ICIWRM – 2000, Proceedings of International Conference on Integrated Water Resources
Management for Sustainable Development, 19 – 21 December, 2000, New Delhi, India

Modelling pollutant movement in the unsaturated aquifer

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Abstract
The most common approach used to model the transport of solutes in the subsurface is a mass balance partial differential equations, which combines two terms, viz., (i) solute displacement by convection with the mean pore flow velocity, and (ii) hydrodynamic dispersion. While the mean velocity convective term has a well-defined meaning, hydrodynamic dispersion in the unsaturated flow zone is still a subject of debate. The relationship found for saturated flow is adopted for unsaturated flow with values of dispersivity for one-dimensional flow taken from break-through-curves (BTC) measured through soil column experiments in the laboratory. The convective – dispersion equation describe the physical processes governing the movement, dispersion and transformation of a solute. An analytical solution describing the transport of solute in the unsaturated porous media with an asymptotic distance – independent dispersion relationship has been developed. The solution has a dispersion function, which is linear near the origin (i.e., for short travel distance), and approaches an asymptotic value as the travel distance becomes infinite. The results were compared with experimental results and with finite difference numerical solutions. The comparision indicates that the theory is reliable and can be used with confidence.

INTRODUCTION

In water resources development, one of the major problems is that of water quality. The sources of groundwater pollution can be divided into four major groups such as, environmental, domestic, industrial and agricultural. Groundwater contains salts carried in solution, which are added to by rainwater, irrigation water, artificial recharge, soluble rock materials, fertilizers etc. Accidental breaking of the sewers and percolation from septic tank may also increase the level of pollution. Contaminants are often leaked from chemical and petrochemical plants and from waste deposits. When radioactive wastes is buried at great depths, the only fluid media that can possibly interact with the wastes is groundwater.

In modern agriculture large quantities of water-soluble fertilizers are frequently applied to the soil surface. A portion of them remain in the root zone, and the rest is carried underground by the moving water. To estimate the magnitude of the hazard posed by some of these chemicals, it is important to investigate the processes that control their movement from the soil surface through the root zone down to the groundwater table. Understanding of these processes will make it possible to develop optimum management schemes for environmental hazard control with the purpose of preventing soil and water pollution.

The greatest challenge at the moment, however, is to develop the capability to predict with a reasonable degree of certainty, the spatial and temporal distribution of contamination in groundwater with the support of mathematical models. To model the behavior of a pollutant/contaminant in the soil is a complex and dynamic system and is inherently a difficult task. Furthermore, a contaminant after coming in contact with the soil, can undergo several biogeo-chemical processes viz., sorption-desorption, transformation/ degradation and leaching. Ideally, a comprehensive transport model should provide accurate predictions of the concentrations resulting from these interactions.

Lakshminarayana V (1968,1990) have solved Richard's equation for flow of water in unsaturated non homogeneous medium using explicit-implicit finite difference scheme and the Galerkin finite element model to solve 1-D and 2-D solute transport in porous medium. Numerous solutions to various forms of the convection-dispersion equations are found in literature (Eshel Bresler, 1973; John Wilson, 1981; Van Genuchten et al., 1991, Yates , 1990, 1992).

In general, the macroscopic rate at which a given solute moves in the soil system depends on the average flow pattern, on the rate of molecular diffusion, and on the ability of the porous material to spread the solute as a result of local microscopic deviations from the average flow. For proper modeling and understanding of the manner of solute transport in a natural soil profile, these phenomena must be considered simultaneously. The present work attempts to identify the level of groundwater contamination and to predict contaminant movement through the aquifer. Theoretical and mathematical tools for analyzing one-dimensional transfer of solutes in unsaturated soil zone is developed.

THEORETICAL CONSIDERATIONS

In dealing with the problem of simultaneous transfer of solute and water, one usually assumes that the transport of the solute is governed by convection and diffusion. In general, molecular diffusion takes place together with the convective transport, and each process contributes to the final dispersion of the solute. It is generally assumed that macroscopic transport by convection must take into account the average flow velocity as well as the mechanical or hydrodynamic dispersion. Solutes are transported by convection at the average velocity of the solution, and in addition they are dispersed about the mean position of the front.

