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Impact of thin aquitards on two-dimensional solute transport in an aquifer

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ABSTRACT

The influence of aquitards on solute transport in an aquifer is an important and often overlooked process for subsurface contaminant transport. In particular, slow advection (leakage) into an aquitard is often neglected in previous analytical treatment of solute transport, making such analytical solutions unsuitable for benchmarking numerical simulations of transport when aquitard leakage exists. In this study, a semi-analytical solution to the two-dimensional conservative solute transport in an aquifer bounded by thin aquitards is derived in the Laplace domain. The governing equation in the aquifer (not aquitard) incorporates terms accounting for advection, longitudinal dispersion, and transverse vertical dispersion. Both one-dimensional vertical advection and molecular diffusion are considered for aquitard transport. The solutions are derived under conditions of steady-state flow and the first- and third-type transport boundary conditions in the aquifer along with assuming the continuity of concentration and vertical mass flux at aquifer and aquitard interfaces. The solutions in the real time domain are obtained by numerically inverting the solutions in the Laplace domain using the Stehfest (1970) algorithm. The semi-analytical solutions are compared with those from Zhan et al. (2009b), which considered aquitard leakage in infinitively thick aquitards. The concentration profiles, breakthrough curves and distribution profiles in the aquifer are different from those of Zhan et al. (2009b) at small ratios of the aquitard/aquifer thickness; whereas, the results of both are consistent for thick bounding aquitards. This study reveals that the residence time distribution (RTD) in the main aquifer is related to the aquitard/aquifer thickness ratios, Peclet numbers and porosities of adjacent aquitards. The results also suggest that MT3DMS (a commonly applied transport code) cannot successfully simulate solute transport at the aquifer–aquitard interfaces. The presented solutions improve available solutions for transport processes in an aquifer bounded by thin aquitards with leakage. The developed solutions can be directly extended to cases when the vertical hydrodynamic dispersion of the aquitards is considered by simply replacing the effective molecular diffusion coefficients of the aquitard by the vertical hydrodynamic dispersion coefficients of the aquitards.

1. Introduction

It is now recognized that aquitards have an important role in controlling contaminant transport between adjacent aquifers (Cherry et al., 2004; Liu et al., 2004; Zhan et al., 2009a, 2009b). Solute transport in aquitards has received much less attention than that in aquifers, partially because of the difficulty of obtaining creditable data within reasonable time frames in aquitards, and partially because of the

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misunderstanding of the role that aquitards play during transport. Oftentimes, aquitards are regarded as impermeable barriers to transport, or at most, allow diffusion to occur (Bear, 1972; Cleary, 1978; Domenico and Schwartz, 1998; Fetter, 1999; Starr et al., 1985; Sudicky and Frind, 1981; Sudicky et al., 1985). In reality, leakage often occurs into the aquitards, resulting in advective transport, particularly in thin aquitards (Barazzuoli et al., 2008; Becker et al., 2009; Chesnaux et al., 2012; Rasmussen et al., 2003; Sayed et al., 1992; Shestakov et al., 2002; Tang and Aral, 1992b; Xu et al., 2008; Zhang et al., 2010). Some studies on solute transport in aquitards indicate that molecular diffusion and advection are the two main controlling factors (Ball et al., 1997a, 1997b; Cherry et al., 2004; Hendry et al., 2003; Hunkeler et al., 2004; Johnson et al., 1989; Liu and Ball, 1999; Parker et al., 2004; Starr et al., 1985; Sudicky et al., 1985; Tang and Aral, 1992a; Tang and Aral, 1992b; Zhan et al., 2009a, 2009b). For the first time, Tang and Aral (1992a, 1992b) considered both diffusion and advection in analytical models of solute transport within aquitards. The importance of advective transport in the aquitards has been recognized before, but often overlooked by many scientists (Tang and Aral, 1992a, 1992b). Cherry et al. (2004) indicated that contaminant migration in deposits with a hydraulic conductivity of less than about 10^{-8} m/s was diffusion-controlled but for a conductivity of higher than about 10^{-7} m/s was advection-controlled, while between these two ranges, both advection and diffusion were controlling.

