Groundwater Contaminant Transport 1-D FDM Approach

AMARSINH B. LANDAGE[1]

1 Asst. Professor, Government College of Engineering, Karad, Maharashtra, India - 415124
amarlandage@yahoo.co.in

Abstract It Management of ground water resources including both quantity and quality requires the ability to establish a regional groundwater balance, to calculate flow of ground water, to predict water regimes in aquifers in response to proposed management schemes, to predict changes in water quality, to predict the transport of response of an aquifer system, both in terms of quantity which is observed as water levels and quality, is provided by flow and solute transport models that describe the response of the considered groundwater system to excitations.

When the contaminant is subject to non-linear degradation or decay, or it is characterized by a chemical constituent that follows a non-linear sorption isotherm, the resulting differential equation is non-linear. Analytical solution of non-linear differential equation is difficult. In the present work analytical model is the practical scenario of an instantaneous spill is studied for situations of non-linear decay, non-linear Freundlich isotherm, and non-linear Langmuir isotherm.

The FDM predictions were found to be in excellent agreement with analytical solutions for a wide range of field conditions with regard to dispersion and source definition. The new developed numerical model can be used for the forecasting of contaminant dispersion in laboratory and field under non-linear reactions, or for the quantitative description of the effect of non-linearity in the sorption parameters, on the time-space distribution of the contaminant. The implicit method used here which is unconditionally stable.

Key words Numerical Model, Analytical Model, FDM, Contaminant Transport, Advection, Diffusion, Dispersion

INTRODUCTION

Contamination of water either on surface or in ground is crucial problem. In most of groundwater contaminant transport investigations it is not practical to monitor all aspects of the groundwater flow and solute distributions. Groundwater models, which replicate the processes of interest at the site, can be used t complement monitoring and laboratory bench-scale studies in evaluating and forecasting groundwater flow and transport. However, every reliable model is based on accurate field data.

The oscillation in FDMs is usually avoided by adapting upwind methods. The upwind methods are reported to introduce large artificial dispersion. An improved FDM has been developed by Hossain and Yonge (1999) to provide oscillation free results with the introduction of minimum artificial dispersion. The improvement has been achieved by developing an expression of the minimum artificial dispersion needed to provide accurate results. The improved FDM provides results in excellent agreement with the analytical solution. A one-dimensional theory of contaminant migration through a saturated deforming porous media is developed by D.W. Smith (2000) based on a small and large strain analysis of a consolidating soil and conservation of contaminant mass. By selection of suitable parameters, the new transport equation reduces to the familiar one-dimensional dispersion-advection equation for a saturated soil with linear, reversible, equilibrium controlled sorption of the contaminant onto the soil skeleton. Analytic solutions for a quasi-steady-state problem have been presented. The solutions presented here provide a useful benchmark for solutions found using numerical methods, and clearly an investigation of the new transport equation under transient and finite mass boundary conditions should be undertaken using finite element analysis. A hybrid method of differential transform and finite difference method is employed by Chen and Ju (2004) to predict the advective–dispersive transport problems. The parameters of the equation are varied and different kinds of input sources are engaged to verify that the differential transform method is suitable for the problem. Some simulation results are illustrated and discussed in compare with the analytic solutions. The results show that the differential transform method can achieve good results in predicting the solution of such problems. A solute transport model developed by Eckhard Worch (2004) that describes non equilibrium adsorption in soil/groundwater systems by mass transfer equations for film and intra particle diffusion. The Freundlich isotherm is used in the model to make it applicable to systems with linear and nonlinear adsorption isotherms. This dispersed flow/film and particle diffusion model (DF-FPDM) was applied to three experimental data sets from column experiments with sandy aquifer material as sorbent and different solutes. The validity was also proved by a comparison with an analytical solution for the limiting case of predominating dispersion. Furthermore, a sensitivity analysis was performed to illustrate the influence of different process and sorption parameters (pore water velocity, intra particle mass transfer coefficient, and isotherm nonlinearity) on the shape of the calculated breakthrough curves. The DF-FPDM is assumed to be applicable also to competitive adsorption.

