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Subsurface solute transport with one-, two-, and three-dimensional arbitrary shape sources

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ABSTRACT

Solutions with one-, two-, and three-dimensional arbitrary shape source geometries will be very helpful tools for investigating a variety of contaminant transport problems in the geological media. This study proposed a general method to develop new solutions for solute transport in a saturated, homogeneous aquifer (confined or unconfined) with a constant, unilateral groundwater flow velocity. Several typical source geometries, such as arbitrary line sources, vertical and horizontal patch sources, circular and volumetric sources, were considered. The sources can sit on the upper or lower aquifer boundary to simulate light non-aqueous-phase-liquids (LNAPLs) or dense non-aqueous-phase-liquids (DNAPLs), respectively, or can be located anywhere inside the aquifer. The developed new solutions were tested against previous benchmark solutions under special circumstances and were shown to be robust and accurate. Such solutions can also be used as a starting point for the inverse problem of source zone and source geometry identification in the future. The following findings can be obtained from analyzing the solutions. The source geometry, including shape and orientation, generally played an important role for the concentration profile through the entire transport process. When comparing the inclined line sources with the horizontal line sources, the concentration contours expanded considerably along the vertical direction, and shrank considerably along the groundwater flow direction. A planar source sitting on the upper aquifer boundary (such as a LNAPL pool) would lead to significantly different concentration profiles compared to a planar source positioned in a vertical plane perpendicular to the flow direction. For a volumetric source, its dimension along the groundwater flow direction became less important compared to its other two dimensions.

1. Introduction

Contaminant fate and transport in the subsurface environment is a complicated problem which attracts attention among the general public and hydrogeologists for decades. The complexity partially comes from the uncertainty of contaminant sources, including source shapes and locations. Taking light non-aqueous-phase liquids (LNAPLs) such as gasoline as an example, spilled LNAPLs on ground surface will migrate downward through unsaturated zone due to gravity, which is also strongly affected by pore structure, moisture content and heterogeneity of the unsaturated zone. If the spill is sufficiently large to reach water table, soluble components will enter the saturated aquifer and move downgradient along the groundwater flow direction. The contaminant source for the saturated zone here is somewhat like a flat pan with various shapes lying on top of the unconfined aquifer. Chrysikopoulos (1995) investigated this problem and proposed a method to calculate solute concentration profile, but his approach has constrained to problems with a regular source shape like rectangular or elliptic geometry. If the contaminants are dense non-aqueous-phase liquids (DNAPLs), they may further penetrate into the aquifer and accumulate at the aquifer base to become a persistent contaminant pool.

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Numerical modeling is commonly employed for describing complicated three-dimensional transport in the subsurface, especially for irregular source shapes. For example, the finite element method (FEM) or the finite volume method (FVM) is capable of dealing with irregular shapes using unstructured grids (Huyakorn and Pinder, 1983; Yeh, 2000; Geiger et al., 2004; Begnudelli and Sanders, 2006). However, both FEM and FVM are computationally expensive for dealing with field-scale transport problems, and they must be validated against benchmark analytical solutions. Sometimes what one needs is a quick and approximate assessment for solute transport in the subsurface for the purpose of screening multiple options of remediation plans, or for understanding the transport process under different possible source types. If numerical modeling is used, a separate model run is needed for each source type, a process that is tedious and time-consuming. The general analytical approach with the capability of handing various source shapes may be a better choice to meet the need. In addition, such developed analytical solutions can serve the purpose of validating the numerical models if needed.

Consequently, many analytical solutions have been proposed for one-(1D), two-(2D) and three-dimensional(3D) problems, along with the development of numerical models for subsurface solute transport over the past many decades. In the following, we briefly reviewed the analytical works that were mostly relevant to this study which was focused on finding a general analytical approach to deal with subsurface solute transport in 1D, 2D and 3D domains with arbitrary source shapes. For more detailed information related to the advancement of analytical and numerical modeling of subsurface transport, one can consult the reviews done by various investigators, including Batu (2005). Wang and Zhan (2015) reviewed different inverse Laplace transform techniques in terms of dealing with subsurface transport problems.

Bear (1972) gave an analytical solution of instantaneous point injection, which can be used to obtain the solution for a continuous point injection by integration over time. Sagar (1982) and (Domenico and Robbins, 1985; Domenico, 1987) proposed a patch-source solution in an unbounded aquifer with different methods. Sagar (1982) used an approximate Green's function method and was more rigorous in terms of mass conservation. The solutions of (Domenico and Robbins, 1985; Domenico, 1987) were heuristic in nature as they were not derived based on a rigorous mass conservation principle. Despite their obvious flaws, the solutions of (Domenico and Robbins, 1985; Domenico, 1987) were found to be good approximations to patch-source transport problems for some practical problems, and the accuracy of such solutions depended on aquifer parameters, as carefully documented by West et al. (2007), Srinivasan et al. (2007).

Wexler (1992) summarized the existing analytical solutions for transport problem that were demonstrated to be accurate and practical by many professionals. For instance, Wexler (1992) provided solutions for aquifers of infinite extent with continuous point sources (Hunt, 1978), aquifers of finite extent with patch sources (Cleary and Ungs, 1978), and aquifers of infinite extent with patch sources (Sagar, 1982). Neville (1998) derived a patch source solution in a confined semi-infinite aquifer using Green's function method by treating the patch-source as a prescribed concentration or the first-type (Dirichlet) boundary. Park and Zhan (2001) made a further step on the basis of Neville (1998), and extended the patch-source to a volumetric source with a prescribed flux or the second-type (Neumann) boundary condition. In addition, a series of solutions of line sources and patch sources were also given by Park and Zhan (2001). However, all the source types discussed in Park and Zhan (2001) had regular shapes. For instance, line sources were either parallel or perpendicular to the aquifer base and patch sources were assumed to be in rectangular shapes. The influence of inclined line sources and sources sitting on top or bottom of the aquifer were not discussed by Park and Zhan (2001).

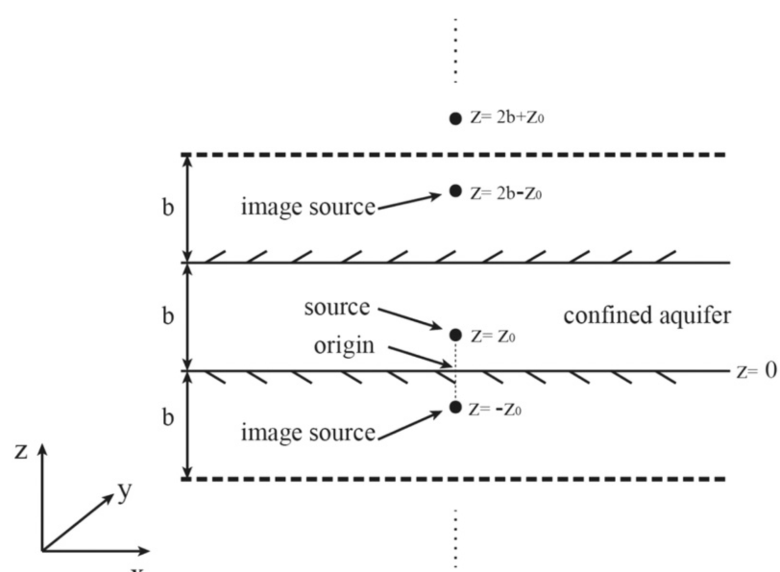

Fig. 1. A schematic diagram of a point source and the associated image sources.