kim et al. (2012). A version of the dual-continuum concept; the dual-permeability concept, was applied for modeling coupled THM processes associated with the Yucca Mountain Project, Nevada (Rutqvist and Tsang, 2003). This included modeling of the Yucca Mountain drift scale test (Rutqvist et al., 2005; 2008) and also part of the previous DECOVALEX studies (Rutqvist et al., 2009a). In these modeling efforts, the emphasis was on high-temperature (above boiling for water) thermally-driven coupled processes in the near field of heated drifts, including heat advection in the fracture system and dryout of matrix rock.

In this paper, we present a linked multicontinuum and crack tensor approach and apply it to a simulation case involving coupled geomechanics, fluid flow, and solute transport in fractured rock. We apply the crack tensor theory to calculate effective block scale properties, including anisotropic permeability and elastic tensors, as well as multicontinuum properties relevant to matrix diffusion. Stress-dependent properties are considered through stress-induced changes in fracture apertures, which in turn, are used to update permeability and elastic tensors as a function of mechanical loading. We test the approach in a simulation study of water flow and solute transport through a 20 × 20 m model domain of fractured rock subject to changing stress conditions (Figure 1 and 2). This simulation case was a part of the international DECOVALEX-2011 project, where it was denoted Task C (Zhao et al., 2012). The rock mass considered in this example is heavily fractured; the model domain contains 7797 individual fractures, with an average fracture spacing of about 0.13 m. The geometric fracture data originate from the Sellafield area, West Cumbria, UK, and have been used as input for several previous DECOVALEX studies (Kobayashi et al., 2001; Blum et al. 2009; Min et al., 2004; Öhman and Niemi, 2003). Four fracture sets are identified having fracture length following a power law with fitted fractal dimension equal to 2.2 (Min et al., 2004). The fracture network was generated for minimum and maximum cutoffs of 0.5 and 250 m trace length, respectively. Despite a minimum cutoff trace length of 0.5 m, the mean trace length is still just 0.92 m, and more than 95% of the fractures are less than 2 m (Min et al., 2004). Baghbanan and Jing (2007) used the same statistical fracture parameters, but generated a fracture network that included a correlation between fracture aperture and length, so that larger fractures would have larger apertures and higher permeability. The aperture-length correlation used, shown in Figure 3, has a profound effect on the fluid-flow distribution, with more fluid going through larger fractures, leading to a more heterogeneous flow field (Baghbanan and Jing 2007).
In this study, we evaluate the effectiveness and accuracy of our linked multicontinuum and crack tensor approach, by comparing our modeling results with that of three independent discrete fracture network (DFN) models applied to the same benchmark problem within the DECOVALEX-2011 project (Zhao et al., 2012). In two of the three alternative DFN models, solute transport was simulated by particle tracking—very different from our standard solute transport model. We compare the results for fluid flow and solute transport through the entire 20 × 20 m model domain, with detailed comparison of total flow rate, its distribution, and breakthrough curves for flow and transport under both high and low pressure gradients with, respectively, low and high impact of fracture-to-matrix diffusion. We show that the multicontinuum approach is indeed a viable option to DFN models for modeling of coupled fluid flow, solute transport, and geomechanics in fractured rock masses, although we identified some needed improvements that will be the subject of future research.

2 LINKED MULTICONTINUUM AND CRACK TENSOR APPROACH

In this section, we describe the approach, implementation, and calculation procedure for the linked multicontinuum and crack tensor approach. We implemented it in TOUGH-FLAC (Rutqvist et al., 2002; Rutqvist 2011), a simulator based on coupling the TOUGH2 multiphase flow simulator (Pruess et al., 1999) with the FLAC3D geomechanical simulator (Itasca, 2009). We also employed the TOUGH2 multiple interaction continuum (MINC) approach (Figure 4), which provided us with an effective way of including important fracture-matrix interactions, including fracture-matrix diffusion.

2.1 General approach and domain discretization

In the linked multicontinuum and crack tensor approach, we divide the model domain into overlapping fracture and matrix continuum elements (Figure 5). For each element, we calculate upscaled (effective) properties, such as permeability and elastic tensors. We also calculate multicontinuum parameters, such as average fracture spacing and fracture volume fraction that are used in the TOUGH2-MINC model. For example, in the DECOVALEX-2011 benchmark test, we divided the 20 × 20 m fractured rock domain into uniform cubic elements. We investigated the use of different element sizes, from a very fine mesh of 400 × 400 elements (i.e., elements of side length 0.05 m) to a very coarse mesh of 4 × 4 m (i.e., side length of 5 m). In the case of a very fine mesh (elements with side length of 0.05 m), only 1 or 2 fractures, or indeed none may intersect each element. The fine-mesh approach could be characterized as a discrete continuum approach, because each fracture trace is
actually discretely represented through distinctly different properties of grid elements along a fracture trace. Such an approach was previously introduced and applied using TOUGH-FLAC in Rutqvist et al. (2009b) for studies related to the excavation disturbed zone around tunnels in fractured rock. However, herein we use a more systematic approach, in which equivalent properties (such as a permeability and elastic tensor) for each fracture continuum element (Figure 5) are calculated analytically, using crack tensor theory.

