Influence of fracture aperture on solute transport in porous media

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ABSTRACT
We study the effect of fracture networks on solute transport in heterogeneous porous media. This is conducted by combining a higher order implicit scheme for solving solute transport equations and a geomechanical finite element model. We investigate the effect of fracture aperture distribution on solute transport based on numerical simulations. Naturally fractured media exhibit anomalous transport when fracture network connectivity is well developed. Our results demonstrate highly disperse plumes and long-tails in breakthrough curves for fractured media. Our findings suggest that using average fracture aperture size is sufficient for studying the dispersive behaviour of heterogeneous porous rocks.

RÉSUMÉ
Cette étude porte sur l'effet du réseau de fractures présentes dans les milieux poreux sur le transport de solutés. Un schéma implicite au second ordre permettant la résolution des équations de transport est combiné à un modèle géomécanique aux éléments finis. Les simulations numériques montrent l'effet de la distribution des ouvertures de fractures sur le transport de solutés. Les milieux fracturés, naturellement hétérogènes, présentent des anomalies de transport lorsque la connectivité du réseau de fractures est bien développée. Les structures de panaches sont hautement dispersives, tout comme la forme des courbes d'avancée du front. Nos résultats montrent également que l'utilisation de l'ouverture moyenne des fractures est suffisante pour étudier le comportement dispersif dans les roches poreuses hétérogènes.

1 INTRODUCTION

Recent numerical studies show that fracture patterns can be realistically recreated by approximating mechanical behaviour using 2D simulations [Ingraffea and Saouma, 1985; Belytschko and Black, 1999; Olson, 1993; Renshaw and Pollard, 1994b; Huang et al., 2003]. Interest in simulating fracture growth extends across a variety of application fields including: hydraulic fracturing [e.g. Boone and Ingraffea, 1990], structural analysis for civil engineering [e.g. Bazant and Verdure, 2007], composite material design for aeronautics [e.g. Camanho et al., 2006], nuclear waste disposal risk assessment [e.g. Shen et al., 2004], and analysis of flow and mechanical properties of fractured reservoirs [cf. Zoback, 2007]. Fractures not only damage rocks making them weaker and causing fragmentation, they also influence their flow properties changing the speed at which they conduct liquids, gases, transport contaminants, among others.

Describing solute transport in terms of average equations is a challenge [Berkowitz, 2002]. It is known that velocity field variation arising from the permeability field is responsible for the dispersive movement of contaminants or tracers in heterogeneous porous media. This yields an anomalous solute transport in porous media which is also referred to as non-Fickian.

It is shown that the dispersive behaviour of solute transport is a function of scale, correlation length and heterogeneity [Berkowitz et. al., 2006; Berkowitz, 2002; Berkowitz and Scher, 1995]. Moreover, if the viscosity or density of a tracer and the background fluid is different, both porous media and fluid properties control the dispersion, e.g. [Nick et. al., 2009]. Therefore, inconstant dispersivity, early breakthrough times, and long tail of breakthrough curves are characteristic of such solute transport.

In this work we demonstrate how heterogeneity caused by geomechanically grown fractures can alter the solute transport in fractured media, and, how macroscopic behaviour emerges from small-scale structure. This paper continues with a description of governing equation used in this study. Then the numerical set-up is presented which is used to study the effect of fracture networks on solute transport in porous media. This section is followed by the results and conclusions.

2 MATHEMATICAL MODEL

In this study we combined two numerical models: deformation and fracture grown model and second order implicit flow and transport model.

2.1 Flow and transport in porous media

The specific discharge $\mathbf{u}$ [LT^{-1}], in Darcy's law,

$$\mathbf{u} = -\frac{k}{\mu}\left(\nabla p - \rho g\right) \quad [1]$$

is a function of k the intrinsic permeability tensor [L^2], μ the dynamic viscosity [$ML^{-1}T^{-1}$], P the pressure gradient [$ML^{-1}T^{-2}$] and ρ the fluid density [ML^{-3}]. Variable **g** is the gravity vector pointing in the negative Z-direction [LT^{-2}].
Conservation of mass is explained by the continuity equation,

$$\frac{\partial(\phi\rho)}{\partial t} + \nabla.(\rho\mathbf{u}) = 0,$$
[2]

Assuming a slightly compressible fluid and porous material for tracer experiments, Equations (1) and (2) yield,

$$c_t \frac{\partial p}{\partial t} + \nabla.(\frac{k}{\mu}\nabla p) = 0, \quad [3]$$

Where c_t [LT^2M^{-1}] can be written as, $c_t = \phi\beta_w + (1-\phi)\,\beta_s$ by assuming density is a function of pressure. Parameters β_w and β_s denote the compressibility of fluid phase and solid phase respectively.

