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Research papers

Quantification of solute penetration in an asymmetric fracture-matrix system

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ABSTRACT

Solute and/or heat penetration into a fracture-matrix system is an important subject in subsurface transport. Solute and/or heat partitions among the fracture and its surrounding rock matrixes are based on coupled transport processes that are closely related to transport properties of the media. The penetration processes in an asymmetric fracture-matrix system are more complicated than that in a symmetric fracture-matrix system, due to different matrix properties. Accurate quantification of plume distribution in such a system is the basis of remediation design and risk assessment of a contaminated fracture-matrix system. Closed-form analytical and semi-analytical solutions (involving integrations) are obtained in this study to quantify the influences of asymmetric matrix properties on solute penetration processes in a fracture-matrix system. Advection, matrix diffusion, sorption, source decay and aqueous phase decay are considered. Numerical simulations are performed using HydroGeoSphere to test the solutions. Well matched curves of the numerical results and the closed-form solutions and semi-analytical solutions are obtained. The matrix porosity and retardation factor appear to significantly affect the spatiotemporal distribution of solute in a fracture-matrix system. Penetration depth in the matrix is a linear attenuation function of the horizontal distance from the source. And a new dimensionless number called the *Z* number (or the matrix penetration number) is defined to quantify the maximal penetration depth into the matrix. The solutions obtained can act as an effective tool for assessment of solute and/or heat transport in a fracture-matrix system. The solutions are also applicable to advection-dominated solute and/or heat transport in a thin aquifer bounded by two different aquitards.

1. Introduction

Groundwater quality and subsurface contaminant transport have drawn much attention in the hydrological and environmental communities over five decades. As key channels of fluid flow and solute/heat transport, fractures and fracture networks play an important role in controlling subsurface environments (Novakowski and Lapcevic, 1994). Consequently, numerous investigators have made great efforts to study the mechanism of transport processes in fractured rocks (Dai et al., 2009; Dejam et al., 2016; Roubinet et al., 2012; Sudicky and Frind, 1982; Tang et al., 1981). Fractured porous medium is typically characterized by less permeable matrix blocks and a more permeable network of fractures. As solutes enter a fracture-matrix system, the plume will penetrate into the fracture as well as into the surrounded matrixes. Solute mass transfer between the fracture and matrix is through molecular diffusion, sometimes accompanied by other chemical reaction processes in the matrix (Dai et al., 2009). Many studies have shown that solute diffusion from a fracture into matrix plays an important role in controlling the transport process and could not be ignored. For instance, matrix diffusion has been proven to retard the solute migration velocity and to decrease the solute peak concentration in the fracture (Jardine et al., 1999; Liu et al., 2004; Maloszewski and Zuber, 1985; Neretnieks, 1980).

A paradigm developed over the past several decades for solute transport in a fracture-matrix system makes use of the assumptions that the matrixes adjacent to the fractures have the same transport properties including porosity, effective diffusion coefficient and reaction rate. Such a paradigm is termed the symmetric matrix scenario, in which one only needs to deal with a half-plane because of the symmetry of the problem (Roubinet et al., 2012; Shahkarami et al., 2015; Tang et al., 1981; Zhu et al., 2016). The symmetric matrix scenario is a special case of a more general asymmetric matrix scenario which allows matrixes bounding the fracture to have different transport properties. Examples of asymmetric matrix scenario are not uncommon in real geological setting. For instance, fractures surrounded by different rock matrixes are commonly seen in interlayer fault zones in which some rapid

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transport pathways can act as conduits for transmitting subsurface flows over large distances (Walker et al., 2013; Fairley et al., 2003). Transport properties vary significantly for different parts of the fault zones, depending on displacement rates, offsets and host rocks (Evans et al., 1997; Fairley and Hinds, 2004). Caine et al. (1996) presented field and laboratory observations in brittle fault zones which are lithologically heterogeneous and structurally anisotropic. Chester and Logan (1986) explored the Punchbowl fault zone which is bounded by extensively damaged host rock, and field observations showed that the texture and fabric of the surrounded layers varied greatly. Cipollari and Cosentino (1995) studied several unconformities controlled by tectonic processes or eustasy and indicated that the layers near the unconformities may have different transport properties. Similar situations were shown by Raffensperger and Garven (1995), who investigated two unconformity-type uranium deposits in Australia and Canada, in which the upper and lower layers are separated by faults. These unconformities could act as preferential pathways for water and solute transport. Zhou and Zhan (2018) have documented various cases of different lithology bounded a single fracture, which will lead to asymmetric matrix diffusion in a fracture-matrix system. For solute transport mentioned above, the symmetric fracture-matrix models are not practicable and asymmetric models are more applicable instead.