2.2 Effective multicontinuum properties using crack tensor theory

The effective multicontinuum properties were derived using Oda’s crack tensor theory (Oda, 1986), but in this case formulated as a discrete summation of contributions from each fracture that intersects an element volume. We can use discrete summation for this case, because each fracture is known by its position and its geometric properties—length, orientation, and aperture. We use Oda’s crack tensor theory, in which fractures are considered as disc shaped in a 3D system. The basic quantities of the crack tensor for each crack intersecting an element can be stated as follows:

\[ F_{ij} = \frac{1}{V_e} \frac{\pi}{4} D^3 n_i n_j \]  
\[ F_{ijkl} = \frac{1}{V_e} \frac{\pi}{4} D^3 n_i n_j n_k n_l \]  
\[ P_{ij} = \frac{1}{V_e} \frac{\pi}{4} D^2 b^3 n_i n_j \]

where \( F_{ij}, F_{ijkl}, P_{ij} \) are basic crack tensors, \( V_e \) is element volume, \( D \) is the diameter of the crack, \( b \) is the aperture of the crack, and \( n \) is the unit vector of normal orientation for each crack with the component \( n_i (i=1,2,3) \).

By using the quantities and the mechanical properties for each fracture, we calculate the anisotropic compliance tensor \( C_{ijkl} \) and permeability tensor \( k_{ij} \), using

\[ C_{ijkl} = \sum_{NCR} \left[ \left( \frac{1}{K_a D} - \frac{1}{K_s D} \right) F_{ijkl} + \frac{1}{4K_s D} \left( \delta_{ik} F_{jl} + \delta_{jk} F_{il} + \delta_{il} F_{jk} + \delta_{jl} F_{ik} \right) \right] \]  
\[ k_{ij} = \sum_{NCR} \frac{1}{12} (P_{ik} \delta_{ij} - P_{ij}) \]
where NCR is number of fractures (or cracks) intersecting an element, $K_n$ is fracture normal stiffness, $K_s$ is fracture shear stiffness, and $\delta_{ij}$ is Kronecker’s delta.

The total elastic compliance tensor can be then be formulated as

$$ T_{ijkl} = C_{ijkl} + M_{ijkl} \quad (6) $$

$$ M_{ijkl} = (1/E)[(1+\nu)\delta_{ik}\delta_{jl} - \nu\delta_{ij}\delta_{kl}] \quad (7) $$

where $M_{ijkl}$ is the elastic compliance tensor of the intact rock that depends on the Young’s modulus, $E$ and Poisson’s ratio, $\nu$.

For a multicontinuum model, we need to calculate the fracture volume fraction in each element. However, in the current model simulation, and in the MINC capability of TOUGH2, one fracture volume fraction, $f_{vf}$ is derived for the entire domain, as follows:

$$ f_{vf} = \frac{\sum \sum \frac{1}{4} \pi D^2 b}{\sum V_e} \quad (9) $$

where $NE$ is the number of elements.

In the current application for the DECOVALEX-2011 benchmark test, we must consider that the problem was defined as a 2D problem, with fractures defined by their end points and aperture. When using Oda’s crack tensor for this 2D system, we divide the domain into cubic blocks and investigate the geometry of each fracture intersecting such a block. The intersection of a fracture plane with an element volume is defined as a polygon with segments. We then calculate an equivalent disc-shaped fracture diameter, preserving a consistent fracture area (and fracture volume). Having the equivalent diameter of the disc-shaped fracture, we can readily apply Oda’s theory.
2.3 Stress Effects on Permeability and Compliance Tensors

The effect of stress on permeability and compliance are considered through constitutive models for hydraulic and mechanical behavior of single fractures under stress. In this case, we use a fracture HM constitutive model defined in the description of the benchmark test. It was derived as a simplified version of the Bandis hyperbolic model (Bandis et al., 1983), constrained by some basic relationships between initial aperture, maximum normal closure, and stiffness that could represent the observed sample size dependency of these parameters. For example, Baghbanan and Jing (2008) defined a normalized critical normal stress, as the fracture is compressed and approaches the maximum closure where normal compliance decreases significantly. For their particular study, which is also used in this study, the normalized critical stress was set to 10. Moreover, they assumed that maximum normal closure \( \delta_m \) over initial (physical) aperture \( h_i \) is constant and equal to 0.9, i.e., \( \delta_m/h_i = 0.9 \). Using these assumptions, Baghbanan and Jing (2008) simplified the Bandis hyperbolic normal closure equation as follows:

\[
\sigma_n = \frac{\sigma_{nc} \delta}{10(0.9h_i - \delta)}
\]

(10)

and then normal stiffness can be linked to the normal stress as given by

\[
K_n = \frac{(10\sigma_n + \sigma_{nc})^2}{9\sigma_{nc}h_i}
\]

(11)

where \( \sigma_{nc} \) is critical normal stress, defined by Baghbanan and Jing (2008) as \( \sigma_{nc}[\text{MPa}] = 0.487 \times h_i[\mu\text{m}] + 2.51 \). This relation for critical normal stress was chosen such that critical normal stress would vary linearly from 3 to 100 MPa for the defined range of initial aperture (1 to 200 \( \mu\text{m} \)).

