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Generalized semi-analytical solutions to multispecies transport equation coupled with sequential first-order reaction network with spatially or temporally variable transport and decay coefficients

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ABSTRACT

This paper presents a semi-analytical procedure for solving coupled the multispecies reactive solute transport equations, with a sequential first-order reaction network on spatially or temporally varying flow velocities and dispersion coefficients involving distinct retardation factors. This proposed approach was developed to overcome the limitation reported by Suk (2013) regarding the identical retardation values for all reactive species, while maintaining the extensive capability of the previous Suk method involving spatially variable or temporally variable coefficients of transport, general initial conditions, and arbitrary temporal variable inlet concentration. The proposed approach sequentially calculates the concentration distributions of each species by employing only the generalized integral transform technique (GITT). Because the proposed solutions for each species' concentration distributions have separable forms in space and time, the solution for subsequent species (daughter species) can be obtained using only the GITT without the decomposition by change-of-variables method imposing the limitation of identical retardation values for all the reactive species by directly substituting solutions for the preceding species (parent species) into the transport equation of subsequent species (daughter species). The proposed solutions were compared with previously published analytical solutions or numerical solutions of the numerical code of the Two-Dimensional Subsurface Flow, Fate and Transport of Microbes and Chemicals (2DFATMIC) in three verification examples. In these examples, the proposed solutions were well matched with previous analytical solutions and the numerical solutions obtained by 2DFATMIC model. A hypothetical single-well push–pull test example and a scale-dependent dispersion example were designed to demonstrate the practical application of the proposed solution to a real field problem.

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1. Introduction

Multispecies reactive transport with sequential first-order reaction network is frequently encountered in contaminated aquifer systems or sites with radioactive wastes, nitrogenous species, and chlorinated solvents. Many analytical solutions have been developed for the multispecies transport equations coupled with sequential first-order reaction network. Several previous workers have developed various methods, such as the Fourier or Laplance transform technique (Cho, 1971; Lunn et al., 1996; Sudicky et al., 2013; van Genuchten, 1985), decomposition with the help of transformation of variable using the existing single-species analytical solutions (Sun and Clement, 1999; Sun et al., 1999a; Sun et al., 1999b), decomposition by matrix diagonalization together with the Laplace transform technique (Quezada et al., 2004; Srinivasan and Clement, 2008a; Srinivasan and Clement, 2008b), and the classic integral transform technique (CITT) or generalized integral transform technique (GITT) (Chen et al., 2012a; Chen et al., 2012b; Perez Guerrero et al., 2009; Perez Guerrero et al., 2010; Suk, 2013).

The standard Laplace or Fourier transforms usually require complicated and cumbersome mathematical derivations and manipulations to perform inverse transform. Accordingly, above integral transform methods are limited for a small number of species, a one-dimensional infinite or semi-infinite domain, and relatively simple initial conditions, specifically when trying to obtain closed explicit analytical solution based on analytical inverse transform expression (Lunn et al., 1996; Srinivasan and Clement, 2008a; Srinivasan and Clement, 2008b; van Genuchten, 1985; van Genuchten and Wierenga, 1976).

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The method of decomposition with the help of transformation of variable using the existing single-species analytical solutions has the limitation of requiring the same retardation values for all species (Sun and Clement, 1999; Sun et al., 1999a; Sun et al., 1999b). The method of decomposition by matrix diagonalization together with a Laplace transform removes the limitation of the same retardation values (Quezada et al., 2004; Srinivasan and Clement, 2008a; Srinivasan and Clement, 2008b). Srinivasan and Clement (2008a, b) improved the method of Quezada et al. (2004) for the coupled multispecies transport problem involving an arbitrary number of species.

However, because of the complicated and difficult solution procedure of deriving the analytical solutions for a finite domain, Perez Guerrero et al. (2009, 2010) used CITT for analytical solutions of coupled multispecies transport equations in a finite domain. Chen et al. (2012a) derived the analytical solution in a finite domain subject to a time-invariant constant source boundary condition. Afterwards, Chen et al. (2012b) improved their solutions for an arbitrary time dependent boundary condition as well as an arbitrary number of species.

Simpson and Ellery (2014) described a method that provides an exact power series solution for linear coupled reactive transport problems for general initial conditions, for which traditional transform inversion techniques are not applicable.

However, all of the aforementioned analytical solutions have great difficulties to deal with either transient flow conditions or temporally varying or spatially varying velocities and dispersion coefficients. Transport properties often encountered in a real field such as velocities and dispersion coefficients are both spatially and temporally variable. Especially, traditional Laplace or Fourier transform methods cannot manage multispecies transport problems with such arbitrary spatially varying transport properties, even single species transport problems.

Recently, coupled multispecies reactive solute transport equation with a sequential first-order reaction network on spatially or temporally varying flow velocities and dispersion coefficients was solved with semi-analytical method proposed by Suk (2013). This semi-analytical method employs general linear transformation method to transform the set of coupled multispecies equations into a set of independent uncoupled equations and then uses GITT to solve these independent equations with spatially or temporally varying flow velocities and dispersion coefficients. However, this method has limitation about retardation coefficients. In other words, it is only applicable for identical retardation values for all reactive solutes, although it is highly flexible approach for dealing with spatially or temporally variable transport coefficients. The objective of this study was to extend the work of Suk (2013) to solve the coupled multispecies reactive solute transport equation with distinct retardation coefficients consisting of a sequential first-order reaction network. Therefore, the proposed approach in this study can handle distinct retardation factors, spatially or temporally varying flow velocities, dispersion coefficients, and decay rates as well as temporally varying boundary conditions and arbitrary initial concentration distributions of the species in a finite domain.

