An Investigation of tracer transport in variably saturated porous media using VS2DI model

Parul Saxena and Manju Agarwal
Dept. of Mathematics and Astronomy,
Lucknow University, Lucknow-226007
pulsxn@gmail.com

Abstract
The present study deals with the tracer transport in variable saturated porous media. The advection –dispersion equation has been used for the purpose. Firstly the results have been deduced using Matlab program. The Concentration analysis has been done against time and dispersion coefficient. The important results are deduced. Further a case study has been done using vs2dt.

Keywords: *Variable saturated porous medium, tracer transport, Advection dispersion equation*

Introduction
Chemical substances have been used as tracers to estimate the migration of contaminant in a porous medium. Oceanographers use a variety of chemical substances to track diffusive and adventive processes in the ocean. These chemical tracers can be divided into two primary categories, conservative and non-conservative tracers.

Transport models can be solved using two methods (i) Analytic approach, (ii) Computational technique. Solving problems numerically suitable methods can be used and can be solved using Matlab software and other software also. Most of the problems have been solved using these approaches. Everts et al. (1989) investigated if the large amount of tracers applied they could potentially affect adversely water quality similar to the pollutants.

The models based on analytic approach contained many boundary conditions are proposed by various scientists (James and Rubin 1986, Wallach and Stenhuis 1998, Nützmann *et al.* 2002. Sato *et al.* 2003, Toride *et al.* 2003).Picken and Grisak 1981 proposed numerical approach to study transport models. The characteristics of the water flow and the solute transport in unsaturated soils has been discussed by Grisak and Picken 1980a, b, James and Rubin 1986, Nützmann *et al.* 2002 and Sato *et al.* 2003.

Here in this paper our focus is to investigate the tracer transport using VS2DT software.Vs2dt is software which is used for transport in variably saturated porous media. There are three softwares provided by US geological survey 1. Vs2DTI, for simulating fluid flow and solute transport, 2. VS2DHI, for studying simulation of fluid flow and heat transport, and 3. VS2POST, A post processor is used for viewing results of simulation.

VS2DT Healy, 1990; Lappala etal., 1987 provided the numerical models used for flow and transport calculations and VS2DH (Healy and Ronan, 1996). This software vs2dt works on a finite-difference model which solves Richard's equation for fluid flow, and the advection-dispersion equation for solute transport. The model can analyze problems many complicated problems in simple way. The results are depicted in terms of pressure head, moisture content, and relative hydraulic conductivity. The basic models which are used in this modeling are Van Genuchten (1980), Brooks and Corey (1964), Haverkamp etal. (1977). Initial hydraulic condition can be specified as static equilibrium, specified pressure head, or specified moisture content. Numerical modeling of Tracer transport in unsaturated porous media has been done by T. Bunsari. et al. (2008), in this paper the author has developed a model for estimating the non-reactive constituent transport in porous media. As result it is obtained that tracer transport in the thick layer took longer elapse time than in thin layer.

In the vs2dt modeling boundary conditions may be added in terms of specified pressure head, specified flux, infiltration with ponding, evaporation, plant transpiration, and seepage faces. Solute transport processes include advection, dispersion, first-order decay, adsorption, and ion exchange. McCord etal. , 1997; and Halford, 1997 have used vs2dt in a variety of field studies.

Governing equations for Tracer transport model

The equation which governs the tracer transport in unsaturated soil in vertical y-direction is given below:

$$D_z \frac{\partial^2 c}{\partial z^2} - q_z \frac{\partial c}{\partial z} = \frac{\partial c}{\partial t} \qquad (1)$$

The dispersion coefficient couples both mechanical and molecular diffusions and the equation was given as

$$D_Z = \lambda v + D_M \qquad (2)$$

Richards equation which is used to determine Darcy's velocity which was presented in Eq.(1) Richards's equation was given as:

$$M \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z}(k_{zz} k_{rw} (\frac{\partial \psi}{\partial z} + 1), \qquad (3)$$