The combined effect of diffusion and convection is derived by combining their mathematical expressions to obtain,

$$J = -D(v, \vartheta)\frac{\partial C}{\partial x} + q\,C \qquad (1)$$

J is total flux of solute;

C is solute concentration of the soil solution;
x is flow direction co-ordinate;
D is combined diffusion-dispersion coefficient;
q is volumetric flux of solution;
v is mean velocity of flow;
θ is moisture content.

In soils, changes in water content due to infiltration, redistribution, evaporation, and transpiration bring about the simultaneous movement of water and salt. A mathematical expression for one-dimensional transient conditions is derived from continuity considerations, which leads to;

$$\frac{\partial(Q+\theta C)}{\partial t} = \frac{\partial}{\partial z}\left(D(v,\theta)\frac{\partial C}{\partial z}\right) - \frac{\partial(qC)}{\partial z} + S \qquad (2)$$

where, Q is local concentration of solute in the adsorbed phase, meq/cm^3 ;
S is any sink or source rate term due to salt uptake, precipitation or dissolution;
t is time of travel of solute.

For water q (z, t), the boundary conditions at the soil surface (z = 0) and at t > 0 are;

$$|q(o, t)| \leq |R(t)|$$

$$\theta_d \leq \theta(0, T) \leq \theta_s$$

$$P_d \leq P(0, t) \leq P_a.$$

Whereas, during infiltration,

$$R(t) > 0, \quad p(0, t) \leq P_o \text{ or } \theta(0, t) \leq \theta_s.$$

During drainage or redistribution, $R(t) = 0$

and during evaporation,

$$R(t) < 0 \quad p(0, t) \geq P_d \quad \text{or} \quad \theta(0, t) \geq \theta_d$$

where q (0 , t) is volumetric flux of water at the soil surface,
p (0, t) is pressure and water contents corresponding to air dry soil;
p_0, θ_0 are highest pressure and soil water content,
R(t) is given potential flux at the soil surface.

The lower boundary at a depth ‘z’ must always be chosen such that it is below the root zone and the wetting front, where the pressure gradient approaches ‘0’.

In a simple case of drainage, the bottom boundary conditions could be zero pressure (p = 0) at the water table. Thus,

$p = 0, \quad z = Z, \quad t \geq 0.$

$P(z, 0) = P_n(z), \quad \theta(z, 0) = \theta_n(z), \quad 0 \leq z \leq Z.$

The boundary conditions at the bottom and the initial conditions are,
$t \geq 0 \quad z = Z \quad = 0;$
$t = 0 \quad 0 \leq z \leq Z; \quad C(z, 0) = C_n(z)$

where $C_n(z)$ is the predetermined initial salt concentration profile.

ANALYTICAL SOLUTIONS

$$\theta \frac{\partial C}{\partial t} = D' \frac{\partial^2 C}{\partial z^2} - q \frac{\partial C}{\partial z} \qquad (3)$$

$$D = \frac{D'}{\theta}, \qquad u = \frac{q}{\theta}$$

$$L\left[\frac{\partial C}{\partial t}\right] = L\left[D \frac{\partial^2 C}{\partial z^2}\right] - L\left[u \frac{\partial C}{\partial z}\right],$$

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial z^2} - u \frac{\partial C}{\partial z} \qquad (4)$$

$$D \frac{D^2 C}{D z^2} - u \frac{DC}{Dz} - SC = 0$$

$$S\, C(z,s) - C(z,0) = D \frac{D^2 C}{D z^2} - u \frac{DC}{Dz}$$

$$\frac{C}{C_o} = e^{\frac{uz}{2D}} \left[\frac{e^{-\frac{uz}{2D}}}{2} Erfc\left(\frac{z - ut}{\sqrt{4Dt}}\right) + e^{\frac{uz}{2D}} \; Erfc\left(\frac{z + ut}{\sqrt{4Dt}}\right) \right]$$

$$Dm^2 - u\,m - s = 0$$

$$m = \left(\frac{1}{2}D\right) [u \pm (u^2 + 4Ds)^{0.5}]$$

The general solution is

$$C = Ae^{\left[z\left\{u + (u^2 + 4D\,s)^{1/2}\right\}\right]} + B\,e^{\left[z\left\{u - \left(u^2 + 4D\,s\right)^{1/2}\right\}\right]} \qquad (5)$$

$$L\,[C\,(0, t)] = L\,(C_o) = \frac{C_0}{s}$$

$$L\,[C\,(\infty, t)] = L\,(0) = 0$$

Then we get the unknown constants B= $\frac{C_0}{s}$ and A=0.

