



Analytical solutions of one-dimensional multispecies reactive transport in a permeable reactive barrier-aquifer system

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ARTICLE INFO

Article history:

Received 6 October 2011
Received in revised form 31 March 2012
Accepted 2 April 2012
Available online 13 April 2012

Keywords:

Multispecies reactive transport
In situ remediation
PRB design equations
Modeling

ABSTRACT

The permeable reactive barrier (PRB) remediation technology has proven to be more cost-effective than conventional pump-and-treat systems, and has demonstrated the ability to rapidly reduce the concentrations of specific chemicals of concern (COCs) by up to several orders of magnitude in some scenarios. This study derives new steady-state analytical solutions to multispecies reactive transport in a PRB-aquifer (dual domain) system. The advantage of the dual domain model is that it can account for the potential existence of natural degradation in the aquifer, when designing the required PRB thickness. The study focuses primarily on the steady-state analytical solutions of the tetrachloroethene (PCE) serial degradation pathway and secondly on the analytical solutions of the parallel degradation pathway. The solutions in this study can also be applied to other types of dual domain systems with distinct flow and transport properties. The steady-state analytical solutions are shown to be accurate and the numerical program RT3D is selected for comparison. The results of this study are novel in that the solutions provide improved modeling flexibility including: 1) every species can have unique first-order reaction rates and unique retardation factors, and 2) daughter species can be modeled with their individual input concentrations or solely as byproducts of the parent species. The steady-state analytical solutions exhibit a limitation that occurs when interspecies reaction rate factors equal each other, which result in undefined solutions. Excel spreadsheet programs were created to facilitate prompt application of the steady-state analytical solutions, for both the serial and parallel degradation pathways.

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1. Introduction

In recent years, the permeable reactive barrier (PRB) technology has proven capable of rapidly reducing the concentration of some chemicals of concern (COCs) by up to several orders of magnitude (EPA, 1998). The purpose of a PRB is not to treat large volumes of an impacted aquifer, but rather to manage plume concentrations as groundwater flows towards receptors or off-site. In its simplest form, a

continuous PRB is a vertically emplaced rectangular porous medium in which influent groundwater passively enters a treatment zone. The reactive media contained in the treatment zone varies depending on the COC being treated, however the most common media is zero-valent iron (Gavaskar et al., 2000). As illustrated in Fig. 1, a continuous PRB is constructed with only the treatment zone, whereas the funnel-and-gate PRB (not illustrated here) is constructed with flanking impermeable walls that funnel captured groundwater to the treatment zone (or the gate).

As the groundwater flows through the treatment zone, the dissolved COCs come in contact with the reactive material and are rapidly degraded (EPA, 1998). The effluent groundwater contains significantly lower concentrations as it re-enters the aquifer and flows towards the plane of compliance (POC), as

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illustrated in Fig. 1. It should be noted that effective implementation of a PRB relies on accurate site characterization to identify the existing COCs, their interactions, and their required residence time in the PRB and down-gradient aquifer. Note that the down-gradient aquifer may also contribute to additional COC degradation through natural attenuation processes. Ensuring adequate residence time in a PRB–aquifer system allows COCs sufficient time to degrade, improving the likelihood that regulatory or target concentrations are achieved at the POC. Therefore, minimizing performance uncertainties (such as inadequate barrier thickness) in the preliminary design phase is critical in avoiding underperformance of the PRB.

To address design uncertainties, prior research has focused primarily on better understanding 1) the geochemistry of the PRB material (Allen-King et al., 1997; Arnold and Roberts, 2000; Johnson et al., 1996; Roberts et al., 1996; Tratnyek et al., 1997), 2) flow characteristics (Gupta and Fox, 1999), and 3) the minimum PRB thickness as determined from current design equations (Eykholt, 1997; Park and Zhan, 2009; Rabideau et al., 2005). The one-dimensional (1D) design equations presented by Eykholt (1997), Rabideau et al. (2005), and Park and Zhan (2009) utilize the advection–dispersion equation (ADE) with the first-order reaction as the governing equation(s) but differ primarily in their application of the boundary conditions. For example, the two equations of Eykholt (1997) were derived using van Genuchten's (1981) analytical solutions of the ADE with a first-type boundary condition $C(x,t)|_{inlet} = C_{in}$ at the influent face of the PRB and a semi-infinite boundary condition $\frac{\partial C}{\partial x}(\infty, t) = 0$ at the effluent face of the PRB, where C represents concentration [ML^{-3}], t is time [T], x is the spatial coordinate along the flow direction [L], and C_{in} is the concentration at the inlet boundary [ML^{-3}]. The two solutions of Rabideau et al. (2005) were derived using the Sun et al. (1999) transformation procedure: the first assumed a third-type influent boundary condition and semi-infinite effluent condition, while the second solution assumed a first-type influent condition and zero concentration gradient $\frac{\partial C(x,t)}{\partial x}|_{outlet} = 0$ effluent condition.