2. Problem formulation and procedures

The general 1-D mass balance equations for a saturated aquifer, which predict the fate and transport of multispecies coupled with sequential first-order reactions, can be written as

$$\begin{aligned} &R_i\theta\frac{\partial C_i}{\partial t}+\frac{\partial}{\partial x}[\theta v(x,t)C_i]-\frac{\partial}{\partial x}\left[\theta D(x,t)\frac{\partial C_i}{\partial x}\right]\\ &\quad=y_i k_{i-1}(x,t)\theta C_{i-1}-k_i(x,t)\theta C_i,\quad \forall i=2,3,\cdots,N\\ &\quad=-k_i(x,t)\theta C_i,\quad i=1,\quad \forall t>0,\quad \text{and}\ \ 0<x<L, \end{aligned} \tag{1}$$

where $v(x, t)$ is the seepage velocity $[LT^{-1}]$, $D(x, t)$ is the dispersion coefficient $[L^2T^{-1}]$, C_i is the concentration of species i $[ML^{-3}]$, y_i is the stoichiometric yield coefficient for the reaction of species $i-1$ to produce species i $[MM^{-1}]$, $k_i(x, t)$ is the first-order decay-rate constant of species i $[T^{-1}]$, L is the length of the porous medium $[L]$, N is the total number of species, $R_i = 1 + \rho_b k_{d,i}/\theta$, R_i is the retardation factor of species i, ρ_b is the porous medium bulk density $[ML^{-3}]$, $k_{d,i}$ is an empirical distribution coefficient of species i $[M^{-1}L^3]$, and θ is the porosity. For the sake of clarity, retardation factors and porosity are assumed to not change with time and space. It should be noted that the retardation factors of each species are distinct and that $v(x, t)$, $D(x, t)$, and $k_i(x, t)$ are assumed to be arbitrary functions of space x and time t. Here, the initial and boundary conditions of Eq. (1) are as follows:

$$\theta v(x,t)C_i(x,t)-\theta D(x,t)\frac{\partial C_i(x,t)}{\partial x}\bigg|_{x=0}=\theta v(x=0,t)f_i(t),\quad \forall i=1,2,3,\cdots,N \tag{2}$$

$$\theta D(x,t)\frac{\partial C_i(x,t)}{\partial x}\bigg|_{x=L}=0,\quad \forall i=1,2,3,\cdots,N \tag{3}$$

$$C_i(x,t)|_{t=0}=F_i(x),\quad \forall i=1,2,3,\cdots,N, \tag{4}$$

where $f_i(t)$ is the inlet concentration of species i on the flux boundary $[ML^{-3}]$, and $F_i(x)$ is the initial concentration of species i $[ML^{-3}]$. Here, the coupling terms are only associated with their parent concentrations.

2.1. Analytical solution for the first species

The solution for the GITT procedure begins with a variable substitution in order to make boundary condition homogeneous, which will facilitate good convergence to solution as follows:

$$C_i(x,t)=U_i(x,t)+f_i(t),\quad \forall i=1,2,3,\cdots,N \tag{5}$$

For the first species, the governing equation can be changed using Eq. (5) as follows:

$$\begin{aligned} &R_1\frac{\partial U_1}{\partial t}+R_1\frac{df_1(t)}{dt}+\frac{\partial}{\partial x}[v(x,t)U_1]+\frac{\partial}{\partial x}[v(x,t)f_1(t)]\\ &\quad-\frac{\partial}{\partial x}\left[D(x,t)\frac{\partial U_1}{\partial x}\right]\\ &=-k_1(x,t)U_1-k_1(x,t)f_1(t), \end{aligned} \tag{6}$$

where $U_1(x, t)$ has the following boundary condition:

$$v(x,t)U_1(x,t)-D(x,t)\frac{\partial U_1(x,t)}{\partial x}\bigg|_{x=0}=0 \tag{7a}$$

$$D(x,t)\frac{\partial U_1(x,t)}{\partial x}\bigg|_{x=L}=0 \tag{7b}$$

and initial condition:

$$U_1(x,t)|_{t=0}=F_1(x)-f_1(0). \tag{8}$$

Applying $\int_0^L \psi_n(x)dx$ to the governing Eq. (6) of U_1 and using Green's theorem:

$$\begin{aligned} &\int_0^L \psi_n(x)R_1\frac{\partial U_1}{\partial t}dx+\int_0^L \psi_n(x)R_1\frac{df_1(t)}{dt}dx\\ &\quad+\psi_n(L)v(L,t)U_1(L,t)-\psi_n(0)v(0,t)U_1(0,t)\\ &\quad-\int_0^L\frac{d\psi_n(x)}{dx}v(x,t)U_1dx\\ &\quad+\int_0^L\psi_n(x)\frac{\partial}{\partial x}[v(x,t)f_1(t)]dx \end{aligned}$$

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