$$C = \frac{C_o}{s}\; e^{\frac{\left(u - \left(u^2 + 4Ds\right)^{0.5}\right)z}{2D}}$$

$$= C_o\, e^{\frac{uz}{2D}} \quad L^{-1}\left[\frac{1}{s} Exp\left(-a\left(b^2 + s\right)^{0.5}\right)\right]$$

$$L^{-1}(C) = C = C_o e^{\frac{uz}{2D}}\; L^{-1}\left[\frac{1}{s} Exp\left[-\frac{\left(u^2 + 4Ds\right)^{0.5} z}{2D}\right]\right]$$

$$a = \frac{z}{D^{0.5}} \qquad b^2 = \frac{u^2}{4D}$$

$$C = C_o\, e^{\frac{uz}{2D}} \int_0^t \frac{a}{2\sqrt{\pi\, t^3}}\, e^{\left[-\left(\frac{a^2 + 4b^2t^2}{4t}\right)\right]}\, dt$$

$$C = C_o e^{\frac{uz}{2D}}\left[\int_0^t \frac{a + 2bt}{4\sqrt{\pi t^3}} e^{\left[-\frac{(a-2bt)^2}{4t}\right]} e^{-ab}\, dt + \int_o^t \frac{a - 2bt}{4\sqrt{\pi\, t^3}}\, e^{-\frac{(a+2bt)^2}{4t}}\; e^{ab}\, dt\right]$$

$$C = C_o e^{\frac{uz}{2D}}\left[Erfc\left(\frac{a - 2bt}{\sqrt{4t}}\right)\frac{e^{-ab}}{2} + \frac{e^{ab}}{2} Erfc\left(\frac{a + 2bt}{\sqrt{4t}}\right)\right].$$

$$Take \qquad \xi = \frac{a - 2bt}{\sqrt{4t}} \qquad \eta = \frac{a + 2bt}{\sqrt{4t}}$$

$$C = C_o e^{\frac{uz}{2D}}\left[\int_{\frac{a-2bt}{\sqrt{4t}}}^{\varpi} e^{-\xi^2}\,\frac{1}{\sqrt{\pi}}\, d\xi\; e^{-ab} + \frac{e^{ab}}{\sqrt{\pi}} \int_{\frac{a+2bt}{\sqrt{4t}}}^{\varpi} e^{-\eta^2}\, d\eta\right]$$

$$\frac{C}{C_o} = \frac{1}{2}\left[Erfc\left(\frac{z-ut}{\sqrt{4Dt}} \right) \; + \; e^{\frac{uz}{D}} \; Erfc\left(\frac{z+ut}{\sqrt{4Dt}} \right) \right] \quad . \tag{6}$$