In the benchmark test description, shear slip was to be modeled using an elasto-perfectly plastic model with a Coulomb failure criterion, including a constant shear stiffness \( K_s = 434 \text{ GPa/m} \) (Zhao et al., 2012). As soon as shear failure is reached, the continued shear displacement \( u_s \), would induce shear dilation \( u_{dil} \), according to

\[
u_{dil} = u_s \tan \phi_d
\]

(12)
where $\phi_d$ is the dilation angle, which in this study was set to $5^\circ$. In the Coulomb failure criterion, the cohesion, $C = 0$, and the internal friction angle is set to $\phi = 24.9^\circ$, a value once determined from laboratory tests on core samples related to fractures from one of the fracture sets.

In our model simulations, we then consider stress-induced aperture change as a result of both current normal stress and shear dilation, as follows:

$$b = b_0 - \delta + \Delta b_{\text{dil}}$$

$$\delta = \frac{9\sigma_n b_0}{\sigma_{nc} + 10\sigma_p}$$

Equation (10), denoting the initial aperture as $b_0$, i.e., $b_0 = h_i$. Note that $b_0 = h_i$ is the aperture under stress-free conditions that might be measured on core samples, but in this study, $b_0 = h_i$ was assigned for each fracture based on the aperture-length correlation shown in Figure 2.

In this study, we propose a pragmatic approach for modeling of fracture shear slip and dilation, by considering the shear stiffness of the rock surrounding the fracture being sheared. We consider the effect of shear failure through reduction in the shear stiffness, and that shear dilation start at the critical shear stress $\tau_{sc}$ dictated by the Coulomb criterion. A useful feature in this approach is that the fracture shear displacement remains a unique function of the current shear stress even after failure. Thus, shear dilation can be directly related to the current shear stress across the fracture.

Figure 6 illustrates how the shear stiffness of the system—defined as $K_s = K_s^{\text{fracture}} + K_s^{\text{rock}}$—changes at the onset of shear failure. $K_s^{\text{fracture}}$ is shear stiffness related to interlocking of the two opposite rough-fracture surfaces, and it is given in the benchmark test description as 434 GPa. $K_s^{\text{rock}}$ is the shear stiffness of the surrounding rock mass felt by the fracture, estimated from an expression related to shear stress drop, $\Delta \tau$ and shear displacement, $u_s$ along a fracture embedded in a linear-elastic medium as (Rahman et al., 2002; Dietreich 1992):

$$K_s^{\text{rock}} = \frac{\Delta \tau}{u_s} = \eta \frac{G}{l}$$
where $G$ is the shear modulus (of the surrounding rock mass), $l$ is the half length (or radius) of the fracture, and $\eta$ is a factor with a value that depends upon the geometry of the slip patch and assumptions related to slip or stress conditions on the patch (Dietreich, 1992). In our case, we may consider a circular crack in which $\eta = 7\pi/24 \approx 0.92$ and $l$ is the radius. For example, in this benchmark test study, the elastic matrix properties given in Table 1 yields a shear modulus, $G = 34.1$ GPa; shear stiffness of the rock would then be

$$K^\text{rock}_s = \eta \frac{G}{l} \approx \frac{31.2 \cdot 10^9}{r}$$

For a fracture length of 0.92 (the mean fracture trace length in this study), $K^\text{rock}_s = 67.8$ GPa/m, i.e., much less than $K^\text{fracture}_s = 434$ GPa/m. Before shear failure, the system stiffness will then be $K_s = K^\text{fracture}_s + K^\text{rock}_s = 434 + 67.8 = 501.8$ GPa/m. After shear failure, the elasto-perfectly plastic assumption corresponds to $K^\text{fracture}_s = 0$, and hence $K_s = K^\text{rock}_s = 67.8$ GPa/m, given by Equation (16). Thus, in this case, shear stiffness drops significantly upon shear failure. Figure 6 also illustrates that longer fractures result in lower $K^\text{rock}_s$, which is also obvious from Equation (15).

For implementation into the TOUGH-FLAC simulation, we take advantage of the fact that shear dilation occurs for shear stress changes happening after the onset of shear slip, and therefore the dilatational normal displacement can be calculated using

$$\Delta h_{dil} = \frac{\tau - \tau_{sc}}{K^\text{rock}_s} \times \tan(\phi_d)$$

In our TOUGH-FLAC model simulation, we calculate a stress-induced aperture change (including normal and shear stress) update to a new aperture and fracture normal stiffness, and use these new values in the calculation of updated permeability and elastic tensors. The work flow for doing this is described in the next section.

### 2.4 Implementation and work flow

Figure 7 presents the calculation procedure for the linked multicontinuum and crack tensor approach. We first calculate the initial (stress free) elastic compliance tensor and permeability tensor, considering fracture geometry and mechanical properties. For a stress ratio $K = 1$, we first assign initial total elastic compliance tensor fields to each element in the FLAC3D model (employing a user-
defined elastic anisotropic constitutive model) and calculate the new stress state. Note that because of the heterogeneous compliance within the model, the new stress state will be heterogeneous, somewhat different from the stress applied at boundaries. Then, we use the new stress fields to calculate the stress induced fracture change and update the permeability and compliance tensor fields. With the permeability tensor defined in each element, we use TOUGH2 to simulate the flow and transport through the model. The same procedures are used for stress ratios K=2, 3, and 5.