Since matrix diffusion can be of considerable importance to transport process in fractured media, the asymmetric matrix properties may significantly affect the solute spatiotemporal distribution, especially for cases in which large parameter differences exist between different matrixes. Determining the impact of different matrix properties on the transport process through a cost-effective way such as using analytical and semi-analytical methods would be instructive regarding physical process that controls the solute transport. Zhou and Zhan (2018) considered different values of properties for the surrounded matrixes bounding a horizontal single fracture when developing a semi-analytical solution using Laplace transform, considering longitudinal dispersion in the fracture (among other factors). Numerical inverse Laplace transform is adopted by Zhou and Zhan (2018) to obtain solutions in real-time domain. As numerical inverse Laplace transform techniques may involve various degrees of numerical errors, if it is not done properly (Wang and Zhan, 2015), the semi-analytical solution developed in such a fashion must be tested, preferably against a closed-form analytical solution, which is unfortunately not available. Alternatively, Zhou and Zhan (2018) compared their semi-analytical solution with a high-resolution finite-element numerical solution using COMSOL, and found that both solutions agreed with each other very well. No closed-form analytical solution was obtained in Zhou and Zhan (2018).

The purpose of this study is to develop closed-form analytical solutions, as well as semi-analytical solutions (involving integrations) to describe the solute penetration process in an asymmetric fracture-matrix system and to evaluate the effect of various matrix parameters on the spatiotemporal concentration profiles in the system. The "closed-form" solutions are simply algebraic functions of spatial and temporal coordinates (which is the case in Section 2.1 for a conservative solute). And the semi-analytical solutions in this work do not involve numerical inverse Laplace transform, but have functions that include integrations which can be computed straightforwardly at almost any given degree of accuracy. Our work differs from the previous studies with symmetric matrix properties on the consideration of different matrix properties. Specially, we try to figure out the extent of influences of different matrix parameters on solute penetration, and to evaluate under what conditions such influences can be ignored. This work can be applied to deal with asymmetric matrix diffusion for heat penetration in a fracture-matrix system, simply by replacing the solute transport properties with the heat transport properties. Furthermore, the work may be applied to study solute and/or heat penetration in an aquifer bounded by two different aquitards from above and below, provided that the transport in the aquifer is advection-dominated (or aquifer dispersions are negligible), which can be true when the aquifer is relatively thin in respect to the scale of transport.

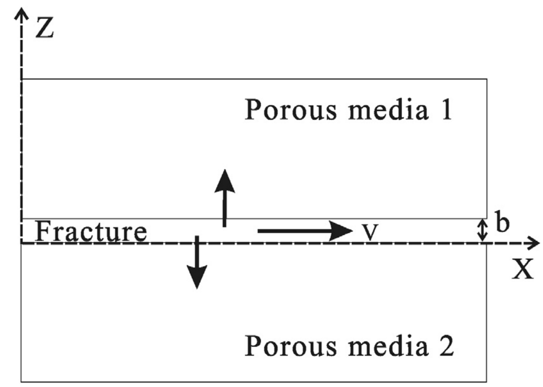

Fig. 1. The diagram of the asymmetric fracture-matrix system.

The paper is organized as follows. A conceptual model of the problem will be established first, followed by the mathematical model and the development of associated closed-form solutions and semi-analytical solutions involving integrations. Closed-form steady-state solutions are also provided. The obtained solutions are tested extensively against the uniquely designed high-resolution numerical simulations using HydroGeoSphere and against previous solutions under special circumstances. The tested solution will be used as a diagnostic tool to assess the impact of different matrix properties on the transport process. After that, applications of the developed solutions will be discussed before summarizing the findings in the conclusion.

2. Conceptual model

The conceptual model presented here takes place in a single horizontal fracture with an aperture of b, adjacent with two semi-infinite rock matrixes which have different transport properties (Fig. 1). Both matrixes are much less permeable as compared to the fracture. Advective transport with a constant flow velocity takes place in the fracture and molecular diffusion takes place in the matrix. The dimensions of matrix and fracture are sufficiently large in the horizontal direction thus the lateral boundaries far from the source will not impose any noticeable influence on the domain of interest. The thicknesses of both matrix blocks are also sufficiently large so that their vertical dimensions will not affect the transport process. This assumption is generally valid as the penetration depth of solute into the matrix via molecular diffusion is usually quite limited to the near-fracture regions (Zhu et al., 2016). Origin of the coordinate system is at the bottom of the fracture on the left boundary from which the solute enters the fracture (see Fig. 1). The x-axis is along the constant flow direction in the fracture (horizontal) and the vertical axis z is positive upward. The fracture-matrix system is free of solute of concern at $t = 0$.

For the sake of developing closed-form analytical solutions, a series of assumptions are inevitable for simplifying the fracture-matrix system. First, the fracture-matrix interfaces are assumed to be two parallel horizontal planes, like that described by Zhou and Zhan (2018). Second, the fracture is assumed to have a constant aperture without any filling, meaning that any hydromechanical effect due to the stress–-strain changes is not a concern, and the fracture porosity is 1. This assumption can be relaxed to deal with a filled single fracture by considering a less than unity fracture porosity, as investigated by Zhou et al. (2017). Third, longitudinal and transverse dispersions in the fracture are neglected, as transport in the fracture is usually advection-dominated with limited dispersive spreading. This is understandable if one recalls that dispersion is caused by velocity variation. For an idealized single fracture as shown in Fig. 1, the only velocity variation inside the fracture is the parabolic velocity distribution along the z-axis over the fracture aperture, which is quite limited.