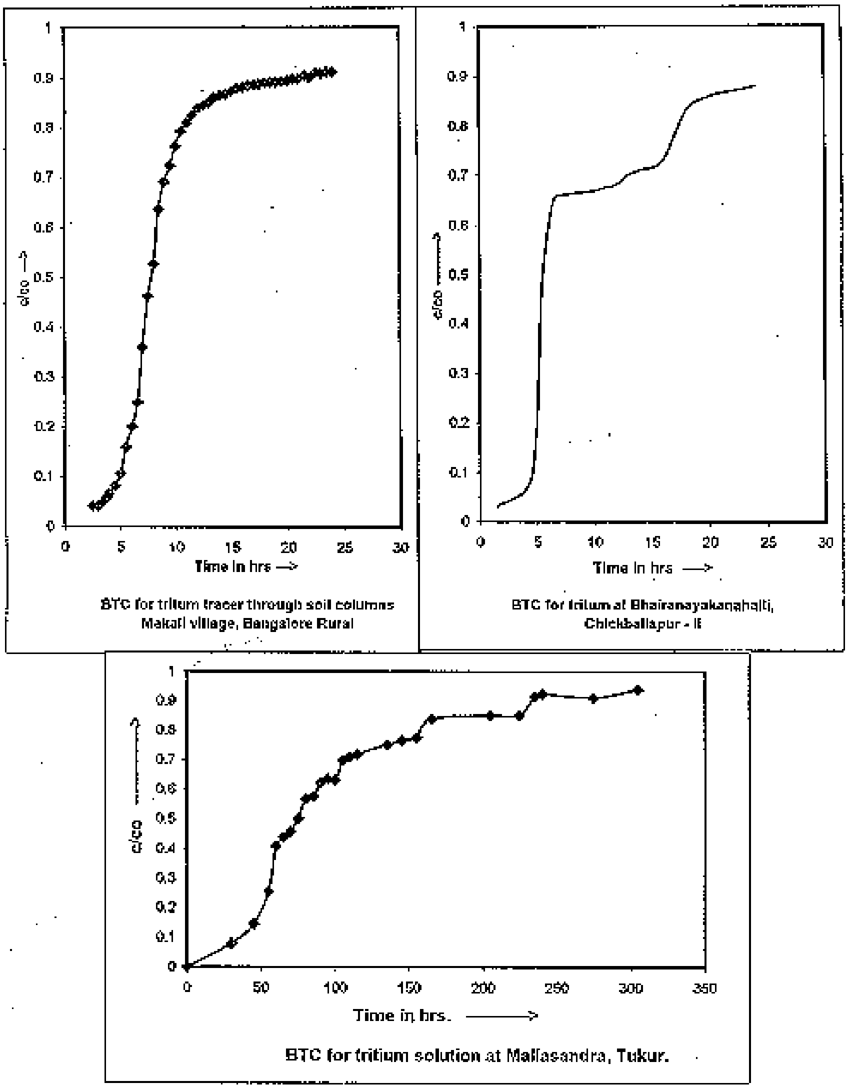

Figure 1. Break Through Curves for tritium solutions as tracer when passing through soil columns.

DISCUSSIONS AND CONCLUSIONS

An analytical solution for the transport of solutes in unsaturated media has been developed for a constant flux and constant concentration. The initial and boundary conditions chosen are,

$C(z, 0) = 0$ ……….Initial condition

$C(0, t) = C_o \quad t \geq 0$

$C(\infty, t) = 0 \quad t \geq 0$ ….. $\Big\}$ .Boundary conditions

The flow velocities and longitudinal dispersion coefficient are determined experimentally by allowing the solute to pass through the soil columns. The undisturbed soil columns were collected from Mallasandra, Chickballapur, and Makali village, Bangalore Rural.