The mass balance for a non-reactive and non-adsorbing solute in a non-deformable porous medium is given by,

$$\phi\frac{\partial c}{\partial t} + \nabla.\left(\mathbf{u}c\right) = 0. \quad [4]$$

where c denotes the concentration [ML^{-3}], t represents time and ϕ is porosity. In this study we neglect the local dispersion J which is the dispersive mass flux [$ML^{-2}T^{-1}$] as we are only interested to examine the effect of fracture network on advection dominated flow.

2.2 Dispersion

Advection, diffusion and dispersion are the main processes facilitating solute transport. The spreading of solutes may be resolved in the direction of fluid flow and perpendicular to it [De Josselin De Jong, 1958]. Molecular diffusion and spatial variability of the transport velocity on the sub-REV scale leads to pore-scale dispersion. When considering the instantaneous injection of a solute into a uniform flow in porous media, the spreading of solute particles around the center of mass is a function of both mechanical dispersion and diffusion, but is dominated by mechanical dispersion when advection is dominating.

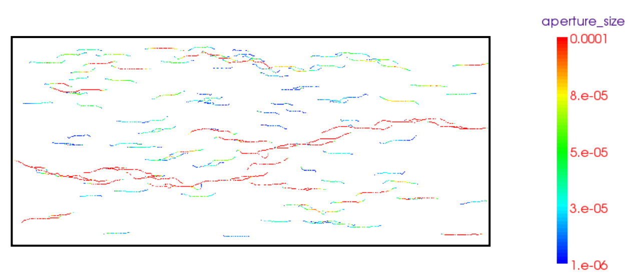
Longitudinal and transverse dispersion have been shown to vary with scale and, therefore, the spatial variability of dispersion is generally assumed to be scale-dependent and in particular due to porous media heterogeneity [Gelhar, 1986]. It is a function of both local and macro-scale velocities.

2.3 2D Fracture growth

Fractures are propagated in a quasi-static manner by deforming a model initially containing a set of randomly distributed and randomly sized flaws. We assume the matrix to be linear elastic, homogeneous, and isotropic. Finite element-based simulations are carried out to deform the 2D model. As the simulation progresses, the diamond shaped flaws grow into fractures represented by 2D polygons. At each loading step the mesh is adapted to capture the emerging fracture geometry. For a fixed set of tensional boundary conditions, the model is progressively deformed until there is no more growth ceases. This is equivalent to a high-level Picard iteration which allows fractures to advance while energy at the tips induces propagation. Mesh nodes remain stagnant as long as the equilibrium state is not reached. Every time the geometry evolves, the previous stress state is invalidated and new updated stresses are recomputed. Once fracture growth stops, nodes are moved to capture deformation. The simulation of fracture propagation is summarized as [Paluszny and Matthai, 2009]:

- Generate random flaws.
- Automatically create mesh.
- Apply boundary conditions.
- Solve deformation using FEM.
- Compute stress intensity factors, propagation lengths, and directions for all tips.
- Extend shapes of all propagating fractures.
- Remesh and mapping of variables.
- Re-compute stresses and accumulate as the stress state determined by the previous deformation step.
- Repeat all steps until no growth is recorded for a fixed boundary condition.

We use the resulting fracture network (Figure 1) to simulate solute transport. Details and validation of this method can be found in Paluszny [2009] and Paluszny & Matthai [2009].



