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A modelling investigation of solute transport in permeable porous media containing a discrete preferential flow feature

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ABSTRACT

Preferential flow features (PFFs, e.g. fractures and faults) are common features in rocks that otherwise have significant matrix permeability. Despite this, few studies have explored the influence of a PFF on the distribution of solute plumes in permeable rock formations, and the current understanding of PFF effects on solute plumes is based almost entirely on low-permeability rock matrices. This research uses numerical modelling to examine solute plumes that pass through a PFF in permeable rock, to explore the PFF's influence on plume migration. The study adopts intentionally simplified arrangements involving steady-state solute plumes in idealised, moderate-to-high-permeability rock aquifers containing a single PFF. A range of matrix-PFF permeability ratios (4.9×10^{-6}–2.5×10^{-2}), typical of fractured sedimentary aquifers, is considered. The results indicate that for conditions representative of high-to-moderate-permeability sedimentary rock matrices containing a medium-sized fracture, the effect of the PFF on solute plume displacement and spreading can be considerable. For example, plumes are between 1.3 and 19 times wider than in associated porous media only scenarios, and medium-sized PFFs in moderately permeable matrices can reduce the maximum solute concentration by up to 10^4 times. Plume displacement and spreading is lower in aquifers of higher matrix-PFF permeability ratios, and where solute plumes are more dispersed at the point of intersection with the PFF. Asymmetry in the plume caused by the passage through the PFF is more pronounced for more dispersive plumes. The current study demonstrates that PFFs most likely govern solute plume characteristics in typical permeable matrices, given that a single PFF of aperture representing a medium-sized fracture (i.e. 5.0×10^{-4} m) produces the equivalent spreading effects of 0.22–7.88 m of plume movement through the permeable matrix.

1. Introduction

There are numerous problems of environmental concern that involve the transport of solutes in rocks containing preferential flow features (PFFs) such as fractures and faults. These include the long-term disposal of high-level radioactive waste (Reeves et al., 2008), groundwater contamination arising from urban development and industrialization (Birkhölzer et al., 1993a), amongst many others. In recent decades, considerable research attention has been given to the transport of solutes in aquifers of low-permeability rock matrices containing PFFs, where the transport of solutes occurs primarily via advection and dispersion within the PFF, and exchanges between PFFs and the rock matrix occur by molecular diffusion (e.g. Grisak and Pickens, 1981; Sudicky and Frind, 1982; Himmelsbach et al., 1998; Bense et al., 2013, Gassiat et al., 2013). This body of work has demonstrated that PFFs can provide pathways through which contaminated fluids can migrate rapidly relative to transport in the rock matrix (i.e. the primary porosity), which can attenuate solute breakthrough curves and cause longer residence times than impermeable rocks containing PFFs (Bear et al., 1993; Singhal and Gupta, 2010).

Flow and transport in aquifers containing PFFs and with moderate-to-high matrix permeability requires consideration of solute advection, mechanical dispersion and molecular diffusion in both the PFF and the porous matrix (Birkhölzer et al., 1993a). These conditions have received far less attention compared to low-permeability matrix settings (Rubin et al., 1997; Odling and Roden, 1997). This is despite that PFFs are common features in high-yielding, permeable rock aquifers (e.g. fractured limestone and sandstone), and are critical factors in the occurrence of many groundwater-dependent ecosystems (e.g. springs and outflows along PFFs in carbonate rocks; Bauer-Gottwein et al., 2011).

Studies of solute transport in permeable matrices containing PFFs include the work of Birkhölzer et al. (1993a; 1993b),

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Rubin and Buddemeier (1996), Rubin et al. (1997), Odling and Roden (1997), Sonnenborg et al. (1999) and Houseworth et al. (2013). Birkhölzer et al. (1993a; 1993b) presented an analytical model to describe advection-dominated solute transport (i.e. diffusion/dispersion is negligible) in a 2D PFF network embedded in a permeable rock matrix. The authors developed a 'diffusion-advection number' to determine the conditions for which diffusive exchange (via molecular diffusion) between the PFF and matrix is insignificant relative to advective PFF-matrix solute exchange. Results from numerical simulations (Birkhölzer et al., 1993b) indicated that solute transport in permeable rocks matrices containing parallel, equidistant PFFs with uniform aperture can be represented using an equivalent porous media (EPM) approach if the representative elementary volume of the network is large enough. Rubin and Buddemeier (1996) demonstrated that in permeable formations, the ratio of transverse to longitudinal dispersivity that is required to reproduce contaminant distributions in an EPM model is sensitive to the orientation of the PFF. Transverse dispersivity may exceed longitudinal dispersivity as the PFF angle relative to the direction of flow (α_{pff}) approaches 90°. As α_{pff} approaches 0°, longitudinal dispersivity increases and advection in the PFF dominates flow in the system. These studies consider formations that can be approximated using the EPM approach, and do not provide insight into the local-scale effects of individual, discrete PFFs on the distribution of solute plumes in permeable matrices.