The multiple domain algorithms solves the one dimensional transient advection dispersion equation and similar partial differential equation numerically using an explicit scheme over a series of spatial domains at a constant time step, facilitating a faster propagation of transport information. This facilitates spreading the effect of the boundary condition across a wider interior domain with reduced computational effort. This study has accomplished integrating this approach for the explicit family of schemes, which are otherwise limited by the CFL condition. Rao and Medina Jr (2005) has been used the second order accurate MacCormack predictor–corrector method as the base numerical scheme in this investigation. However, this method is subject to another numerical difficulty: excessive diffusion of the wave front near the location of the moving front, thus possibly limiting its application for a select class of problems. In this numerical model proposed combine effect of decay and sorption on account for the solution of governing equation of contaminant transport.

CONTAMINANT TRANSPORT MECHANIS

Advection

Advection is the mass transport caused by the bulk movement of flowing ground water. The deriving force is the hydraulic gradient. The average transport velocity is calculated as the Darcy flux is divide by the effective porosity.

Dispersion

Dispersive spreading, within and transverse to, the main flow direction causes a gradual dilution of the contamination plume. Dispersion is an undesirable because it spreads contaminants very fast which in turn increases the volume of the contaminated ground water.

Diffusion

Diffusion is the net flux of the solutes from a zone of higher concentration to a zone of lower concentration. Diffusion does not depend on any bulk movement of the solution. The driving force is the random movement of the ionic and molecular constituents under the influence of their kinetic activity called Brownian motion

Decay

Not all contaminants that are adsorbed or desorbed follow the principle of fast reactions. Reactions that are relatively slow in comparison to the average travel time of the contaminants are described by kinetics. Reactions of the first order are applied to describe radioactive decay and/or simple degradation processes.

Sorption

Sorption refers to adsorption and desorption. Adsorption describes the adhesion of molecules or ions to the grain surface in the aquifer. The release from the solid phase is called desorption. Adsorption causes diminution of concentrations in the aqueous phase and a retardation of contaminant transport compared to water movement.

GOVERNING EQUATION FOR CONTAMINANT TRANSPORT

It is assumed that soil is homogeneous and isotropic. The porosity of soil, saturated hydraulic conductivity, ground water pore velocity is constant. One-dimensional ground water flow is considered. Hydrodynamic dispersion coefficient, Freundlich and Langmuir parameters and retardation is constant.

The one-dimensional advective-dispersive equations in an infinite aquifer subject constant point source and linear biological or radioactive decay.

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} + aC = 0 \text{ ----------------------- } -\infty < x < \infty, 0 < t \text{ and } C(\pm\infty, t) = 0$$

The one-dimensional advective-dispersive equations in an infinite aquifer subject to a general non-linear sorption isotherm of the form

$$R_d\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} = 0 \text{ ----------------------- } -\infty < x < \infty, 0 < t \text{ and } C(\pm\infty, t) = 0$$

Where, Rd is retardation factor

(a) Freundlich retardation factor by Freundlich sorption Isotherm

$$F = C_s = K_F C^b$$

Partition or Distribution coefficient $K_p = \frac{dF}{dC}$

$$\frac{dF}{dC} = K_F b C^{b-1}$$

$$R_d = 1 + \frac{\rho_b}{\theta}\left[K_F b C^{b-1}\right]$$

(b) Langmuir retardation factor by Langmuir sorption Isotherm

$$F = C_s = \frac{\alpha\beta C}{1 + \alpha C}$$

Partition or Distribution coefficient $K_p = \frac{dF}{dC}$

$$K_P = \frac{dF}{dC} = \frac{\alpha\beta(1 + \alpha C) - \alpha\beta\alpha C}{(1 + \alpha C)^2}$$

$$K_P = \frac{dF}{dC} = \frac{\alpha\beta}{(1 + \alpha C)^2}$$

$$R_d = 1 + \frac{\rho_b}{\theta}\left[\frac{\alpha\beta}{(1 + \alpha C)^2}\right]$$