Where M and kzz k_{rw} are non-linear hydraulic parameters and could be evaluated using basic model Van Genuchten (1980). The associated equations are given below:

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{\left(1 + (p|\psi|^n\right)^m}, \qquad k_{zz} k_{rw} = k_{zz} \frac{[1 - (p|\psi|)^{n-1} [1 + (p|\psi|^n]^{-m}]^2}{\left(1 + (p|\psi|^n\right)^{m/2}} \qquad (4)$$

Method and solution:

US geological survey provided VS2DT which has been used here for investigating tracer transport in variably saturated porous media. In this model the flow equation has been solved using finite difference scheme. This model is developed by considering Darcy equation and advection dispersion equation both. The model is useful and can analyze problems with various geometries. Boundary conditions are specified in the model. There are several options for using them varies with different constraints that are specific to flow under unsaturated conditions: infiltration with ponding, evaporation, plant transpiration, and seepage faces. Solute transport which is our considered case and its options include first-order decay, adsorption, and ion exchange. For case study, the effect of tracer in variable saturated porous media. the transport model (with ion exchange) in VS2DT is considered. For texture class we use following parameters:

For Sandy loam: K_{zz}/ K_{hh} = 1.0, Saturated K_{hh} = 8.1E-6, Specific storage = 1E-4, RMC = 0.15, Alpha = 0.847, beta = 4.8
Alpha-L: (L) Longitudinal dispersivity
Alpha-T: (T) Transverse dispersivity
Coef. of mol. Diff. (L^2/T): Coefficient of molecular diffusivity in porous medium
Decay Constant (1/T) : Constant of first order decay
Bulk density [M/L^3]: Mass of porous medium per bulk volume
K_m : ion exchange selectivity coefficient
Q^: ion exchange capacity
C_0: Total solution concentration

Table parameters are given below for the model consideration:

Table: 1

1.Texture class	Alpha - L	Alpha - T	Mol. Diff.	decay	density	Km	Q^	C_0	
Sandy Loam	0.25	0.45	0.34	0.21	0	0	0	0	
2.Initial equilibrium profile	z-coordinate of water table	Min. pressure head							
	-0.8	0							
3.Domain	height	width							

size									
	5.0cm.	20.0 cm.							
4.Initial concentration	Contour value 1	Contour value 2	Contour value 3	Contour value 4					
	0.45	0.65	0.5	0.7					
5. Recharge period	Period Limit	Initial Time step	Time step multiplier	Max. Time step	Min Time Step	Time step Reduction factor	Max. Head change	Steady state heat criterion	Maximum hight of ponding
	500	10	20	50	10	0.56	8.9	10.5	40.0
6. Boundary conditions	On above boundary	On above boundary	On below boundary	On below boundary	On side1 boundary	On side1 boundary	On side 2 boundary	On side 2 boundary	
	Pressure	Concentration	Pressure	Concentration	Pressure	Concentration	Pressure	Concentration	
	0.35	0.65	0.26	0.32	0.56	0.32	0.67	0.78	

Table: 2

Input parameters for Richard's equation:

Parameters	Values
Domains	5 cm(thin) and 20 cm (thick)
Boundary conditions	Upper and lower ψ are -.0064 and -520 cm.H_2O, respectively
Time Domain	9 hours approx.for both thick and thin
Number of time steps; nt	1000steps per hour (thin) and 1100 steps per hour (thick)

Nodal spacing; dz	0.14 cm(thin) and 0.35 cm (thick)

Results and discussions:

The advection – dispersion equation (1) is solved using Matlab programming with solver pdepe. The proper boundary conditions are used. The graphs are plotted to view the effect on concentration profile with time and different dispersion coefficient. It is observed from fig. 1 that with increasing time concentration increases and attains a constant value at certain distance. Simultaneously the mesh effect has been shown. The values are run up for 100 meshes, which shows numerical solution of the problem. In Fig. 3, the graph has been plotted for different dispersion coefficient and it is observed that with increasing D, the concentration decreases.

