Finite difference approach for modeling multispecies transport in porous media

N.Natarajan[1*] and G. Suresh Kumar[2]

[*] Corresponding author

[1] Research Scholar, EWRE Division, Department of Civil Engineering, Indian Institute of Technology – Madras, Chennai-36

[2] Associate Professor, Department of Ocean Engineering, Indian Institute of Technology – Madras, Chennai-36.

ABSTRACT

An alternative approach to the decomposition method for solving multispecies transport in porous media, coupled with first-order reactions has been proposed. The numerical solution is based on implicit finite difference method. The task of decoupling the coupled partial differential equations has been overcome in this method. The proposed approach is very much advantageous because of its simplicity and also can be adopted in situations where non linear processes are coupled with multi-species transport problems.

Keywords: Multispecies transport, Finite difference, Porous media.

1. Introduction

Modeling of reactive solute transport is inevitable for the comprehensive understanding of the processes occurring in groundwater. Multispecies transport in subsurface media has received much attention because multiple reactive contaminants occur in many field situations. For example, the nuclear waste can get contaminated with radioactive materials which degrade to produce many daughter products such as PCE (tetrachloroethylene) and TCE (trichloroethylene) and many byproducts (Clement et al 1998, 2000). Analytical models have been derived for predicting the fate and transport of single species in groundwater (Bear 1972, Ogata and Banks 1961, van Genuchten and Alves 1982). Analytical solutions for multispecies transport are complicated when compared to single species but a few researchers have derived them. van Genuchten (1985) adopted Laplace transform for four species transport while Lunn et al. (1996) used Fourier transform for three species transport in a one dimensional soil column, considering adsorption of the first species. Sun et al. (1999a) developed a general method for deriving analytical solution of any number of species with first order sequential degradation in multiple dimensions. Sun et al. (1999b) developed a decomposition method for decoupling any number of reactive species coupled by sequential first order reactions. In their method, the coupled partial differential equations are decomposed into independent auxiliary problems for each species in the reaction network. The initial and boundary conditions also need to be transformed into the auxiliary domain and after estimating the concentrations, it has to be converted back to the real domain. Further, this method can be applied only to the species with distinct reaction rates. This disadvantage was overcome by Slodicka and Balazova (2007) who designed a new decomposition method which can also be used for species with identical reaction rates for all dimensions. Slodicka and Balazova (2009) developed a decomposition method which does not need any temporary transformation. Earlier studies have indicated that the researchers have been developing decomposition methods for solving the coupled partial differential equations. To the authors' knowledge there are no previous studies where the multispecies equations have been solved without decoupling. The objective of the present work is to apply finite difference approach for solving the coupled partial differential equations without decoupling them. Finite difference approach has been adopted for its simplicity. The advantage of this numerical approach is that any other non linear processes can be coupled with the existing sequential reactions, if necessary, thus enhancing the conceptualization of the physics underlying the process. We have demonstrated the application of the numerical solution for two species and three species transport problem in a one dimensional domain. The dataset has been adopted from Slodicka and Balazova (2009).

2. Governing equations

The basic equation for describing single species transport for one dimensional case in porous media is of the form (Bear 1979).

$$\frac{\partial c}{\partial t} = -v\frac{\partial c}{\partial x} + D_x\frac{\partial^2 c}{\partial x^2} + f \tag{1}$$

Where c is the species concentration (ML^{-3}); x indicates the dimension (L); t is the time (T); D is the hydrodynamic dispersion coefficient (L^2T^{-1}); v is the flow velocity (LT^{-1}) and f is the reaction rate ($ML^{-3}T^{-1}$).
When first order reaction rate is assumed, equation (1) can be rewritten as,

$$\frac{\partial c}{\partial t} = -v\frac{\partial c}{\partial x} + D_x\frac{\partial^2 c}{\partial x^2} - kc \tag{2}$$

Where k is the first order reaction rate (T^{-1}).The above equation can be extended for describing the multispecies reactive transport. For example, chlorinated solvent contaminants such as PCE (tetrachloroethylene) degrades to produce daughter products such as TCE (trichloroethylene), DCE (dichloroethylene) and VC (vinyl chloride)(Sun and Clement 1999).

