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On the effects of preferential or barrier flow features on solute plumes in permeable porous media

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ABSTRACT

Despite that discrete flow features (DFFs, e.g. fractures and faults) are common features in the subsurface, few studies have explored the influence of DFFs on solute plumes in otherwise permeable rocks (e.g. sandstone, limestone), compared to low-permeability rock settings (e.g. granite and basalt). DFFs can provide preferential flow pathways (i.e. 'preferential flow features'; PFFs), or can act to impede flow (i.e. 'barrier flow features'; BFFs). This research uses a simple analytical expression and numerical modelling to explore how a single DFF influences the steady-state distributions of solute plumes in permeable aquifers. The analysis quantifies the displacement and widening (or narrowing) of a steady-state solute plume as it crosses a DFF in idealised, 1 × 1 m moderately permeable rock aquifers. Previous research is extended by accounting for DFFs as 2D flow features, and including BFF situations. A range of matrix-DFF permeability ratios (0.01 to 100) and DFF apertures (0.25 mm to 2 cm), typical of sedimentary aquifers containing medium-to-large fractures, are considered. The results indicate that for the conceptual models considered here, PFFs typically have a more significant influence on plume distributions than BFFs, and the impact of DFFs on solute plumes generally increases with increasing aperture. For example, displacement of peak solute concentration caused by DFFs exceeds 20 cm in some PFF cases, compared to a maximum of 0.64 cm in BFF cases. PFFs widen plumes up to 9.7 times, compared to a maximum plume widening of 2.0 times in BFF cases. Plumes crossing a PFF are less symmetrical, and peak solute concentrations beneath PFFs are up to two orders of magnitude lower than plumes in BFF cases. This study extends current knowledge of the attenuating influence of DFFs in otherwise permeable rocks on solute plume characteristics, through evaluation of 2D flow effects in DFFs for a variety of DFF apertures, and by considering BFF situations.

1. Introduction

Discrete flow features (DFFs) such as fractures, faults, sand lenses and clay layers are common geologic features in groundwater systems. DFFs can provide preferential pathways (i.e. 'preferential flow features'; PFFs) or act as barriers (i.e. 'barrier flow features', BFFs) to fluid flow and solute transport. DFFs are common in rock aquifers where the parent rock permeability ranges from virtually impermeable (e.g. granite and basalt) to permeable (e.g. sandstone and limestone). Considerably less research attention has been paid to the role of PFFs in modifying groundwater flow and solute transport in permeable rock aquifers, compared to low-permeability rocks (Rubin et al., 1997; Odling and Roden, 1997). The influence of BFFs has been studied to a lesser degree than PFFs. Nonetheless, previous studies of low-permeability rocks (e.g. Thoma et al., 1992; Kessler and Hunt, 1994) have shown that fluid flow and solute transport can be altered significantly by the restrictions to flow caused by BFFs.

Solute transport in low-permeability rocks containing PFFs typically occurs via solute advection and mechanical dispersion within the PFF only, and exchanges between PFFs and the rock matrix occur by molecular diffusion (e.g. Grisak and Pickens, 1981; Sudicky and Frind, 1982). However, in permeable rock aquifers containing PFFs, solute transport more likely occurs via advection, mechanical dispersion and molecular diffusion in both the PFF and the rock matrix (Birkhölzer et al., 1993a). Hence, consideration of these transport processes is required to ascertain the impacts of PFFs on solute transport in otherwise permeable rocks.

Previous studies of solute transport in permeable rocks containing PFFs include Birkhölzer et al. (1993b), Rubin and Buddemeier (1996), Odling and Roden (1997), Houseworth et al. (2013), Willmann et al. (2013), Sebben et al. (2015) and Sebben and Werner (2016). Birkhölzer et al. (1993b) examined solute transport in frac-

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tured rock formations and found that solute transport in permeable rocks containing parallel, equidistant PFFs with uniform aperture can be represented using the equivalent porous media (EPM) approach (i.e. PFFs are not incorporated explicitly into the model) if the representative elementary volume of the network is large enough. Rubin and Buddemeier (1996) found that 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. Odling and Roden (1997) used numerical modelling to study 2D flow and solute transport in permeable rocks containing naturally occurring PFF geometries. They concluded that the orientation and density of PFFs can be as influential as PFF connectivity on contaminant transport rates and solute plume heterogeneity. However, the effect of transport processes at the scale of an individual PFF was not considered, and therefore the key factors driving solute transport within their PFF networks were not revealed, despite that these small-scale processes can influence solute transport at larger scales (Grisak and Pickens, 1980).

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. The authors incorporated several factors not previously included in analytical solutions for comparable transport problems, including 2D flow in the matrix and a general solute source position. Houseworth et al. (2013) considered the case where advective velocities in the matrix are sufficiently small that matrix diffusion dominates in comparison to matrix dispersion. Hence, the effect of a PFF on a solute plume in a matrix that is subjected to both advection and dispersion remains unexplored. Willmann et al. (2013) developed a particle-tracking method that accounts for advection and diffusion explicitly in both the PFFs and surrounding matrix. Mass exchanges from the PFF into the matrix are dependent on the advective flux perpendicular to the matrix, the PFF aperture, and the diffusive component. The authors recommended further research to ascertain whether a transport-related PFF aperture should be used in preference to the hydraulic aperture.