The one-dimensional advective-dispersive equations in an infinite aquifer subject to constant point source and non-linear biological or radioactive decay and sorption

$$R_d\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} + aC = 0 \text{ ----------------- } -\infty < x < \infty, 0 < t \text{ and } C(\pm\infty, t) = 0$$

$$\left(1+\frac{\rho_b}{\theta}\frac{dF}{dC}\right)\frac{\partial C}{\partial t}-D\frac{\partial^2 C}{\partial x^2}+u\frac{\partial C}{\partial x}+aC=0$$

Where,

Retardation factor $R_d=\left(1+\frac{\rho_b}{\theta}\frac{dF}{dC}\right)$ and Partition or Distribution coefficient $K_p=\frac{dF}{dC}$

NUMERICAL SOLUTION FOR DECAYING CONTAMINANT SPECIES TRANSPORT

The one-dimensional advective-dispersive equations in a semi infinite aquifer subject to constant point source and linear biological or radioactive decay.

$$\frac{\partial C}{\partial t}-D\frac{\partial^2 C}{\partial x^2}+u\frac{\partial C}{\partial x}+aC=0 \tag{1}$$

The above equation may be solved for a variety of boundary and initial conditions. However, the following boundary and initial conditions were considered.

B.C.

$C\left(x=0,t>0\right)=C_0$ and $C\left(x=L,t\geq 0\right)=0$

I.C.

$C\left(0<x\leq L,t=0\right)=0$

So the 1-D advection-dispersion equation becomes, in FDM form:

$$\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial x^2}-u\frac{\partial C}{\partial x}-aC$$

In matrix form :

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & . & . & . & . & 0 & 0 & 0 & 0 & 0 \\ P & Q & R & 0 & 0 & 0 & . & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & P & Q & R & 0 & 0 & . & . & . & . & 0 & 0 & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & 0 & 0 & . & . & . & 0 & 0 & P & Q & R & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & . & . & . & 0 & 0 & 0 & P & Q & R \\ 0 & 0 & 0 & 0 & 0 & 0 & . & . & . & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} C_1^j \\ C_2^j \\ C_3^j \\ . \\ . \\ . \\ C_{n-2}^j \\ C_{n-1}^j \\ C_n^j \end{bmatrix} = \begin{bmatrix} C_0 \\ C_2^{j-1} \\ C_3^{j-1} \\ . \\ . \\ . \\ C_{n-2}^{j-1} \\ C_{n-1}^{j-1} \\ C_n^{j-1} \end{bmatrix}$$

$$\left[M^F\right]\left[C^j\right]=\left[R^F\right]$$

The matrix $\left[M^F\right]$ is tridiagonal and is constant. At each time step, systems of equations are solved for concentrations at the nodes by forward and backward substitutions using Gauss Elimination Technique.

NUMERICAL SOLUTION FOR SORBING CONTAMINANT SPECIES TRANSPORT MODEL

The one-dimensional advective-dispersive equations in a semi infinite aquifer subject to a general non-linear sorption isotherm of the form

$$R_d\frac{\partial C}{\partial t}-D\frac{\partial^2 C}{\partial x^2}+u\frac{\partial C}{\partial x}=0 \tag{2}$$

The above equation may be solved for a variety of boundary and initial conditions. However, the following boundary and initial conditions were considered.

B.C.

$$C(x=0, t>0) = C_0 \text{ and } C(x=L, t \geq 0) = 0$$

I.C.

$$C(0 < x \leq L, t=0) = 0$$

So the 1-D advection-dispersion equation becomes, in FDM form:

$$R_d \left[\frac{C_i^j - C_i^{j-1}}{\Delta t}\right] = D\left[\frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{\Delta x^2}\right] - u\left[\frac{C_{i+1}^j - C_{i-1}^j}{2\Delta x}\right]$$