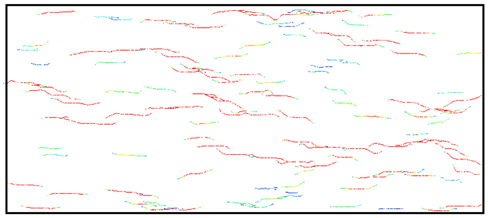


Figure 1. Two mechanically grown fracture networks after 80 iterations with maximum aperture size of 0.0001 m.

The computations presented below were conducted using the CSMP++ multi-physics simulator [Matthai et. al., 2004, Matthai et. al., 2007]. Its kernel relies on the systems algebraic multigrid method (SAMG) to solve ensuing FEM linear algebraic equations [Stuben, 2001; Stuben et. al., 2003].

2.4 Model set-up

We perform the flow and transport simulation on a 2 x 1 m subregion of the grown model. We uniformly distribute a tracer, c=1 kg/m3, initially in a 1 cm thick slit along the left side of the model. Elsewhere, concentration is set to zero. A fluid with zero concentration is injected from the left boundary ensuing from 1 MPa pressure difference between the left and right boundaries. Note that there is no density or viscosity variation in this study. These initial conditions apply to all our numerical experiments. Matrix porosity is 30%. We assume fractures to be open and calculate fracture permeability from local aperture using the parallel plate law such that $k_f = a_f^2/12$. This assumes that the flow is laminar and the fracture has smooth, stepwise parallel walls with a local separation of a_f [Kranz et al., 1979; Witherspoon et al., 1980]. We use a mixed-dimensional FV discretization method where fractures are represented by lower dimensional line discretization elements. This resolves the problem of having fracture elements with large aspect ratios. Fracture permeability, k_f, is defined as a piecewise constant value along the line elements [Geiger et. al., 2004].

3 RESULTS

A series of careful simulations is conducted on several realizations of fracture networks to study the effect of strong heterogeneity on transport.

3.1 Fracture matrix flux ratio

Bodin et al. [2003] present an extensive review of mass transport in fracture-only models. In the frequent case that fracture networks are assumed to be well-interconnected, flow is often modeled only through fractures. However, in poorly interconnected fracture networks, flow in the rock matrix is as important as that in the fracture network. The fracture-matrix flux ratio, q_f/q_m is calculated from the block-scale Darcy velocity, q_v, so that,

$$\frac{q_f}{q_m} = \frac{q_v - q_m}{q_m}. \qquad [5]$$

The matrix flux, q_m, computed from the applied far-field fluid pressure gradient, ∇P, in the direction of flow such that,

$$q_m = \frac{v_m k_m A \nabla P}{\mu\left(v_m + v_f\right)}, \qquad [6]$$

where v_m and v_f are the matrix and fracture pore volumes, A is the cross sectional area of the model perpendicular to the direction of flow.

