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Scale dependent solute dispersion with linear isotherm in heterogeneous medium

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SUMMARY

This study presents an analytical solution for one-dimensional scale dependent solute dispersion with linear isotherm in semi-infinite heterogeneous medium. The governing advection–dispersion equation includes the terms such as advection, dispersion, zero order production and linear adsorption with respect to the liquid and solid phases. Initially, the medium is assumed to be polluted as the linear combination of source concentration and zero order production term with distance. Time dependent exponentially decreasing input source is assumed at one end of the domain in which initial source concentration is also included i.e., at the origin. The concentration gradient at the other end of the aquifer is assumed zero as there is no mass flux exists at that end. The analytical solution is derived by using the Laplace integral transform technique. Special cases are presented with respect to the different forms of velocity expression which are very much relevant in solute transport analysis. Result shows an excellent agreement between the analytical solutions with the different geological formations and velocity patterns. The impacts of non-dimensional parameters such as Peclet and Courant numbers have also been discussed. The results of analytical solution are compared with numerical solution obtained by explicit finite difference method. The stability condition has also been discussed. The accuracy of the result has been verified with root mean square error analysis. The CPU time has also been calculated for execution of Matlab program.

1. Introduction

Pollutants can originate from either point sources or nonpoint sources. Once the pollutants enter into the subsurface region, they may have every possibility to reach shallow aquifers in due course of time. Meanwhile, some pollutants adsorbed by soil and some dissolved in water, and some are transported downstream which moves along flow pathways. These pollutants are very often found in groundwater as a result of waste disposal or leakage of urban sewage and industrial wastes, surficial applications of pesticides and fertilizers used in agriculture, atmospheric deposition or accidental releases of chemicals on the earth surface. Pollutants dissolved in groundwater typically experience complex physical and chemical processes such as advection, diffusion, chemical reactions, adsorption, and biodegradation & decay. To predict the fate and transport of solutes in groundwater through understanding and simulating these processes is very complex. The transformation of these phenomenons in mathematical equation commonly represents Advection Dispersion (AD) equation which depends upon fundamental equation of conservation of mass. We may rely on AD equation for describing the migration and fate of pollutants in groundwater bodies supported by existing literature.

There are considerable body of literature available on solute transport which may be enlisted and it has been dealt with AD equation since last four five decades. Ebach and white (1958) studied the longitudinal dispersion problem for an input concentration that varies periodically with time. Ogata and Banks (1961) discussed for the constant input concentration. Hoopes and Harleman (1965) studied the problem of dispersion in radial flow from fully penetrating well; homogeneous, isotropic non adsorbing confined aquifers. Bruce and Street (1967) established both longitudinal and lateral dispersion effect with semi-infinite non adsorbing porous media in a steady unidirectional flow fluid for a constant input concentration. Bear (1972) studied the transport of solutes in saturated porous media is commonly described by the advection–dispersion equation. Marino (1974) obtained the input concentration varying exponentially with time. Hunt (1978) proposed the perturbation method to longitudinal and lateral dispersion in non-uniform, steady and unsteady seepage flow through heterogeneous aquifers. Wang et al. (1978) studied the

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concentration distribution of a pollutant arising from instantaneous point source in a two dimensional water channel with non-uniform velocity distribution. Kumar (1983a,b) discussed the dispersion of pollutants in semi-infinite porous media with unsteady velocity distribution. Kumar (1983a,b) studied the significant application of advection diffusion equation. Lee (1999), Batu (1989), and Batu (1993) presented two dimensional analytical solutions considering solute transport for a bounded aquifer by adopting Fourier analysis and Laplace transform technique. Aral and Liao (1996) obtained a general analytical solution of the two dimensional solute transport equation with time dependent dispersion coefficient for an infinite domain aquifer. Serrano (1995) established the scale-dependent models to predict mean contaminant concentration from point sources i.e., well injection, and non-point sources i.e., ground surface spills in heterogeneous aquifers. Schafer and Kinzelbach (1996) presented transport of reactive species in heterogeneous porous media. Zoppou and Knight (1997) explored the analytical solutions for advection and advection–diffusion equations with spatially variable coefficients in which the diffusion coefficient proportional to the square of the velocity concept employed. Delay et al. (1997) predicted solute transport in heterogeneous media from results obtained in homogeneous ones: an experimental approach. Liu et al. (1998) evaluated an analytical solution to the one-dimensional solute advection–dispersion equation in multi-layer porous media by using a generalized integral transform technique. Verma et al. (2000) discussed an overlapping control volume method for the numerical solution of transient solute transport problems in groundwater. Diaw et al. (2001) presented one dimensional simulation of solute transfer in saturated–unsaturated porous media using the discontinuous finite elements method. Saied and Khalifa (2002) presented some analytical solutions for groundwater flow and transport equation. McKenna et al. (2003) discussed the longitudinal and transverse dispersivities in three dimensional heterogeneous fractured media. Ptak et al. (2004) reviewed over the tracer investigation of heterogeneous porous media and stochastic modeling of flow and transport of contaminant in the groundwater flow. Huang et al. (2006) employed a parabolic distance-dependent dispersivity for solving one dimensional fractional ADE. Kim and Kavvas (2006), Huang et al. (2008), and Du et al. (2010) presented transport processes in heterogeneous geological media by Fractional Advection–Diffusion Equation (FADE).