3 MODEL SETUP

We construct the model for testing and comparison to alternative DFN models for fluid flow and transport in fractured rock under mechanical loading. As mentioned, in our approach, we use a standard solute transport calculation rather than particle tracking, and we also use multiple continua, including fracture and matrix continua. In this section, we describe how data and tasks defined in the benchmark description were adapted for the current multicontinuum approach.

3.1 Multicontinuum material properties

The basic parameters for matrix and fractures are given in Table 1, whereas parameters related to fracture-matrix interaction and diffusion are given in Table 2. Notably, only elastic parameters with no permeability were defined for the matrix, which in such a case would be linear elastic and impermeable. These are the material parameters used in the UDEC simulations of this fracture network in Baghbanan and Jing (2008). For our multicontinuum model, we assigned a matrix permeability of $1 \times 10^{-20}$ m$^2$, which is so small that matrix flow is insignificant, compared to the total rock-mass flow. Overall, the permeability of the fractured rock mass in this case is approximately $1 \times 10^{-13}$ m$^2$. Such a high permeability would not be realistic for sites in competent granitic rocks, but was encountered in the volcanic tuff of the Yucca Mountain site, in Nevada, which is also intensively fractured (Rutqvist et al., 2008; Rutqvist and Tsang 2003).

In the TOUGH2-MINC model, we applied both dual-continuum (one fracture and one matrix continuum) and multicontinuum (one fracture and three matrix continua) approaches, with the multicontinuum approach achieving better results, because steep gradients between fracture and matrix could be better resolved. The input to TOUGH2-MINC includes fracture volume fraction and average fracture spacing, used for internal mesh properties (such as element volumes, connection distances, and interface areas). The fracture volume fraction was calculated using Equation (9) for
each loading case, resulting in a decreasing fracture volume fraction with increasing load. The average fracture spacing can be calculated from the inverse of \( P32 \), which is defined as the fracture surface area per unit volume, leading to a fracture average spacing of \( 1/P32 \approx 0.13 \) m. However, in the simulations, as listed in Table 2, a fracture average spacing of 0.2 m was assumed to be consistent with some of the other teams who assumed a matrix diffusion distance of 0.1 m.

### 3.2 Applied mechanical loading and pressure gradients

According to the benchmark test description various boundary stresses were applied on the model domain to generate deformed states for the fluid flow and transport analysis (Figure 1 and 2). A constant vertical normal compressive stress of 5 MPa was specified at the top and bottom boundaries, and a horizontal normal compressive stress, varying from 5, 10, 15 to 25 MPa, was applied at the left and right boundaries. In this way, the stress ratio, defined as \( K = \text{horizontal/vertical stresses} \), increased from \( K = 0, 1, 2, 3, \) to 5 stepwise. (\( K = 0 \) represents the free state when both horizontal and vertical stresses are zero.) Thus, the shear stress and therefore the potential for inducing shear slip along fractures will increase with each loading step.

Fluid flow through the model under various stress ratios was simulated under the specified hydraulic pressure gradients illustrated in Figures 2b and c. The hydraulic boundary conditions allowed the fluid and solutes to exit from three outlet boundaries, except in some cases where closed (impermeable) lateral boundaries were assigned and the solute could exit only through the downstream boundary. Two sets of hydraulic conditions were defined to obtain the macroscopic flow in vertical and horizontal directions, respectively (Figure 2b and c). Moreover, two different values of hydraulic gradient were applied. Initially, a gradient of 10 kPa/m was defined, leading to fast fracture flow, in which the solute transport and breakthrough curves basically depended on the distribution of advective flow within the fracture system, without any significant effect of matrix diffusion. Actually, a gradient of 10 kPa/m is much higher than the conditions expected at a site for an underground radioactive waste repository. Therefore, an additional case of applying a more realistic gradient of 10 Pa/m was defined with matrix diffusion significantly affecting the transport.

### 3.3 Solute injection and monitoring

In our model simulations, using the linked multicontinuum and crack tensor approach, we used a standard solute transport model which is part of the TOUGH2 code and applied the TOUGH2 EOS1 equation of state module (Pruess et al., 1999). In the benchmark for the DECOVALEX-2011 project,
the solute transport was described in terms of particle tracking (Zhao et al., 2012); Solute particles were to be introduced at an amount proportion to the flow rate at each inlet location. Particles collected at each outlet boundary as a function of time were presented in the form of breakthrough curves (Zhao et al., 2012). In our standard solute-transport approach, we used TOUGH2/EOS1 and injected a second water component (water component 2) at the inlet boundary in a pulse over a short time period (e.g., 10 seconds). We then monitored the mass flow of water component 2 at each outlet boundary to calculate breakthrough curves.