The simulation has been done with the help of VS2DT software and the entities pressure head, concentration effect, velocity has been shown graphically at different time steps. The computational domain is considered with proper boundary conditions. The results are declared in terms of pressure head, saturation, concentration profiles

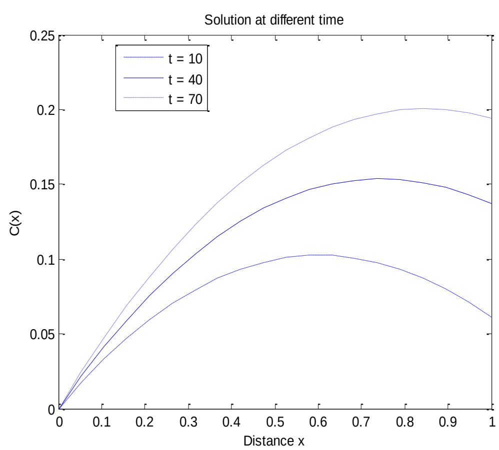

Fig. 1

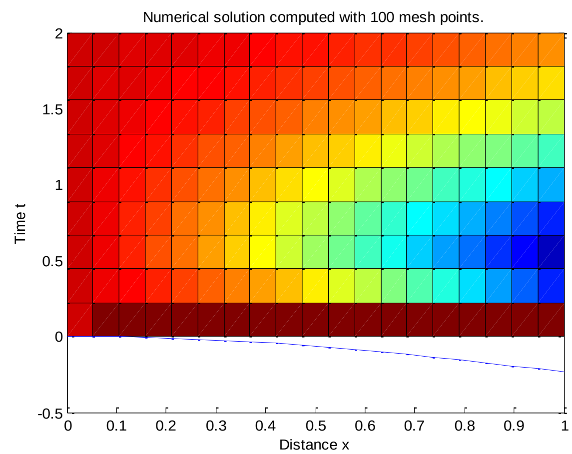

Fig. 2

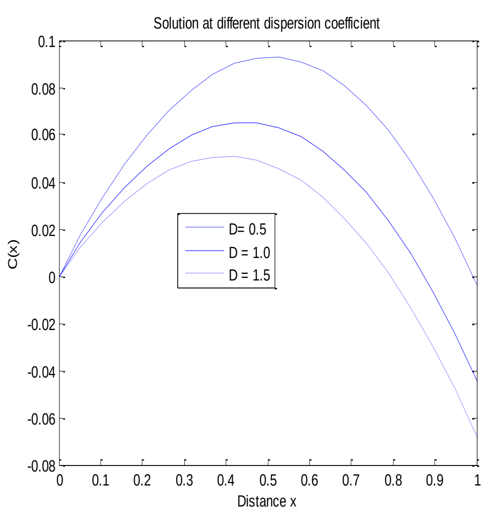

Fig. 3

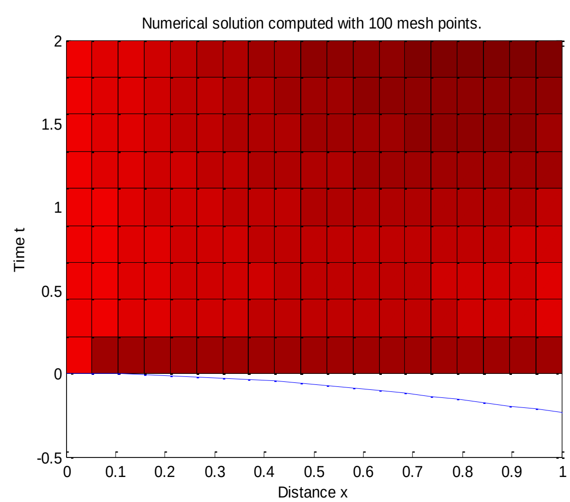

Fig. 4

In Fig. 5 and 6 the effect of porosity of porous media has been shown on tracer concentration which also influences the movement of these tracers in media. It has been observed with increasing value of porous parameter the concentration increases but with distance it decreases very slowly. A case study has been done using vs2dt. In Fig. 7, 8, 9, 10, 11, 12 the variation in pressure head has been shown with time. A table has been given above, the values of which has been used for the purpose.