$c_1 \rightarrow c_2 \rightarrow c_3 \rightarrow \ldots c_i \rightarrow \ldots c_n$ (Sun et al. 1999a)

Where c_i is the species concentration in the ith generation. Species i, which is produced from species i-1, also reacts to produce species i+1 and this further reacts to produce more species. The generalized form of such a sequential transport system can be described using the following equations.

$$\frac{\partial c_i}{\partial t} = -v\frac{\partial c_i}{\partial x} + D_x\frac{\partial^2 c_i}{\partial x^2} - k_i c_i + y_{i-1}k_{i-1}c_{i-1}, \quad i = 1, 2, 3, \ldots n, \tag{3}$$

Where i is the index of the species, k_i is the first order reaction rates (T^{-1}), k_0 =0, y is the yield coefficient and n is the number of species.

3. Numerical Solution

3.1 Two species transport problem

The governing equations for two species transport in a porous media are of the form:

$$\frac{\partial c_1}{\partial t} = -v\frac{\partial c_1}{\partial x} + D\frac{\partial^2 c_1}{\partial x^2} - k_1 c_1 \tag{4}$$

$$\frac{\partial c_2}{\partial t} = -v\frac{\partial c_2}{\partial x} + D\frac{\partial^2 c}{\partial x^2} - k_2 c_2 + y_1 k_1 c_1 \tag{5}$$

The initial and boundary conditions for the above equations are:

$$c_1(x,0) = c_2(x,0) = 0 \qquad x \ge 0 \tag{6}$$

$$c_1(0,t) = 1.0 \qquad t > 0 \tag{7}$$

$$c_2(0,t) = 0 \qquad t > 0 \tag{8}$$

$$c_1(L,t) = c_2(L,t) = 0 \qquad t > 0 \tag{9}$$

Where c_1 and c_2 are the concentrations of the first and second species; k_1 and k_2 are the first order reaction rates; y_1 is the stochiometric yield coefficient and L is the length of the domain. The equations are solved using the implicit finite difference method for maintaining numerical stability. The advection term was discretised using the Upwind scheme and the dispersion term using the central difference. The parameters used for this model are shown in table 1.

Table 1. System parameters for two species reaction system

Dispersion coefficient	D	0.3	$cm^2\ h^{-1}$
Velocity	v	0.2	$cm\ h^{-1}$
Decay rate of species 1	k_1	10	h^{-1}
Decay rate of species 2	k_2	10	h^{-1}
Yield coefficient	y_1	1	h^{-1}

The decay rate constants are assumed to be the same as it is observed form the table. A domain length of 3cm and total simulation time of 1 day is considered for the simulation.

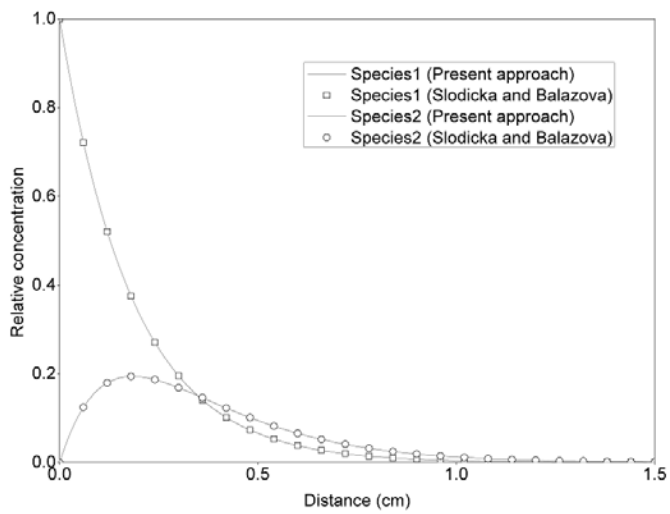

Figure 1. Comparison of the finite difference solution for identical reaction rates with that of Slodicka and Balazova (2009).