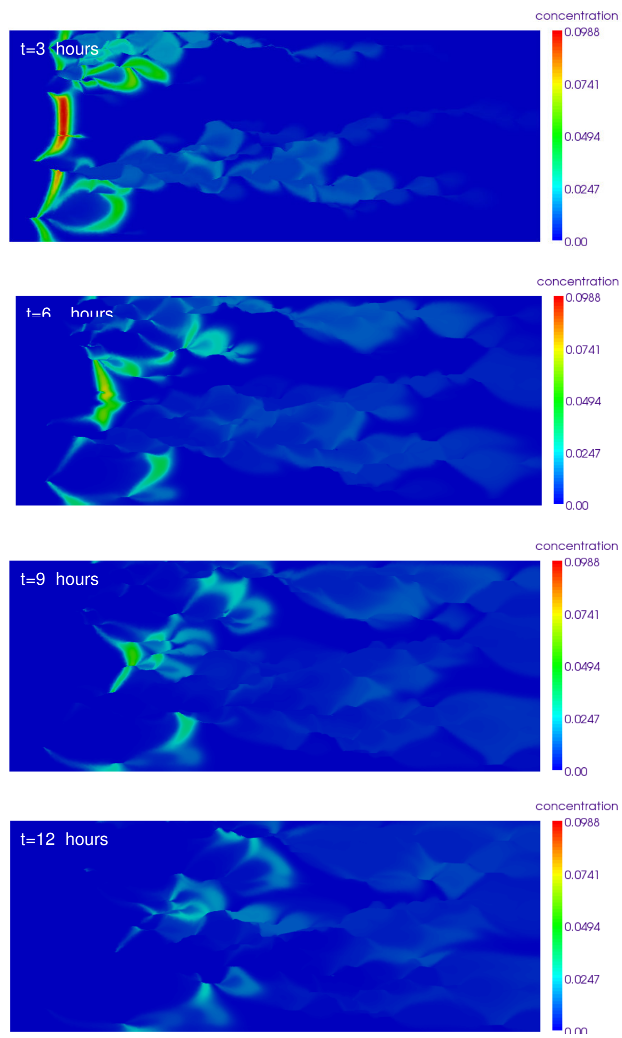


Figure 2. Concentration fronts at different time steps for one realization with k_m=8mD.

Matthai and Belayneh (2004) show the controlling role of fracture-matrix flux ratio on fluid flow in fractured media. This ratio is indicative of the permeability contrasts in the system and can be used to understand solute transport behaviour in rocks where there is significant interaction between rocks and fracture. Four different q_f / q_m ratios are gained by altering the rock matrix permeabilities, k_m= 10, 8, 6, 4 mD. Simulations are conducted on 7 different realizations of fracture networks. Figure 2 illustrates concentration fronts for one realization at different time steps. Concentration profiles for one realization are shown in Figure 3. Results indicate that the plume transverses slower in the model with lower matrix permeability. This slow movement of the plume in the matrix and higher fracture matrix flux ratio leads to stronger anomalous behaviour. This has an explicit effect on the dispersive behaviour of the system. Figure 4 reveals breakthrough curves for different q_f / q_m ratios. For each matrix permeability the breakthrough curves of 7 realizations are averaged (see Figure 5). It is clear that smaller matrix permeability value cause a stronger localization of flow in fractures. Hence, higher fracture-matrix flux ratio yields more dispersive behaviour. Our simulation results indicate that the standard advection-diffusion equation, ADE, is inadequate to represent flow and transport in fractured media for large scale as it results a Gaussian behaviour. This is in accordance with the findings of Berkowitz [2002] and Berkowitz et. al., [2006].

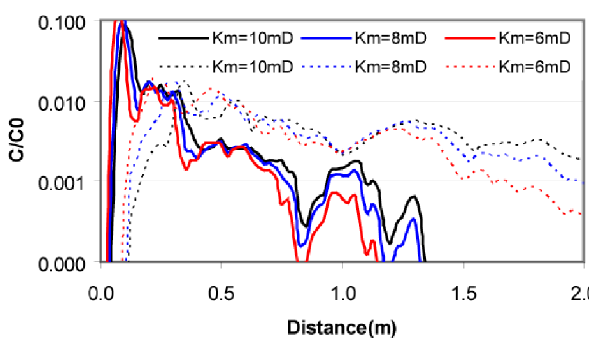


Figure 3. Concentration profiles for one realization with different permeabilities at two different times. The bold lines are the profiles after 1 hour and the dash lines are the concentration profiles after 5 hours.

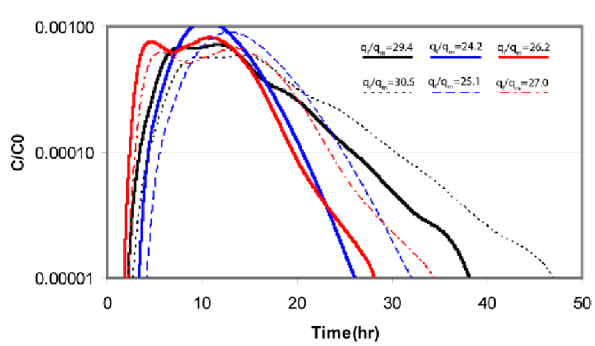


Figure 4. Breakthrough curves for three realization with different fracture matrix flux ratios.