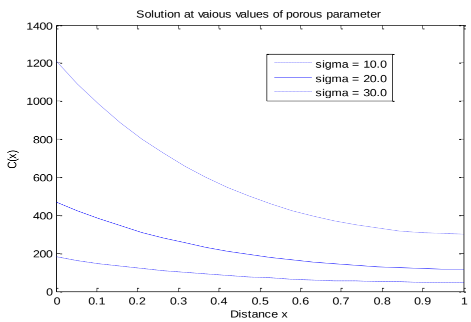

Fig. 5

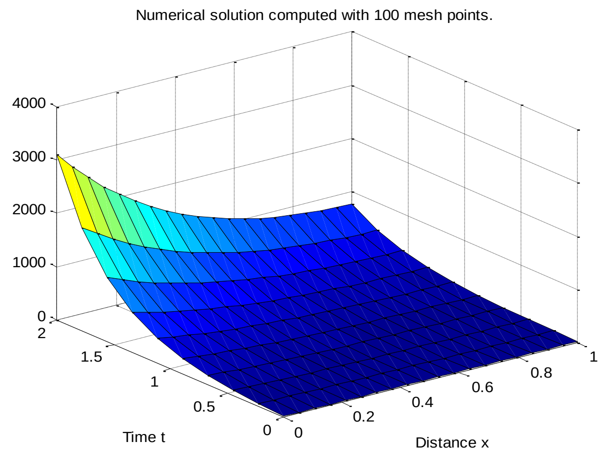

Fig. 6

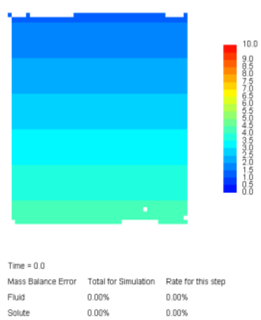

Fig. 7: Pressure head versus time t =0

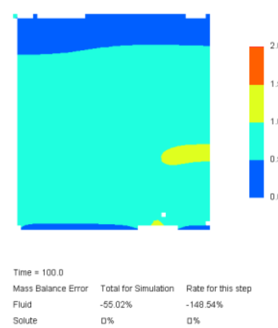

Fig. 8: Pressure head versus time at t = 100.0

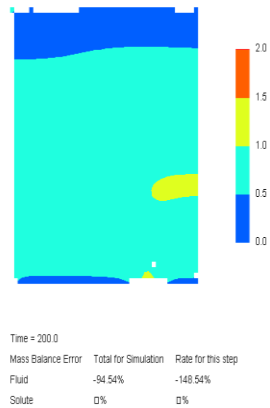

Fig. 9: Pressure head versus time at t = 200.0

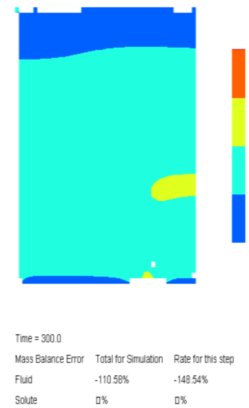

Fig. 10: Pressure head versus time at t = 300.0

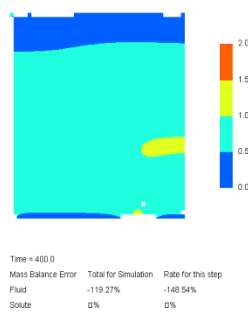

Fig. 11: Pressure head versus time at t = 400.0

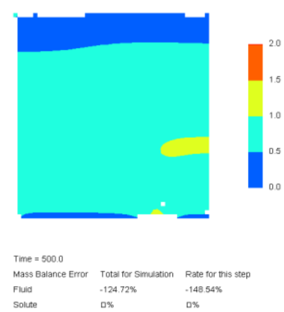

Fig. 12: Pressure head versus time at t = 500.0

The concentration analysis is described graphically below.