Figure 1 illustrates the comparison of the results obtained from the present numerical model with that obtained by Slodicka and Balazova (2009). It is observed from the figure that there is perfect agreement between the same. It is observed from Fig.1 that the profile of the first species with exponential decaying nature, decays to nothing after a distance of 1.0 cm while the second species exhibits skewed Gaussian profile with an elongated tailing along the descending limb. The relative concentration of the second species reaches maximum at a very short distance from the inlet of the soil column, resulting from the decay of the first species, although its initial concentration is zero. The concentration further deteriorates along the length of the column resulting in a longer tailing towards the end of the domain. The first species undergoes rapid decay nearer to inlet itself due to very high reaction rate constant and consequently its concentration reaches zero at 1 cm from the inlet of the column. As the reaction rates are same, it is observed from the Fig.1 that both the species reach zero concentration at the same distance from the inlet of the domain. The model was also validated for various Courant numbers for ensuring its stability before applying the model for the three species reactive transport system.

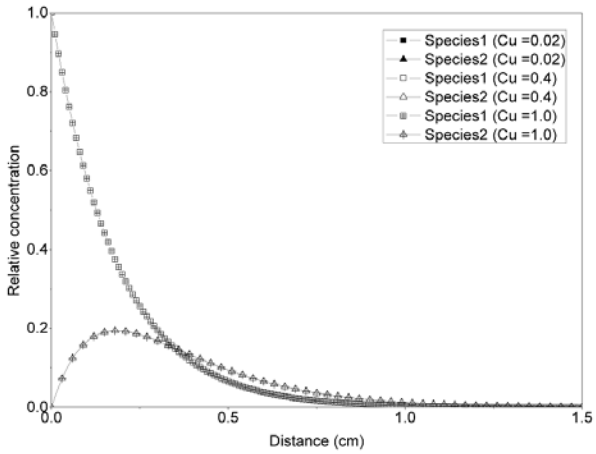

Figure 2. Spatial distribution of concentration obtained from the finite difference model for different Courant numbers.

Figure 2 illustrates the spatial distribution of relative concentration of both the species for Courant numbers ranging over an order of magnitude. Courant number is an indication of the stability of the model. An implicit solution can have a maximum value of 1.0 as the Courant number. It is observed from Fig.2 that the numerical solution is unaffected by the Courant number for the range of values considered.

3.2 Three species transport problem

The numerical model was further extended to the three species reactive system. The equations for describing the system are of the form:

$$\frac{\partial c_1}{\partial t} = -v\frac{\partial c_1}{\partial x} + D\frac{\partial^2 c_1}{\partial x^2} - k_1 c_1 \tag{10}$$

$$\frac{\partial c_2}{\partial t} = -v\frac{\partial c_2}{\partial x} + D\frac{\partial^2 c_2}{\partial x^2} - k_2 c_2 + y_1 k_1 c_1 \tag{11}$$

$$\frac{\partial c_3}{\partial t} = -v\frac{\partial c_3}{\partial x} + D\frac{\partial^2 c_3}{\partial x^2} - k_3 c_3 + y_2 k_2 c_2 \tag{12}$$

The initial and boundary conditions for the above equations are:

$$c_1(x,0) = c_2(x,0) = c_3(x,0) = 0 \qquad x \geq 0 \tag{13}$$

$$c_1(0,t) = 1.0 \qquad t > 0 \tag{14}$$

$$c_2(0,t) = c_3(0,t) = 0 \qquad t > 0 \tag{15}$$

$$c_1(L,t) = c_2(L,t) = c_3(L,t) = 0 \qquad t > 0 \tag{16}$$

Where c_1,c_2,c_3 are the concentrations of the first, second and third species; k_1 ,k_2,k_3 are the first order reaction rates, y_1, y_2 are the stochiometric yield coefficients and L is the length of the domain. The parameters used for this model are shown in table 2.