3.4 Matrix diffusion

In the benchmark test description, a matrix pore diffusion coefficient, $D_p = 10^{-11}$ m$^2$/s was given as well as a matrix porosity of 0.136%, whereas effective diffusion used in the TOUGH2 continuum model is defined as $D_e = D_p n_e$, where $n_e$ is the effective transport porosity (Neretnieks, 1980). Specifically, in TOUGH2, the diffusive mass flux component $\kappa$ in phase $\beta$ is calculated as

$$f^\kappa_\beta = -n_e \tau_0 \tau_\beta \rho_\beta d^\kappa_\beta \nabla X^\kappa_\beta$$

where $\tau_0 \tau_\beta$ is the tortuosity, which includes a porous medium dependent factor $\tau_0$ and a coefficient, $\tau_\beta$, that depends on the phase saturation, $\rho_\beta$ is density, $d^\kappa_\beta$, is the diffusion coefficient of component $\kappa$ in phase $\beta$, and $\nabla X^\kappa_\beta$ is the gradient of the mass fraction of component $\kappa$ in phase $\beta$. In this case, we have a single phase (liquid), with two water components (water 1 and water 2), in which water 2 corresponds to the injected solute. Therefore, $\tau_\beta = 1$, and the effective and pore diffusion coefficients would correspond to $D_e = n_e \tau_0 d_\beta^\kappa$ and $D_p = \tau_0 d_\beta^\kappa$, respectively. We interpret this such that within the matrix continuum, the molecular diffusion coefficient for the tracer (or solute) in water would be $10^{-9}$ m$^2$/s, with a tortuosity factor, $\tau_0 = 0.01$—whereas in the fracture continuum, the fracture porosity is set to 1, and the tortuosity factor is equal to the fracture volume fraction calculated from Equation (9). As mentioned, in our current model, we assign a homogenous fracture volume fraction in the entire model domain.

4 RESULTS AND COMPARISON

Here we present the modeling results for flow and transport through the $20 \times 20$ m model domain under increasing boundary stresses. We focus on the linked multicontinuum and crack tensor results
denoted LBNL, but also compare with results from the alternative DFN model simulations. The DFN model simulations were conducted by research teams from Imperial College (IC), UK, using the NAPSAC DFN model; the Royal Institute of Technology (KTH), Sweden, using distinct element method simulations with UDEC; and the Technical University of Liberec (TUL), using their FEM code Flow123 (Zhao et al., 2012). The IC and KTH teams used particle tracking, whereas the TUL team used a standard solute-transport model, equivalent to the one used in our model. Further details about the DFN models and results can be found in the accompanying paper by Zhao et al. (2012).

4.1 Fluid flow without mechanical loading

A great deal of effort was spent on development and testing of the algorithms for calculating the permeability tensor using Oda’s theory. The permeability field developed by the Oda’s crack tensor was compared to that calculated by an alternative numerical DFN flow calculation according to Jackson et al. (2000), using the NAPSAC DFN code. Moreover, we also compared our TOUGH2 finite volume flow simulations with that of an alternative finite element method (FEM) simulation, using the NAMMU code (Jackson et al., 2000). We investigated the effect of dividing the 20 × 20 m model into 400 × 400, 100 × 100, 40 × 40, 10 × 10, and 4 × 4 elements. Thus, the size or side length of these elements are 0.05, 0.2, 0.5, 2, and 5 m, respectively. The results of this comparison indicated some problems when using Oda’s crack tensor theory and TOUGH2 finite volume scheme “as is” in particular when element sizes became small compared to the density of the fracture network.

Figure 8 presents an example of vertical flow distributions using a TOUGH2 simulation and a 400 × 400 mesh for the numerically evaluated (using NAPSAC) and analytically evaluated (using Oda’s theory) permeability tensor. The black lines inside the model have a width proportional to the flow rate; outflow distribution is also shown. The TOUGH2 model simulation provided a flow distribution similar to the DFN modeling, with flow dominant along larger fractures, but with the total outflow only amounting to about 70% of the DFN model results. The problem was identified to be associated with (1) element size being smaller than a representative elementary volume, and/or (2) finite-difference-method (FDM) space discretization approximations in TOUGH2. The second item becomes more apparent when imagining the case of only one fracture intersecting an element. If it is a diagonal fracture, and if TOUGH2 uses a standard 5-points finite-difference approximation, there are only vertical and horizontal connections between numerical elements, and the permeability along each such connection is projected from the permeability tensor at each element. In the case of a diagonal fracture, the fluid must flow a longer path in the 5-point differencing (Figure 9a). We tried to remedy
this problem by using 9-point differencing (Pruess et al., 1992) that allows flow between diagonal-element connections (Figure 9b). However, for a very fine mesh, the flow rate was still low compared to the DFN model results.

When element size increased, the total flow rate through the model stabilized to values in reasonable agreement with the NAPSAC DFN simulation results (Figure 10). The flow rate stabilized for element side lengths of 0.5 m or larger (i.e., when the model was divided into 40 × 40 elements or less). The 40 × 40 element case was chosen for a more detailed comparison with other DFN results, including fluid flow and transport changes under increasing load. In the 40 × 40 element case, the total flow rate through the 20 × 20 m model is similar to the DFN, so the average solute transit time should be comparable. But as shown in Figure 10, some of the heterogeneities have been smoothed out, which in theory could lead to a less dispersed (sharper) breakthrough.