Most studies on solute transport in aquifer–aquitard systems considered diffusive processes at the aquifer–aquitard interface similar to diffusion at the fracture-matrix boundary which approximated the diffusive mass flux at the interfaces as a volumetric sink/source term (Chen, 1985; Fujikawa and Fukui, 1990; Liu et al., 2004; Tang and Aral, 1992a, 1992b; Tang et al., 1981). This was based on the assumption that complete mixing across the fracture aperture occurred for all times due to a parabolic velocity profile and the roughness of the fracture walls (Davis and Johnston, 1984; Sudicky and Frind, 1982; Tang et al., 1981). This approximation becomes questionable for aquifer–aquitard systems since the aquifer thickness is often much larger than any perceivable fracture apertures. Furthermore, the flow velocity in the aquifer is often much smaller than that in a single fracture; therefore, the complete transverse mixing may not occur within an aquifer (Zhan et al., 2009a, 2009b). The experimental results of Sudicky et al. (1985) revealed that the solution for transport in a fractured system was not valid for a similar process in an aquifer–aquitard system, partially because the relaxation time for the complete transverse mixing in an aquitard was much longer. Based on this argument, Sudicky et al. (1985) solved the solute transport equations by describing the diffusive flux at the aquifer–aquitard interfaces as a boundary condition; whereas, it was heretofore considered as a source/sink term. Recently, Zhan et al. (2009a, 2009b) adopted this idea to derive semi-analytical solutions in the Laplace domain for two-dimensional solute transport in an aquifer–aquitard system for conservative and reactive solutes, respectively. They showed that by describing the diffusive flux at the aquifer–aquitard interfaces as a boundary condition, the results more closely mimicked physical processes than those obtained by the source/sink assumption.

The thicknesses of aquitards were considered infinite in the solute transport studies by Starr et al. (1985), Tang and Aral (1992a, 1992b), and Zhan et al. (2009a, 2009b). In reality, the aquitard thicknesses are not infinite and often are quite thin. For a thin aquitard bounded by two adjacent aquifers, leakage will occur across the aquitard when a hydraulic head difference exists between those two aquifers, which is often the case (Bradbury et al., 2007; Cherry et al., 2004; Yoon et al., 2002). In such a circumstance, the aquitard is no longer a barrier for transport; instead, it becomes a pathway for exchanging water and contaminant mass among different aquifers. Such cross-formation transport is an important and often overlooked process in aquifer remediation or contaminant attenuation.

The purpose of this study is to use an analytical approach to explore the impact of thin aquitards on two-dimensional solute transport in an aquifer considering one-dimensional diffusion and slow advection in the bounding aquitards. The solutions aim to be useful for benchmarking numerical simulations which often suffer from non-negligible numerical errors at the aquifer–aquitard interfaces, particularly when the physical, chemical, and biological parameter values are significantly different in the aquifer and aquitard (Bester et al., 2005; Zhan et al., 2009a, 2009b). The solutions of this study can be easily extended by including the retardation factor if a linear sorption isotherm exists for transport.

2. Material and methods

2.1. Conceptual model

We consider the case of a horizontal-layer aquifer bounded by two parallel thin aquitards with aquifers above and below the aquitard layers (Fig. 1). The origin of the Cartesian coordinate system is fixed at the left boundary and sits at the plane of symmetry in the aquifer. The length of the aquifer–aquitard system is considered infinite along the x and y directions. The y-axis is perpendicular to the x-axis in the horizontal plane. The main aquifer and bounding aquitards are homogeneous and horizontally isotropic with finite thicknesses in the z direction. In the generalization of natural groundwater flow in a flat-lying aquifer–aquitard system as shown in Fig. 1, flow within aquitards is typically vertical or near-vertical and in aquifers is mainly horizontal when the hydraulic conductivities of the aquitards are a few orders of magnitude smaller than those of the aquifers (Cherry et al., 2004; Hantush, 1955; Zhan et al., 2009a). Therefore, the steady and unidirectional groundwater flow is considered horizontal (along the x direction) in the main aquifer and vertical (in the z direction) within adjacent aquitards. It is assumed that the main aquifer is of constant longitudinal and vertical dispersivities. The bounding aquitards have different thicknesses and physical parameter values such as leakage velocity, dispersivity, etc. The solute concentrations in the aquifers and aquitards are assumed