Table 2. System parameters for three species reaction system

Dispersion coefficient	D	0.18	$cm^2\ h^{-1}$
Velocity	v	0.2	$cm\ h^{-1}$
Decay rate of species 1	k_1	0.05	h^{-1}
Decay rate of species 2	k_2	0.03	h^{-1}
Decay rate of species 3	k_3	0.02	h^{-1}
Yield coefficient	y_1, y_2	1	-

A domain length of 40 cm and simulation time period of 400 hours was considered for this case.

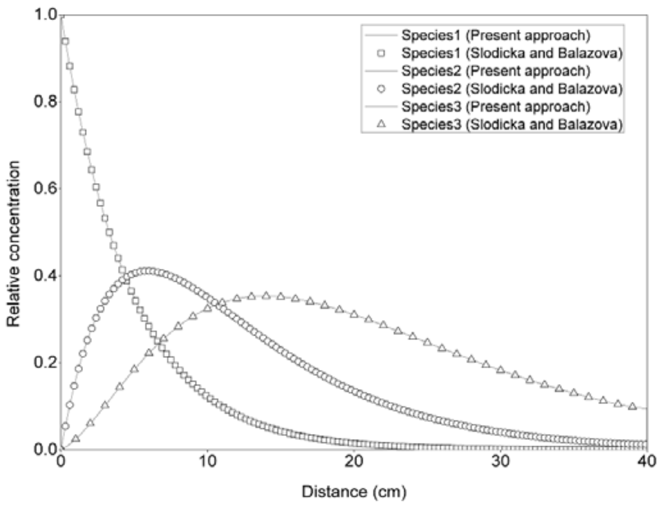

Figure 3. Comparison of the finite difference solution for three species reactive transport system with that of Slodicka and Balazova (2009).

Figure 3 provides the comparison of the concentration of all the species with the profiles obtained by Slodicka and Balazova (2009). A perfect agreement is observed between the results obtained using the present model and that of the new decomposition method developed by them. In this case, the model has been simulated for different reaction rates although the yield coefficients were kept constant. The yield coefficients have been considered to be constant in all the above cases. It is observed from the Fig.3 that the first and the second species are showing a similar behavior as in the case of two species transport as observed in Fig.2. However it is also observed that they do not reach zero concentrations at the same location as seen in Fig.2 but at different locations along the length of the domain as observed in Fig.3. This difference results from the difference in reaction rates between species 1 and 2. Since the reaction rate constant for third species is significantly small, with no further decaying, a significant concentration is observed at the end of the solution domain as seen in Fig.3 is quite expected. To test the validity of the model for different yield coefficients and different reaction rates, the following dataset from Sun et al. (1999b) was adopted.

Table3. System parameters for three species transport with different yield coefficients

Dispersion coefficient	D	4	$m^2\ d^{-1}$
Velocity	v	0.4	$m\ d^{-1}$
Decay rate of species 1	k_1	0.2	d^{-1}
Decay rate of species 2	k_2	0.1	d^{-1}
Decay rate of species 3	k_3	0.02	d^{-1}
Yield coefficient	y_1	0.5	-
Yield coefficient	y_2	0.3	-

A domain length of 40m and total simulation period of 40days was considered for the simulation.

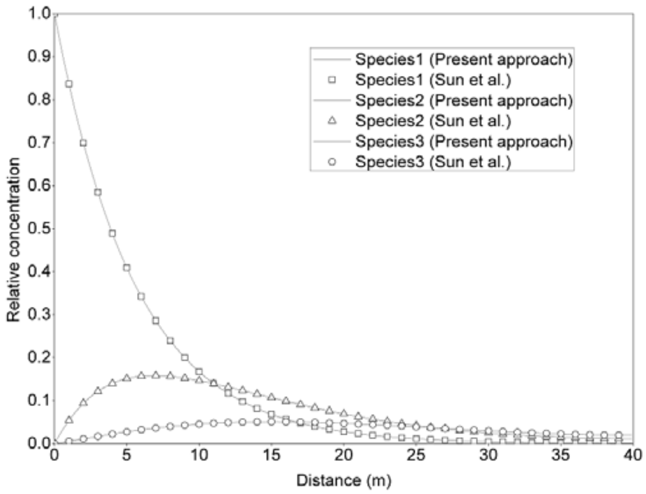

Figure 4. Spatial distribution of relative concentration for three species transport with different yield coefficients.