In matrix

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & . & . & . & . & 0 & 0 & 0 & 0 & 0 \\ P & Q & R & 0 & 0 & 0 & . & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & P & Q & R & 0 & 0 & . & . & . & . & 0 & 0 & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & 0 & 0 & . & . & . & 0 & 0 & P & Q & R & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & . & . & . & 0 & 0 & 0 & P & Q & R \\ 0 & 0 & 0 & 0 & 0 & 0 & . & . & . & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} C_1^j \\ C_2^j \\ C_3^j \\ . \\ . \\ . \\ C_{n-2}^j \\ C_{n-1}^j \\ C_n^j \end{bmatrix} = \begin{bmatrix} C_0 \\ C_2^{j-1} \\ C_3^{j-1} \\ . \\ . \\ . \\ C_{n-2}^{j-1} \\ C_{n-1}^{j-1} \\ C_n^{j-1} \end{bmatrix}$$

$$\left[M^F\right]\left[C^j\right] = \left[R^F\right]$$

NUMERICAL SOLUTION FOR DECAYING AND SORBING CONTAMINANT SPECIES TRANSPORT MODEL

The one-dimensional advective-dispersive equations in a semi infinite aquifer subject to constant point source and non-linear biological or radioactive decay and sorption

$$R_d \frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} + aC = 0 \quad (3)$$

The above equation may be solved for a variety of boundary and initial conditions. However, the following boundary and initial conditions were considered.

B.C.

$$C(x=0, t>0) = C_0 \text{ and } C(x=L, t \geq 0) = 0$$

I.C.

$$C(0 < x \leq L, t=0) = 0$$

So the 1-D advection-dispersion equation becomes, in FDM form:

$$R_d \frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - u\frac{\partial C}{\partial x} - aC$$

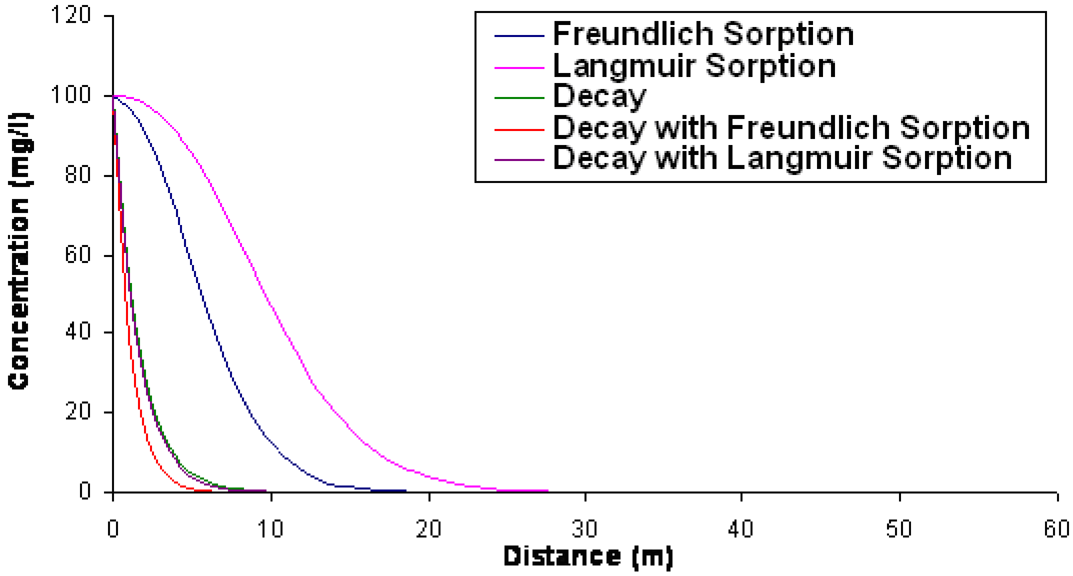
In matrix form:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & . & . & . & . & 0 & 0 & 0 & 0 & 0 \\ P & Q & R & 0 & 0 & 0 & . & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & P & Q & R & 0 & 0 & . & . & . & . & 0 & 0 & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & 0 & 0 & . & . & . & 0 & 0 & P & Q & R & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & . & . & . & 0 & 0 & 0 & P & Q & R \\ 0 & 0 & 0 & 0 & 0 & 0 & . & . & . & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} C_1^j \\ C_2^j \\ C_3^j \\ . \\ . \\ . \\ C_{n-2}^j \\ C_{n-1}^j \\ C_n^j \end{bmatrix} = \begin{bmatrix} C_0 \\ C_2^{j-1} \\ C_3^{j-1} \\ . \\ . \\ . \\ C_{n-2}^{j-1} \\ C_{n-1}^{j-1} \\ C_n^{j-1} \end{bmatrix}$$