4.2 Fluid flow under increasing mechanical load

Figure 11 presents the results of horizontal and vertical permeability calculated from the downstream boundary flow rate under horizontal and vertical gradients, respectively. The figure shows that, overall, permeability is high (on the order of 1×10⁻¹³ m²), and that under increasing mechanical load, the vertical permeability decreases more than the horizontal. This is reasonable, considering that most of the loading is horizontal and therefore tends to preferentially compress vertical fractures to a smaller aperture. Moreover, TOUGH-FLAC modeling results for the 40 × 40 element model is in close agreement with alternative DFN models, even with increasing stress ratios. The TUL results shown in Figure 11 correspond to TUL_2 in Zhao et al. (2012), in which the rock-mass shear stiffness was chosen to be similar to that of IC and LBNL. The results by the KTH team, using the UDEC DFN model simulation, show a somewhat larger decrease in permeability than other teams. This might be caused by a difference in the normal closure model (the KTH team used a tri-linear approximation of the hyperbolic closure model), or it might result from the UDEC model being based on the distinct element method (DEM), the only one of the four models that allows for block rotations, which might cause additional localized fracture closure at block corners (Zhao et al., 2012).

The results also showed that shear dilation had a minor impact on permeability in this case. This might be a surprising result, considering that the highest horizontal-to-vertical stress ratio of 5 is quite extreme. In fact, shear failure along optimally oriented fractures (fractures dipping about 30°) started to occur at a stress ratio of 3, and a large number of fractures had failed in shear at a stress ratio of 5.
However, while many fractures are in a shear failure mode, most of them are smaller fractures confined within the rock mass, which prevents them from sliding sufficiently to cause significant shear dilation. Moreover, small fractures that might be sheared may connect to other fractures of different orientation that are not sheared, and no continuous path of shear-dilated fractures forms.

With a simple calculation using Equation (17), we can find an explanation for the lack of shear induced permeability in this case. For example, at the highest stress ratio, i.e., 5 MPa vertical stress and 25 MPa horizontal stress, the maximum shear stress upon an optimally oriented fracture will be

$$\tau_m = \frac{1}{2} (\sigma_1 - \sigma_3) = \frac{1}{2} (25 - 5) = 10 \text{ MPa}$$

(19)

Shear failure for such a case can be determined using the Mohr-Coulomb criterion, written in the form

$$\sigma_1 = \frac{2C \cos \phi}{1 - \sin \phi} + \frac{1 + \sin \phi}{1 - \sin \phi} \sigma_3$$

(20)

which for $C = 0$ and $\phi = 24.9^\circ$ yields $\sigma_1 = 2.45 \sigma_3$. Consequently, for a vertical stress of 5 MPa, failure would occur at a horizontal stress of $2.45 \times 5 = 12.25$ MPa, and in that instance, the maximum shear stress would be $\tau_m = 3.6$ MPa. This means that a shear-stress increment of $\Delta \tau = 10 - 3.6 = 6.4$ MPa can occur after shear failure.

For a mean fracture length of 0.92, we previously estimated $K'_s = 67.8$ MPa/m, which, according to Equation (17), would result in a dilation of $\Delta b_{dil} = (\Delta \tau / K'_s)^{\tan \phi_d} = (6.4 \times 10^6 / 67.9 \times 10^6) \tan 5 \approx 8.2 \times 10^{-6}$ m, i.e., 8.2 $\mu$m. According to Figure 2, a 0.92 m long fracture has an initial aperture of about 30 $\mu$m, which means that transmissivity through such a fracture might increase according to the cubic law by about $[(30 + 8.2)/30]^3 \approx 2.1$, i.e., a factor of 2.1.

For a 20 m fracture, the initial aperture is already close to the maximum allowable aperture of 200 $\mu$m, so no significant increase can occur. This means that the permeability of the most open and permeable large scale fractures will not increase very much even optimally oriented for shear. As a result, the overall permeability change by shear dilation is expected to be quite small in this case.

### 4.3 Fracture-dominant advective transport
Under the relatively high gradient of 10 kPa/m, the solute transport is dominated by advection within the fracture system. This is illustrated in Figure 12, which shows the results of the total solute transport through the fracture system, with a negligible amount of solute residing in the matrix. Thus, under this high hydraulic gradient, matrix diffusion and fracture-matrix interactions are negligible.

Figure 13 presents breakthrough curves for the three outlet boundaries with comparison to the results of the three alternative DFN models. For $K = 0$, which corresponds to the initial unstressed case, there is excellent agreement in the breakthrough curves between the different teams. At increasing stress ratios, some differences can be observed. In general, the results of our multicontinuum and solute transport approach are very similar to that of the TUL, even under increasing mechanical load. The results for KTH and IC indicate a relatively slower breakthrough under increasing load. It is not clear what is causing this systematic difference in the breakthrough (considering that the permeability and total flow through the model domain are very similar for the different models). It appears that the two teams (KTH and IC) that used particle tracking obtained a delayed breakthrough compared to the two teams (LBNL and TUL) that used standard solute-transport simulation.