The solutions of Eykholt (1997) and the second solution of Rabideau et al. (2005) tend to overestimate mass in the PRB system (particularly at early time) by assuming that the concentration gradient across the influent boundary is initially zero (van Genuchten and Parker, 1984; Wexler, 1992). However, the second solution of Rabideau et al. (2005) with a finite PRB width forces a zero concentration gradient at the exit face of the PRB; hence it is useful in that it yields the largest PRB width (Park and Zhan, 2009). Alternatively, the first solution of Rabideau et al. (2005) with the third-type or total flux influent condition (Kreft and Zuber, 1978) is more accurate; however, it incorrectly implies that PRBs have large thicknesses due to the semi-infinite effluent condition. Additionally, the Eykholt (1997) and Rabideau et al. (2005) design equations are of limited use because they are unable to account for the entirely distinct flow and chemical processes occurring in the down-gradient aquifer. For example, solute degradation in a PRB is typically induced by a strong (abiotic) reaction while the reaction in aquifers tends to be weaker (biologically driven) natural attenuation (EPA, 1998). As such, these solutions are unable to model the solute concentration at the down-gradient POC in the aquifer.

Both the first solution of Rabideau et al. (2005) and the Park and Zhan (2009) solution consider the dissolved

influent solute to be well-mixed and therefore described completely by the advective mass flux condition or flowing concentration flux, which upon entering the PRB is subject to dispersive and advective fluxes. Hence, the third-type boundary condition is more physically sound and tends to conserve mass (van Genuchten and Parker, 1984) at the inlet boundary when applied to the ADE, without reaction. In reality, before entering the PRB, the influent solute is not well-mixed due to the porous nature of the up-gradient aquifer. Unlike the Rabideau et al. (2005) and Park and Zhan (2009) studies, this study includes the influent boundary condition that considers dispersive and advective fluxes in the up-gradient aquifer.

The difference between the first solution of Rabideau et al. (2005) and that of Park and Zhan (2009) is that Park and Zhan (2009) assumed a finite PRB width, maintained total flux and concentration continuity at the PRB–aquifer interface, and assigned a separate governing equation to the aquifer, which permitted modeling solute concentrations at the POC. The Park and Zhan (2009) solution, however, is limited to one reactive species in the PRB–aquifer system. Most groundwater plumes have multiple chemicals present and many plumes have reactive solutes which decay to produce daughter chemicals. A common example is tetrachloroethene (PCE), which degrades to produce trichloroethene (TCE), then dichloroethene (DCE), with vinyl chloride (VC) as the final chlorinated daughter product. Given this limitation, the objective of this study is to expand the Park and Zhan (2009) model to handle multispecies reactive transport in the PRB–aquifer system. Furthermore, the inlet boundary condition of Park and Zhan (2009) (see Eq. (3) there) has been modified to include both advective and dispersive fluxes. The results will focus on the closed-form steady-state analytical solutions of the aquifer, but it is noted that the transient solutions can be extracted from the supplemental derivations with minimal effort and programmed into a numerical Laplace inversion algorithm. Due to the length of the solutions, an electronic supplement is provided. Two Excel programs were preprogrammed with the steady-state analytical solutions of the serial and parallel degradation pathways and are available upon request.

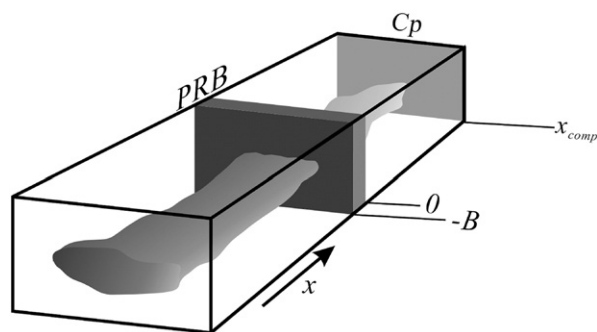


Fig. 1. Schematic of installed continuous PRB, solute plume, and aquifer. The x axis is along the groundwater flow direction and the PRB is of thickness B . The down-gradient PRB–aquifer interface is located at $x = 0$ and x_{comp} is the plane of compliance (POC), which could be a property boundary or a predetermined location where solute concentrations must achieve a target concentration. Figure adapted from Park and Zhan (2009) (with permission from American Geophysical Union).

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