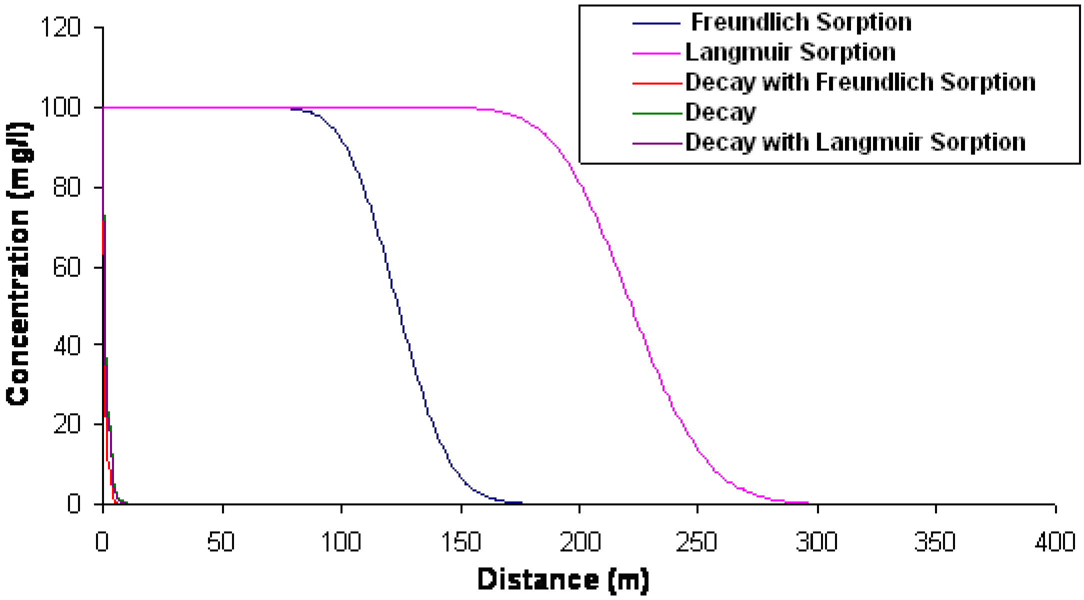
$$\left[M^F\right]\left[C^j\right]=\left[R^F\right]$$

RESULT AND DISCUSSION

Contaminant concentration distribution species for decaying and sorbing species at different time