Figure 14 presents results for breakthrough curves of different model discretizations. The figure shows that the breakthrough becomes sharper as element sizes decrease. This might be counterintuitive, because for smaller grid sizes we should be able to resolve a heterogeneous flow pattern more precisely, and thereby the breakthrough should be more dispersed. The results in Figure 14 show that the breakthrough curve for the $100 \times 100$ grid is somewhat delayed as a result of the above-discussed reduced total flow rate in the case of finer mesh. Moreover, as shown in Figure 15, for very large element sizes, we see some additional fraction of injected solute exit by diagonal flow through lateral boundaries. Specifically, Figure 15b shows a relatively larger fraction of the solute exit through the top and bottom boundaries, which are lateral boundaries relative to the inlet, and consequently a relatively smaller fraction exit through the left boundary, which in this case is the downstream outlet boundary. However, one critical issue with large grid sizes, such as in the cases of $10 \times 10$ and $4 \times 4$ grids, is numerical dispersion, which in fact is the main cause of the observed more disperse breakthrough curves.

We investigated the effect of numerical dispersion by simulations in which we distinguish between the regular FDM numerical grid and a property grid in which the material properties, including permeability and elastic tensors, are homogenized and defined. Figure 16 presents two such cases. In
Figure 16a, we present the results for a $10 \times 10$ property grid, whereas the numerical grid is either $10 \times 10$ or $100 \times 100$. Likewise, in Figure 16b, we present the results for a $4 \times 4$ property mesh, but with $4 \times 4$ or $40 \times 40$ numerical grids. The result in Figure 16 shows that a much sharper breakthrough is obtained for a finer numerical grid resolution, signifying the profound effect of numerical dispersion in the transport calculation. Remedies to cope with numerical dispersion exist, such as total-variation-diminishing or flux-limiter schemes, which have also been implemented in special versions of the TOUGH2 code (Wu and Forsyth, 2006). Without such remedies, another possibility would be to use different grid resolutions for the numerical analysis and evaluation of equivalent properties. That is, use a fine numerical grid that can resolve sharp fronts of solute transport, and use a larger grid (a property grid) to evaluate continuum properties.

### 4.4 Fracture-matrix diffusion retarded transport

Figure 17 and 18 present simulation results for the case of a much lower hydraulic gradient of 10 Pa/m. In this case, the transit time through the network increases, and matrix diffusion becomes much more significant. Figure 18 shows that the importance of matrix diffusion increases with load, because fracture permeability decreases and transit time increases. For the high load case (Figure 18b), at one point of time as much as 60% of the injected solute resides within the matrix, causing a significant additional delay in the breakthrough. Note that in this case, no advective transport takes place between fracture and matrix, because the pressure is steady state and uniform at all times (thus, there is no pressure gradient between fractures and matrix).

The comparison of breakthrough curves between our multicontinuum model results and two DFN modeling results, in Figure 17, shows good agreement in overall transport behavior, in particular at $K = 0$ (Figure 17a). Note that in the DFN model simulations, the rock matrix is not discretized, but matrix diffusion is modeled using a 1D diffusion model that results in an extra “retarded” travel time. The good agreement in the matrix-diffusion results between the multicontinuum and DFN approaches are encouraging, because the low gradient case of strong fracture-matrix interaction behavior is more realistic from a repository-performance perspective. A dependency on numerical grid size was also observed for the low gradient case, affecting the advective transport in the fracture system, whereas grid size is not expected to directly impact the calculated matrix diffusion.
5 CONCLUDING REMARKS

In this paper, we presented and applied a linked multicontinuum and crack tensor approach for modeling of coupled geomechanics, fluid flow, and solute transport in fractured rock. We used the crack tensor theory to calculate effective block-scale properties, including permeability and elastic tensors, as well as multicontinuum properties relevant to matrix diffusion. In the modeling, we considered stress dependent properties through stress-induced changes in fracture apertures that were used to update permeability and elastic tensors as a function of mechanical load. We evaluated the effectiveness and accuracy of our linked multicontinuum and crack tensor approach by comparing our modeling results with that of three independent discrete fracture network (DFN) models. In two of the three alternative DFN models, solute transport was simulated using particle tracking, i.e., a very different method from the standard solute transport used in our multicontinuum modeling. We compared the results for flow and solute transport through a $20 \times 20 \text{m}$ model domain of fractured rock—with detailed comparison of total flow rate, its distribution, and breakthrough curves. In our modeling, we divided the $20 \times 20 \text{m}$ model domain into regular blocks, or continuum elements for the numerical simulations. We selected a model discretization of $40 \times 40$ elements (having a side length of 0.5 meter), which resulted in flow rates equivalent to that of the DFN models. Using such a model discretization, our results were in reasonably good agreement with the alternative DFN models, for advective dominated transport (under high hydraulic gradient) as well as for matrix diffusion retarded transport (under low hydraulic gradient). We think these are encouraging results, especially since our modeling approach could be readily applied for studying large-scale coupled processes in three dimensions. Of course, we must also consider that in using the large block-scale homogenized properties, we miss out on some of the heterogeneities, leading to a less dispersed transport. One potential remedy is the possibility of using the crack tensor to calculate the dispersivity of each element and adding such capability to the solute transport modeling. However, we also found that numerical dispersion has a pronounced impact on the flow when using larger grid spacing. Thus, it appears that the best way to cope with these issues is to use a property mesh that is large enough to achieve representative continuum properties and a numerical grid that is sufficiently fine to minimize numerical dispersion. Finally, using the crack tensor and TOUGH2 finite volume scheme, we encountered some difficulties when element sizes are so small that only one or a few fractures would intersect an element. In such a case, we are practically modeling the fractures discretely, albeit approximately, and this is an area where improvements are currently being pursued.
ACKNOWLEDGMENTS

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REFERENCES


Tables

Table 1 model properties of intact rock and fractures

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<th>Properties</th>
<th>Value</th>
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<tr>
<td>Elastic modulus, $E$ (GPa)</td>
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Table 2 Parameters for multicontinuum model

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Figures

Figure 1. 20 × 20 m model domain and the 2D fracture network with 7797 fractures.