The methodology of Birkhölzer et al. (1993a; 1993b) was employed by Rubin et al. (1997) to examine solute transport in permeable media containing PFFs when the flow velocities inside PFFs are slow (i.e. the flow velocity inside the PFF is of the same order of magnitude as the matrix flow velocity). They found that the larger the deviation of the matrix-PFF velocity ratio from unity, the greater the effective dispersivity of the fractured permeable formation (Rubin et al., 1997). Odling and Roden (1997) used numerical modelling to study 2D flow and solute transport in permeable rock containing PFFs arranged according to naturally occurring geometries. They found that in permeable matrices (i.e. unlike for low-permeability rock), PFF orientation and density can be as influential as PFF connectivity on contaminant transport rates and solute plume heterogeneity. Hence, matrix-PFF hydraulic conductivity contrasts and PFF orientation are likely to influence the distribution of solutes in permeable rock matrices that are subject to both advective and dispersive transport processes. The effect of an individual PFF on solute transport in permeable matrices was not considered in the abovementioned studies; despite that transport processes at small scales can influence dramatically solute transport at larger scales (Grisak and Pickens, 1980).

Laboratory experiments and numerical modelling were carried out by Sonnenborg et al. (1999) to examine 2D flow and solute transport in a permeable matrix with variable aperture PFFs. They demonstrated that the EPM approach may be justified for modelling preferential flow systems where physically realistic values for macro-porosity and macro-dispersivity could be obtained. Further experimental and theoretical work was recommended to test the range over which the EPM approach might be valid. Houseworth et al. (2013) obtained a closed-form analytical solution for solute transport during steady-state saturated flow in a single PFF embedded within a porous, permeable rock matrix. Unlike existing analytical solutions, Houseworth et al. (2013) incorporated lateral matrix diffusion, and flows through both the matrix and PFF. Their study considered the case where matrix diffusion dominates in comparison to matrix dispersion, and hence they did not provide insight into the effect of a PFF on a solute plume in a matrix that is subjected to both advection and dispersion.

Case studies of solute transport in karst aquifers (i.e. PFFs that are formed by fractures, faults and/or karst conduits) include Bonacci and Roje-Bonacci (1997) and Arfib et al. (2007). Mechanisms of seawater intrusion (SWI) through coastal karst springs were investigated in Blaž, Croatia (Bonacci and Roje-Bonacci, 1997) and central Crete, Greece (Arfib et al., 2007). Both studies demonstrated that PFFs can alter the distribution of seawater in coastal aquifers compared with the classical description of a 'seawater wedge' in porous media. A recent study by Sebben et al. (2015) employed numerical models to investigate the characteristics of SWI in permeable rock matrices containing simple PFF network geometries. Their study demonstrated that PFFs can either widen or narrow the seawater wedge relative to porous media only (PMO) formations, depending on the PFF location and orientation. While Sebben et al. (2015) offer macro-scale descriptions of PFF effects on SWI plumes, the mechanisms that underlie solute plume widening (or narrowing) as it passes through an individual PFF were not explored because of the complex effects of heterogeneities on the density-dependent flow field. Quantitative analyses of solute plumes that intercept a PFF are needed at local scales to explain the integrated, macro-scale solute behaviour of previous PFF-permeable matrix studies.

The purpose of the current study is to explore within a modelling framework the influence of a single PFF (representing a medium-sized fracture) on the distribution of solutes in a permeable rock matrix. Numerical simulations are conducted to investigate PFF effects on a 2D solute plume caused by a point source, under steady-state groundwater flow conditions where regional flow is oblique to the PFF. Results are compared with associated PMO models, to determine the influence of PFFs on both the horizontal displacement of peak solute concentrations and the spreading of contaminant plumes in permeable rock matrices. We examine the distribution of solutes for a variety of matrix-PFF permeability ratios (given in terms of hydraulic conductivity, i.e. the matrix hydraulic conductivity is modified) and contaminant source locations, adopting aquifer properties that are representative of sedimentary rocks (e.g. sandstone and limestone) in which preferential flow through discrete features and flow in the matrix are known to occur (e.g. Webb et al., 2010; Al Ajmi et al., 2014).

2. Methodology

2.1. Conceptual model

The discrete fracture network (DFN) approach, wherein individual PFFs are incorporated explicitly into an n-dimensional model as (n-1)-dimensional features (e.g. Smith and Schwartz, 1984), was employed in numerical modelling experiments. PFFs within a DFN are assumed to contain water that is fully-mixed across the PFF width, such that solute concentration is uniform across the PFF's aperture. The model used here to evaluate PFF effects simulates groundwater flow and solute transport in a 1 m × 1 m 2D cross section through a homogeneous, isotropic, confined aquifer containing a single, discrete horizontal PFF at $z = 50$ cm. The small domain size was chosen because very fine grid spacing perpendicular to the PFF-matrix interface ($\Delta z \approx$ PFF aperture) is required if grid-independent results are to be achieved (Weatherill et al., 2008). Computational restrictions (i.e. avoiding excessively long run times) currently limit the application of DFN models to small-scale solute transport problems, if grid-independent results are sought (e.g. Tang et al., 1981; Graf and Simmons, 2009).

The model set up, including flow and transport boundary conditions, is shown in Fig. 1. Constant head boundaries are prescribed so that the groundwater flow direction (α_f) is 45° relative to the orientation of the PFF. An α_f of 45° was chosen so that displacement of streamlines is expected to occur (i.e. $0^\circ < \alpha_f < 90^\circ$). The flow field in the matrix is unaffected by the introduction of the PFF, because the model set up is such that the superposition principle applies to the flow field. A continuous mass flux