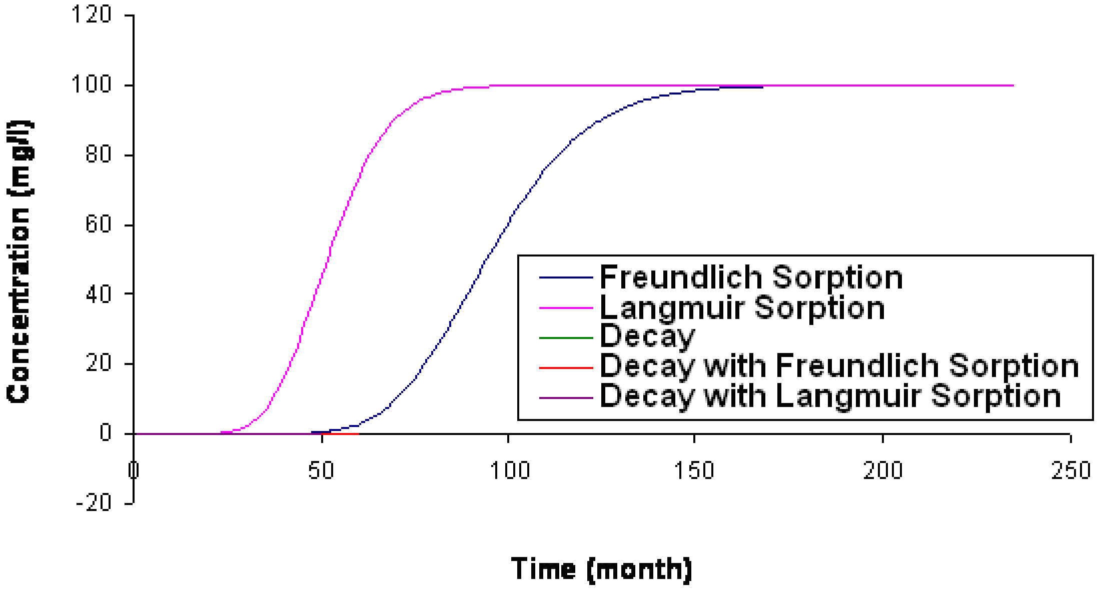
Concentration Distribution at 1 month



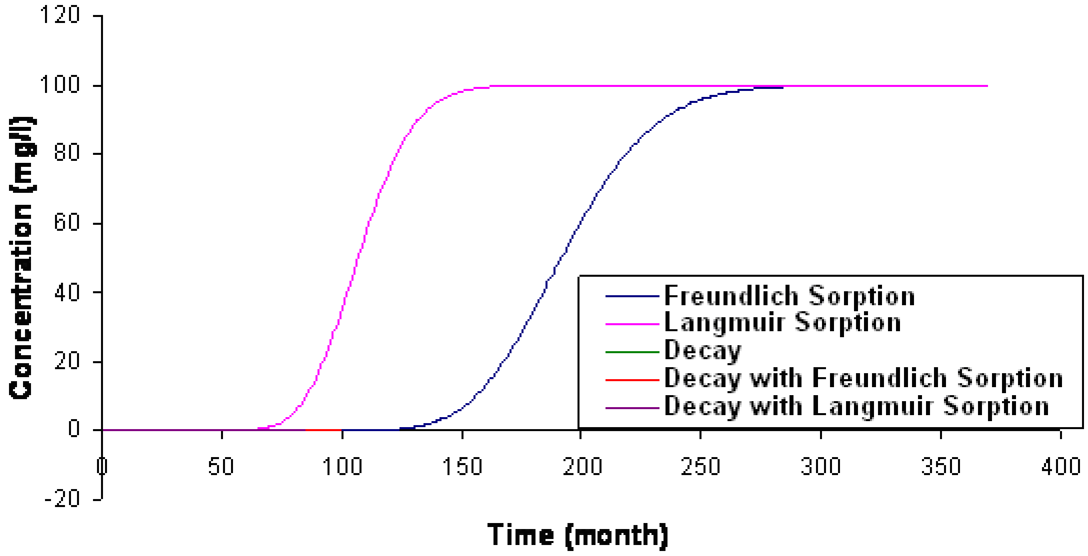
Concentration Distribution at 240 month

Figures show concentration distribution of contaminant species at different time in longitudinal direction.
It is observed that at initial time contaminant species rapidly reduces in domain due to sorption and decay. Contaminant specie dose not travel more distance As time increases plot clearly difference between decay, Freundlich sorption and Langmuir sorption. Contaminant species diminish due to decay. In case of Freundlich sorption and Langmuir sorption solute particle travel long distance in the direction of ground water velocity and slowly reduces its movement and existance. Because of high value of Freundlich retardation factor contaminant species velocity less than velocity of species due to Langmuir sorption.
At the initial few months it is observed that front of concentration distribution curve is smooth and concentration slow decrease. However, as time increases front become sharp. It indicates that after traveling certain distance in long time concentration reduces rapidly.

Contaminant concentration distribution species for decaying and sorbing species at different distance



Concentration Distribution at 50 meter



Concentration Distribution at 100 meter

Figures show concentration distribution of contaminant species at different distance for continuous time

It is observed that plume of contaminant species reaches early period in case of Langmuir sorption, shows that contaminant species velocity in the longitudinal direction of ground water is high. In case of Freundlich sorption, plume takes more time to reach at particular distance than Langmuir sorption. It indicates that contaminant species velocity more affected due Freundlich sorption than Langmuir sorption.

Contaminant species almost diminishes due to decay. When we take combine effect of decay and sorption, decay is always dominant than sorption. Because of that species concentration reduces rapidly in aquifer.