Figure 2. Mechanical and hydraulic boundary conditions for investigating flow and transport under mechanical load. P1 and P2 are upstream and downstream boundary fluid pressures, and $\sigma_v$ and $\sigma_h$ are vertical and horizontal boundary stresses.

Figure 3. Hydraulic aperture correlation with fracture trace length according to Baghbanan and Jing (2007). In this case the solid line correlation function for $b = 1.0$ was used.
Figure 4. Schematic diagrams for the multiple porosity model and MINC concept according to Pruess and Narashimhan (1985). Left: A composite porous medium which consists of several distinct types of porous materials. Right: A conceptual diagram for a MINC model (Kim et al., 2012).

Figure 5. Scheme of multicontinuum approach used in this study. The original fracture network was simulated using overlapping fracture and matrix continua with equivalent properties of the fractured continuum elements calculated using Oda’s crack tensor theory, for comparison purpose the equivalent permeability was also calculated numerically using DFN modeling with NAPSAC.
Figure 6. Approach for modeling of dilatational normal displacement as a result of shear slip in fractures embedded in a rock mass.

Figure 7. Workflow of effective property calculation using crack tensor.
Figure 8. TOUGH2 steady state flow results under a vertical hydraulic gradient of 10 kPa/m for a 400 × 400 grid (160,000 grid-blocks and 0.05 m side-length) with comparison of results in which the permeability tensor were evaluated numerically (using an approach developed by Jackson et al., 2000) or analytically (using Oda’s crack tensor theory due to Oda (1989)). The red to blue contours are pressure going from 0.3 MPa (red) to 0.1 MPa (blue) resulting in a pressure gradient of 10 kPa/m. The thickness of the black lines within the model domain are proportional to the mass flow rate and the distribution of flow is shown at the bottom in terms of volumetric rate (m³/s) flowing out of each 0.05 m sized grid element at the bottom of the model domain.

Figure 9. Schematics of FDM schemes in TOUGH2 applied in this study: (a) Schematic representation showing how flow along a diagonal fracture trace would require longer flow distance along vertical and horizontal connections following a staircase path when using 5-point FDM grid, and (b) 9-point differencing that include additional diagonal connections.
Figure 10. TOUGH2 flow distribution and total flow rates through the bottom boundary for different grid sizes and comparison to total mass flow rate to DFN model results in the case of a vertical hydraulic gradient of 10 kPa/m. The TOUGH2 flow total flow are given below each model case and compared in terms of percentage of the total NAPSCA DFN model results.

Figure 11. Model simulation comparison of load dependent equivalent permeability calculated from the downstream boundary flow rate in the case of (a) horizontal and (b) vertical hydraulic gradients.
Figure 12. Solute concentration variation in fractures and rock matrix when (a) $K = 0$, and (b) $K = 5$ under a horizontal hydraulic gradient of 10 kPa/m.

Figure 13. Comparison of breakthrough curves for tracers exiting from all the three outlet for stress ratios (a) $K = 0$, (b) $K = 1$, (c) $K = 3$, and (d) $K = 5$, under a horizontal hydraulic gradient of 10 kPa/m. DFN results (IC, TUL and KTH) used for comparison were extracted from Zhao et al. (2012).
Figure 14. Effects of grid size on the breakthrough curves of tracers exiting from (a) all the three outlet boundaries and (b) the down stream boundary under a horizontal hydraulic gradient of 10 kPa/m and no mechanical load ($K = 0$).

Figure 15. Breakthrough curves of tracers exiting through various boundaries under a horizontal hydraulic gradient of 10 kPa/m and no mechanical load ($K = 0$) in the case of (a) $40 \times 40$ and (b) $4 \times 4$ element discretization.
Figure 16. Investigation of the effects of numerical dispersion by comparing breakthrough under a horizontal hydraulic gradient of 10 kPa/m and no mechanical load ($K = 0$) using a property mesh and different numerical grid resolutions: (a) $10 \times 10$ property mesh with $10 \times 10$ or $100 \times 100$ FDM grid blocks and 3 outlet boundaries and (b) $4 \times 4$ property mesh with $4 \times 4$ or $40 \times 40$ FDM grid blocks and 1 outlet boundary.

Figure 17. Comparison of breakthrough curves for tracers exiting from all the three outlet boundaries for stress ratios (a) $K = 0$, (b) $K = 1$, (c) $K = 3$, and (d) $K = 5$, under a horizontal hydraulic gradient of 10 Pa/m. DFN results (IC and KTH) used for comparison were extracted from Zhao et al. (2012).
Figure 18. Solute concentration variation in fractures and rock matrix when (a) $K = 0$, and (b) $K = 5$ under a horizontal hydraulic gradient of 10 Pa/m
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