Figure 4 provides the comparison of the concentration of different species obtained using finite difference for a system with different yield coefficients with that of Sun et al. (1999). The results are in perfect agreement as observed in the figure. It is observed from the figure that all the species follow a similar behavior as that of the previous case but the relative concentration of the second and the third species is very low since the domain is dispersion dominant due to very high dispersion coefficient accompanied with high reaction rate. Thus it is observed from all the above case studies that the model can be implemented for different combinations of reaction rates and yield coefficients.

Conclusion

An implicit finite difference solution has been developed for modeling two species and three species transport. The model has been validated for identical as well as distinct reaction rates. This method serves as a good alternative for decomposition method adopted for multispecies transport adopted by various researchers, at least for the examples illustrated in this paper. The numerical approach is highly advantageous and handy when non linear processes are involved in the transport of contaminants in groundwater.

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References

[1] J. Bear. Dynamics of Fluids in Porous Media. Elsevier, New York (1972).
[2] J. Bear. Groundwater Hydraulics. Mc-Graw-Hill, New York (1979).
[3] T.P. Clement, Y. Sun, B.S. Hooker, J.N. Petersen. Modeling multi-species reactive transport in groundwater aquifers. Groundwater Monitoring Remediation, 18(2):79-92 (1998).
[4] T.P. Clement, C.D. Johnson, Y. Sun, G.M. Klecka, C. Bartlett. Natural attenuation of chlorinated solvent compounds: Model development and field-scale application. Journal of Contaminant Hydrology, 42: 113-140 (2000).
[5] M.Lunn, R.J. Lunn, R. Mackay. Determining analytic solutions of multiple species contaminant transport, with sorption and decay. Journal of Hydrology, 180:195-210 (1996).
[6] A. Ogata, R.B. Banks. A solution of the differential equation of longitudinal dispersion in porous media, U.S. Geol. Surv. Prof. Pap 411-A (1961).
[7] Y.Sun, T.P. Clement. A generalized decomposition method for solving coupled multi-species reactive transport problems. Transport in Porous Media, 37(3): 327–346 (1999).
[8] Y.Sun, J.N. Petersen, T.P. Clement. A new analytical solution for multiple species reactive transport in multiple dimensions. Journal of Contaminant Hydrology, 35(4): 429-440 (1999a).
[9] Y.Sun, J.N. Petersen, T.P. Clement, R.S.Skeen. Development of analytical solutions for multispecies transport with serial and parallel reactions. Water Resources Research, 35(1): 185–190 (1999b).

[10] M.Slodicka, A. Balazova. Singular value decomposition method for multi-species first-order reactive transport with identical decay rates. Transport in Porous media, (2007) doi: 10.1007/s11242-007-9175-7.
[11] M.Slodicka, A. Balazova. Decomposition method for solving multi-species reactive transport problems coupled with first-order kinetics applicable to a chain with identical reaction rates. Journal of Computational and Applied Mathematics, doi:10.1016/j.cam.2009.04.021.
[12] M. Th. van Genuchten, W.J. Alves. Analytical Solutions of the One-dimensional Convective-dispersive Solute Transport Equation, U. S. Department of Agriculture, Technical Bulletin No. 1661, pp.151 (1982).
[13] M.Th. van Genuchten. Convective-dispersive transport of solutes involved in sequential first-order decay reactions, Computational Geosciences, 11:129-147(1985).