Liu et al. (2007) explored the numerical experiments to investigate potential mechanisms behind possible scale-dependent behavior of the matrix diffusion for solute transport in fractured rock. Chen et al. (2008) developed an analytical solution to solute transport with the hyperbolic distance-dependent dispersivity in a finite column. Guerrero et al. (2009) studied the formal exact solution of the linear advection–diffusion transport equation with constant coefficients for both transient and steady-state regimes by using the integral transform technique. Guerrero and Skaggs (2010) obtained a general analytical solution for the linear, one-dimensional advection–dispersion equation with distance-dependent coefficients in heterogeneous porous media. Chen and Liu (2011) presented the generalized analytical solution for one-dimensional solute transport in finite spatial domain subject to arbitrary time-dependent inlet boundary condition. Hayek (2011) presented a non-linear convection–diffusion reaction equation, considered as generalized Fisher equation with convective terms. Exact and traveling-wave solutions for convection–diffusion–reaction equation with power-law nonlinearity in which density independent and density dependent diffusion were studied. Roubinet et al. (2012) developed the semi analytical solution for the Fracture-matrix interactions of solute transport in fractured porous media and rocks. Ranganathan et al. (2012) analyzed the modeling and numerical simulation study of density-driven natural convection during geological CO_2 storage in heterogeneous formations by using Sequential Gaussian Simulation method. Davit et al. (2012) developed the transient behavior of homogenized models for solute transport in two-region heterogeneous porous media. Chen et al. (2012) solved multi-species advective–dispersive transport equations sequentially coupled with first-order decay reactions. Singh et al. (2012) discussed the analytical solution for the one dimensional heterogeneous porous media. Gao et al. (2012) developed the mobile-immobile model (MIM) with an asymptotic dispersivity function of travel distance to embrace the concept of scale-dependent dispersion during solute transport in finite heterogeneous porous media.

Recently, You and Zhan (2013) studied the semi-analytical solution for solute transport in a finite column is developed with linear-asymptotic or exponential distance-dependent dispersivities and time-dependent sources. Guerrero et al. (2013) presented analytical solutions of the advection–dispersion solute transport equation solved by the Duhamel theorem with the time dependent boundary condition. van Genuchten et al. (2013) presented a series of one- and multi-dimensional solutions of the standard equilibrium advection–dispersion equation with and without terms accounting for zero-order production and first-order decay. Vasquez et al. (2013) introduced the modeling flow and reactive transport to explain mineral zoning in the Atacama salt flat aquifer. Maraqa and Khashan (2014) established the effected of the single-rate nonequilibrium heterogeneous sorption kinetics in the modeling of the solute transport. Singh and Kumari (2014) presented one-dimensional contaminant prediction along unsteady groundwater flow in aquifer with unit Heaviside type input concentration. Fahs et al. (2014) explored extensively about a new benchmark semi-analytical solution for verification of density-driven flow codes in porous media with synthetic square porous cavity subjected to different salt concentration at its vertical wall.

The traditional advection–dispersion equation is a standard model for solute transport. Analyses of many solute transport problems required the use of mathematical models corresponding with the application. Analytical models are useful for providing physical insight to the system. Initial or approximate studies of alternative pollution scenarios may be conducted to investigate the effects of various parameters included in transport processes through the modeling approach.

The objective of the present work is to apply the Laplace integral transform technique for solving one dimensional AD equation with zero order production term in which linear isotherm concept is employed. The AD equation is solved under the initial and boundary conditions taken into consideration. The heterogeneous medium is taken into consideration in which the velocity is the function of the space as well as time dependent. The dispersion is directly proportional to the square of the seepage velocity employed. The various transformations are used for reducing the problem into the simplest form. The exponentially decreasing and increasing form of the flow pattern with respect to the time are considered. The non-dimensional Peclet and Courant numbers are also studied. The equilibrium relationship between the Peclet and Courant number are also depicted. The numerical solution is obtained by explicit finite difference method in which the stability condition has also been discussed. The accuracy of the result has been verified with root mean square error analysis.

2. Mathematical formulation

The solute transport in heterogeneous porous media is generally modeled by assuming a time as well as space dependent spatially average transport velocity and solute dispersion, linear equilibrium adsorption, and first-order decay. Mathematically,