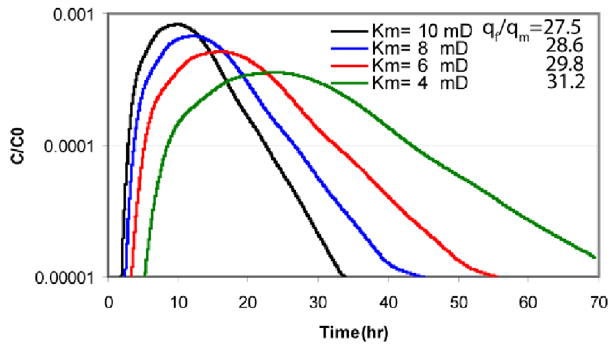


Figure 5. Average breakthrough curves for different fracture matrix flux ratios.

3.2 Average fracture aperture size

We calculate fracture aperture size distribution based on the accurate geomechanical model. This detailed data captures permeability variations which have a strong influence on the effective permeability of the system [Paluszny et al., 2009]. Here, we calculate average permeability using the mechanical simulation results, i.e. considering fractures with inconstant aperture sizes. Then by using an iterative method we determine a constant average aperture size which results the same average permeability.

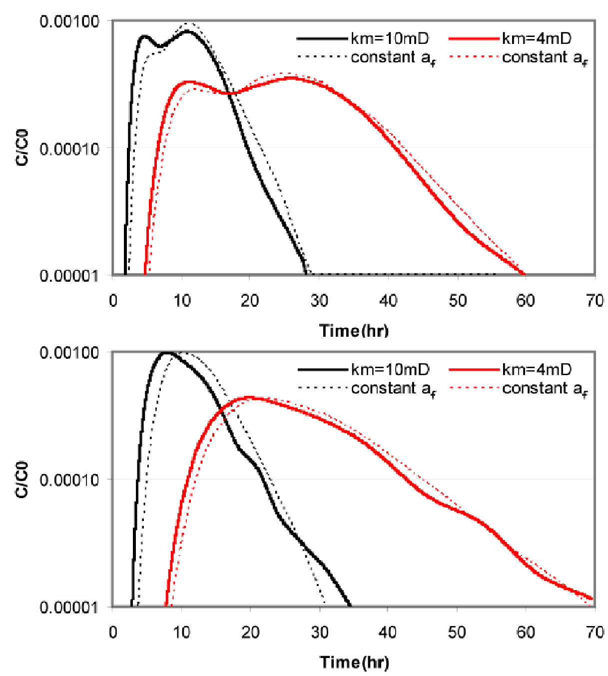


Figure 6. Two realizations are used to compare the breakthrough curves of the models with actual aperture distribution and the ones with the average aperture sizes.

Now, we can use the calculated average aperture size value to conduct the same flow and transport simulation to study the discrepancy of this simplified model result with the result of simulation using detail information of aperture distribution. This comparison is shown in Figure 6 for two different realizations. The main difference is the time to breakthrough which is slightly smaller for the model with detailed aperture size information. For the simplified model, later arrival of solute to the output boundary is due to uniform distribution of fracture aperture size in comparison to the simulation with the inconstant aperture size. In the latter, the aperture size variation provides more channelling in the flow. Surprisingly, the slopes of the breakthrough curves are very similar which can be used to evaluate dispersive behaviour of such system. In order to show the effect of matrix permeability this comparison is done for the system with two different rock matrix permeabilities, 10 mD and 4 mD. The discrepancy between breakthrough curves are small, and, less pronounced for the smaller matrix permeability. Our results imply the efficiency of using average aperture size for transport simulations.

4 CONCLUSIONS

This paper reports numerical results of the solute transport in geomechanically grown fractured porous media. We investigate the role of fracture aperture and network on solute transport. The following conclusion arising from this analysis can be drawn:

- Long-tails in the breakthrough curves and early breakthrough indicate anomalous transport of solute in fractured media.
- The standard advection-diffusion equation is inadequate to represent flow and transport in fractured media for large scale.
- Large variation of permeability field induced by existence of open fractures yields anomalous transport even without incorporating diffusion at local scale.
- The fracture matrix flux ratio can be used to quantify the average dispersive behaviour of solute transport in naturally fractured media.
- The average aperture size calculated based on the average permeability of the media is sufficient for flow and transport modeling.

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