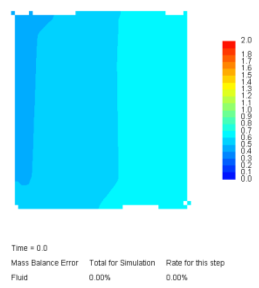

Fig. 13: Concentration of tracers in unsaturated porous media at t = 0.0

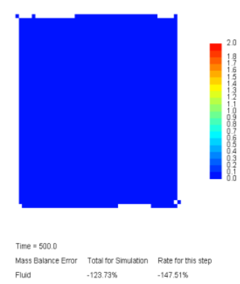

Fig. 14: Concentration of tracers in unsaturated porous media at t = 500.0

The values of pressure head and concentration are shown in above figures. The value of pressure head with respect to water content has been shown and the values differ with increasing simulation time. The approximate values can be estimated through color domain. As we can see that at time t = 0.0 the color domain range is 0 to 10 which changes to 0 to 2 with increasing time. The graphics also changes accordingly. It is observed the effect of high strength tracer concentration is to overcome the interference of background concentration in the soil. If the soil layer is thick, using diffusion mechanism the tracer time can be extended. Spreading of tracers can be affected highly due to dispersion.

Conclusions

The investigation has been carried out for tracer transport analysis in variable saturated porous media. The Matlab program is used for concentration analysis and pressure head analysis with time. A proper case study has also been done using vs2dt. Numerical solution has been shown with 100 meshes. The graphs predict that the effect on concentration with time and distance in porous media and it is deduced that the tracer concentration get affected by porous media significantly. With the effect of porous parameter the concentration reduces exponentially with distance. The graphs also show the importance of dispersion coefficient in approach of tracer transport analysis. The vs2dt modeling helps us to deduce the result for a specific case of porous medium i.e. sandy loam and using colored domain the variation in pressure head and concentration has been shown.

Acknowledgement

The author, Parul Saxena is thankful to the Dept. of Science and technology, New Delhi for financial support and to the Dept. of Mathematics and Astronomy, Lucknow University, Lucknow for providing research facilities during the work.

References

Bunsri, T., Sivakumar, M. and Hagare, D. 2008, Numerical Modelling of tracer transport in unsaturated porous media, Journal of Applied fluid mechanics, Vol.1, No.2, pp. 62-70.

Grisak, G.E. and J.F. Picken (1980a). Solute transport through fracture media 1. The effect of matrix diffusion. *Water Resources Research* 16(4), 719-730.

Healy, R.W., and Ronan, A.D., 1996, Documentation of computer program VS2DH for simulation of energy transport in variably saturated porous media -- modification of the U.S.Geological Survey's computer program VS2DT: U.S. Geological Survey Water Resources Investigations Report 96-4230, 36.

James, R.V. and J. Rubin (1986). Transport of chloride ion in a water-unsaturated soil exhibiting anion exclusion. *Soil Science Society of America Journal* 50, 1142-1149.

Lappala, E.G., Healy, R.W., and Weeks, E.P., 1987, Documentation of computer program VS2D to solve the equations of fluid flow in variably saturated porous media: U.S. Geological Survey Water-Resources Investigations Report 83-4099, 184.

Nützmann, G., S. Maciejewski and K.Joswig (2002).Estimation of water saturation dependence of dispersion in unsaturated porous media: experiment and modelling analysis. *Advance Water Resources* 25, 565-576.

Nützmann, G., S. Maciejewski and K. Joswig (2002) Estimation of water saturation dependence of dispersion in unsaturated porous media: experiment and modeling analysis. *Advance Water Resources* 25, 565-576.

Sato, T., H. Tanahashi and H.A. Loáiciga (2003).Solute dispersion in variably saturated sand. *Water ResourcesResearch* 39(6), 1155-1161.

Wallace, R. and T.S. Steenhuis (1998). Model for nonreactive solute transport in structure soils with continuous preferential flow path. *Soil Science Society of America Journal* 63, 703 712.