CONCLUSION

The FDM predictions were found to be in excellent agreement with analytical solutions for a wide range of field conditions with regard to dispersion and source definition. The new developed numerical model can be used for the forecasting of contaminant dispersion under non-linear reactions, or for the quantitative description of the effect of non-linearity in the sorption parameters, on the time-space distribution of the contaminant. The solution for numerical values of state variable only at specified points in the space and time domains defined for the problem. The above FDM model solved by using implicit scheme is unconditionally stable. The proposed models are flexible, stable, and could be used for laboratory or field simulations at early or prolonged contamination scenarios.

REFERENCES

Basak, V. and Murty,V.V.N. (1978) Pollution of groundwater through nonlinear diffusion. *Journal of Hydrology*, 38,243-247.

Chen, C.K., Ju, S.P. (2004) Application of differential transformation to transient advective–dispersive transport equation. *Applied Mathematics and Computation*, 155, 25-38.

Craig, J.R. and Rabideau, A.J. (2006) Finite difference modeling of contaminant transport using analytic element flow solutions. *Advances in Water Resources* 29, 1075-1087.

Hossain, M.K. and Yonge,D.R. (1999) Simulating advective-dispersive transport in groundwater: an accurate finite difference model. *Applied Mathematics and Computation*,05, 221-230.

Jaco J. A. and Kooten,V.(1994) Groundwater contaminant transport including adsorption and first order decay. *Stochastic Hydrology and Hydraulics*,8,185-205.

Lee, K. Y. and Chrysikopoulos, C. V. (1995) Numerical modeling of three-dimensional contaminant migration from dissolution of multicomponent NAPL pools in saturated porous media. *Environmental Geology*, 26,157-165.

Li, J., Chen, Y. and Pepper, D. (2003) Radial basis function method for 1-D and 2-D groundwater contaminant transport modeling. *Computational Mechanics* 32, 10-15.

Liu, J.J. and Soni, B.K. (1998) 2D Groundwater Contaminant Transport Modeling by using the Finite Volume Method on an Unstructured Grid System. *Applied Mathematics and Computation*, 89, 199-211.

Lunn, R.J. and Mackay, R. (1995) Solution of multispecies transport in the unsaturated zone using a moving point method, *Journal of Hydrology*,168,29-50.

Panday, S. , Huyakorn, P.S., Therrien, R. and Nichols, R.L. (1993) Improved three-dimensional finite-element techniques for field simulation of variably saturated flow and transport. *Journal of Contaminant Hydrology*, 12, 3-33.

Pang, L. and Hunt, B. (2001) Solutions and verification of a scale-dependent dispersion model. *Journal of Contaminant Hydrology*, 53, 21-39.

Rao, P. and Medina, M.A. (2005) A multiple domain algorithm for modeling one-dimensional transient contaminant transport flows. *Applied Mathematics and Computation*,167,1-15.

Serrano, S.E. (2001) Solute transport under non-linear sorption and decay. *Water Resources*, Volume 35, No.6, 1525-1533.

Sheu, T. and Chen, Y.H. (2002) Finite element analysis of contaminant transport in groundwater. *Applied Mathematics and Computation*, 127, 23-43.

Smith, D. W.(2000) One-dimensional contaminant transport through a deforming porous medium: theory and a solution for a quasi-steady-state problem. *International Journal for Numerical and Analytical Methods in Geomechanics*, 24,693-722.

Suna, Y., Petersen, J.N. and Bearc, J. (2001) Successive identification of biodegradation rates for multiple sequentially reactive contaminants in groundwater, *Journal of Contaminant Hydrology*, 51, 83-95.

Sun, Y., Petersen, J.N., Buscheck, T.A. and Nitao,J. J.(2002) Analytical Solutions for Reactive Transport of Multiple Volatile Contaminants in the Vadose Zone. *Transport in Porous Media*, 49,175-190.

Tartakovsky, D.M. (2000) An analytical solution for two-dimensional contaminant transport during groundwater extraction. *Journal of Contaminant Hydrology*, 42, 273-283.

Worch, E. (2004) Modelling the solute transport under nonequilibrium conditions on the basis of mass transfer equations, *Journal of Contaminant Hydrology*, 68, 97-120.