The influence of simple PFF network geometries on seawater intrusion in otherwise permeable coastal aquifers was examined by Sebben et al. (2015). They employed discrete fracture network (DFN) modelling to demonstrate that PFFs can either widen or narrow the seawater wedge relative to homogenous porous media formations, depending on the location and orientation of the PFFs. Sebben et al. (2015) describe PFF effects on seawater intrusion at the macro-scale; however, the complex effects of heterogeneities on the density-dependent flow field precluded examination of the mechanisms that underlie solute plume widening (or narrowing) as it crosses an individual PFF. Local-scale, quantitative analyses of solute plumes that intercept a PFF are therefore needed to explain the integrated, macro-scale solute behaviours observed in previous PFF-permeable matrix studies (Sebben and Werner, 2016).

Sebben and Werner (2016) used DFN modelling to explore the influence of a single PFF on the distribution of solutes in moderate-to-high permeability rock matrices (10^{-6} m/s–10^{-3} m/s, e.g. sandstone and limestone). Numerical simulations were performed to investigate PFF effects on a 2D solute plume under steady-state groundwater flow conditions. Their study considered the influence of PFFs that represent medium-sized fractures (0.25 mm–0.5 mm fracture aperture). Further, PFFs were assumed to be fully mixed, open channels (i.e. flow through PFFs was calculated according to the cubic law (Berkowitz, 2002; Graf and Therrien, 2007)) that can be treated as 1D flow features. The authors found that the degree of spreading that occurs when solute plumes pass through medium-sized PFFs in moderate-to-high permeability matrices is highly dependent on the ratio of the matrix hydraulic conductivity (K_m) to the hydraulic conductivity of the PFF (K_f), and on the concentration of the plume where it encounters the PFF. In cases with low K_m/K_f values, PFFs were found to dilute solute plumes by factors of greater than 100.

Sebben and Werner (2016) encountered seemingly anomalous behaviour arising out of the advection-dispersion equation in the form of higher-than-expected solute concentrations up-gradient of the PFF. It is hypothesised that these are non-physical effects attributable to 'back dispersion' (termed 'upstream dispersion' by Konikow (2011)), which is the anomalous movement of solutes from the PFF back into the matrix against the direction of groundwater flow. Back dispersion has been recognised by Al-Niami and Rushton (1977), Marino (1978) and Kumar (1983). In reality, dispersion of solutes in opposition to the flow of groundwater is expected only in low-permeability sediments, where solute transport by molecular diffusion may exceed advective transport rates (e.g. Grisak and Pickens, 1980; Harrison et al., 1992). It is likely that this effect is not physically realistic for the PFF situations examined by Sebben and Werner (2016), given the moderate-to-high permeability of the rock matrices considered. Back dispersion has also been observed previously in numerical investigations of seawater intrusion (e.g. Segol et al., 1975; Frind, 1982), solute transport in aquifers containing structured heterogeneities (e.g. Liu et al., 2004), and surface-subsurface solute exchanges in hillslope settings (e.g. Liggett et al., 2014). Presently, there is no guidance on the extent of errors in solute predictions for situations where back dispersion is thought to have impacted modelling results. Further analyses were recommended by Sebben and Werner (2016) to ascertain the extent to which back dispersion adversely impacts the results of numerical experiments of DFF situations.

In some cases, DFFs contain material that is less permeable than the host rock, and hence, form BFFs (e.g. Laubach, 2003; Bense and Person, 2006). For example, fractures may be partially or completely clogged as a result of mineral deposition formed by weathering reactions (e.g. Thoma et al., 1992; Kessler and Hunt, 1994). Previous studies of BFFs in permeable rock matrices have focussed primarily on characterising the flow regime rather than solute transport processes. For example, Antonelli and Aydin (1994) used mini-permeameters and image analysis to characterise the porosity and permeability of fault zones in sandstone outcrops. They found that low-permeability deformation bands (0.5–2 mm thick) can have permeabilities one to four orders of magnitude lower than the host rock. Bense et al. (2003) characterized faults in the Roer Valley Rift System (the Netherlands), and showed that in some cases, vertical faults may act as barriers to horizontal fluid flow (i.e. perpendicular to the fault). Groundwater level fluctuations, spring discharge rates and packer tests were analysed by Celico et al. (2006) to help refine the conceptual model of the Matese fractured limestone aquifer (Italy); in particular, by characterising the fault zone hydraulic conductivity. Their analyses highlighted the presence of low-permeability zones within the fault that act as barriers to groundwater flow perpendicular to the fault.

Bense and Person (2006) examined the conduit-barrier behaviour of the Baton Rouge Fault, which traverses sedimentary sediments in south Louisiana (USA). Large changes in hydraulic head were observed across the fault, indicating low permeabilities normal to the fault, whereas geochemical data showed enhanced vertical fluid flows (i.e. along the fault). Numerical modelling of 2D steady groundwater flow and solute transport demonstrated that the anisotropic nature of faults can partly explain the dual conduit-barrier behaviour observed in field studies.

Studies of solute transport across BFFs include analyses of contaminant migration across clay liners (e.g. Johnson et al., 1989) or barrier walls (e.g. Zhang and Qiu, 2010). These studies found that low-permeability clay liners beneath waste disposal sites may not prevent contamination of underlying aquifers (Johnson et al., 1989), and that contaminant migration is largely influenced by the barrier's depth and hydraulic conductivity (Zhang and Qiu, 2010).