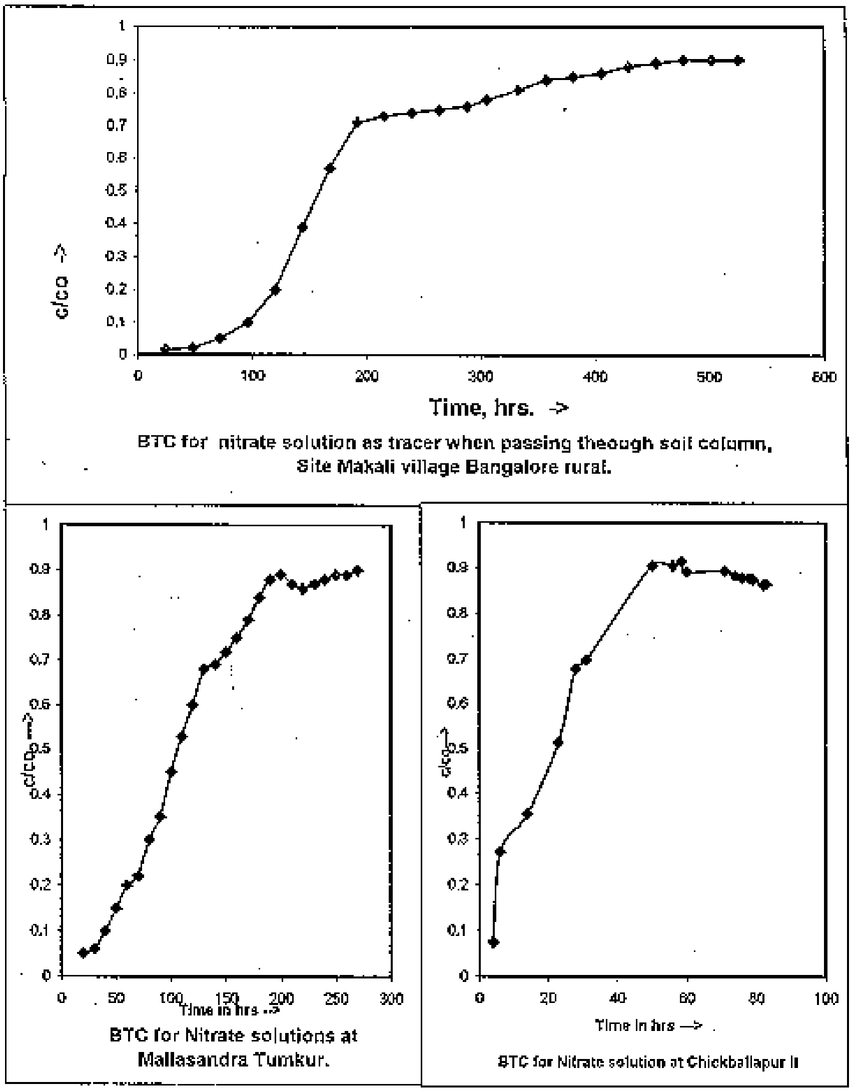

Figure 2. Break Through Curves for artifical nitrates (KNO_3) solutions as tracer when passing through soil columns.

Basak and Murthy (1978, 1979) have attempted to provide useful and unique method for quick determination of the hydrodynamic dispersion coefficients from soil column experimental data. The percolated effluents from soil columns were collected and the concentration of solutes (tritium and nitrates) were measured (Ranganna, 2000).

Figure (1) shows the break through curves resulted when tritium solution is passed through soil columns. Figure. (2) shows the break through curves obtained after artificial nitrate solution is allowed to pass through the soil columns collected from three different sites. Using the diffusion coefficients and average flow velocities computed from the soil columns experiments, the equation (6) is solved and the results are plotted Figure. (3) show the results obtained from the analytical solution for different diffusion coefficients and places. A finite difference solution of the one dimensional transport model has also been developed to check the accuracy of the analytical solutions. Figure. (4) show the results of the finite difference solutions of the transport equations.

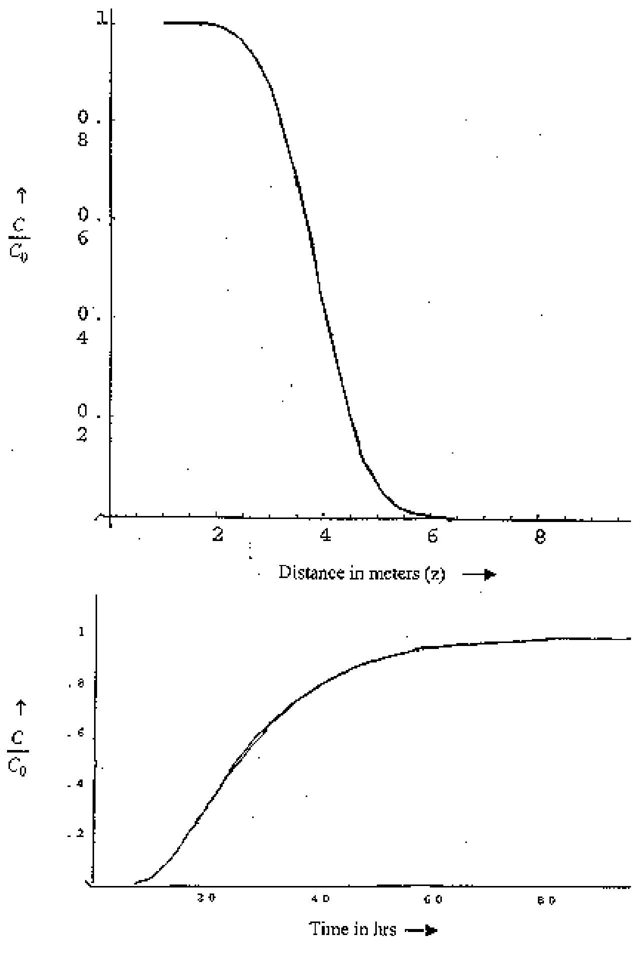

Figure 3. Analytical solution obtained for computed diffusion coefficients and velocity of flow.

The analytical expressions developed herein should prove helpful in making quantitative predictions on the possible contamination of groundwater supplies resulting from seepage of high salt concentrations in drainage ditches, canals and streams and from groundwater movement through buried wastes. The analytical solutions may be useful for verifying the numerical accuracy of more comprehensive finite difference and finite element solutions to the transport equations as well as for investigating some aspects of the transport process in porous media which has a distance dependent dispersion function of the described form.

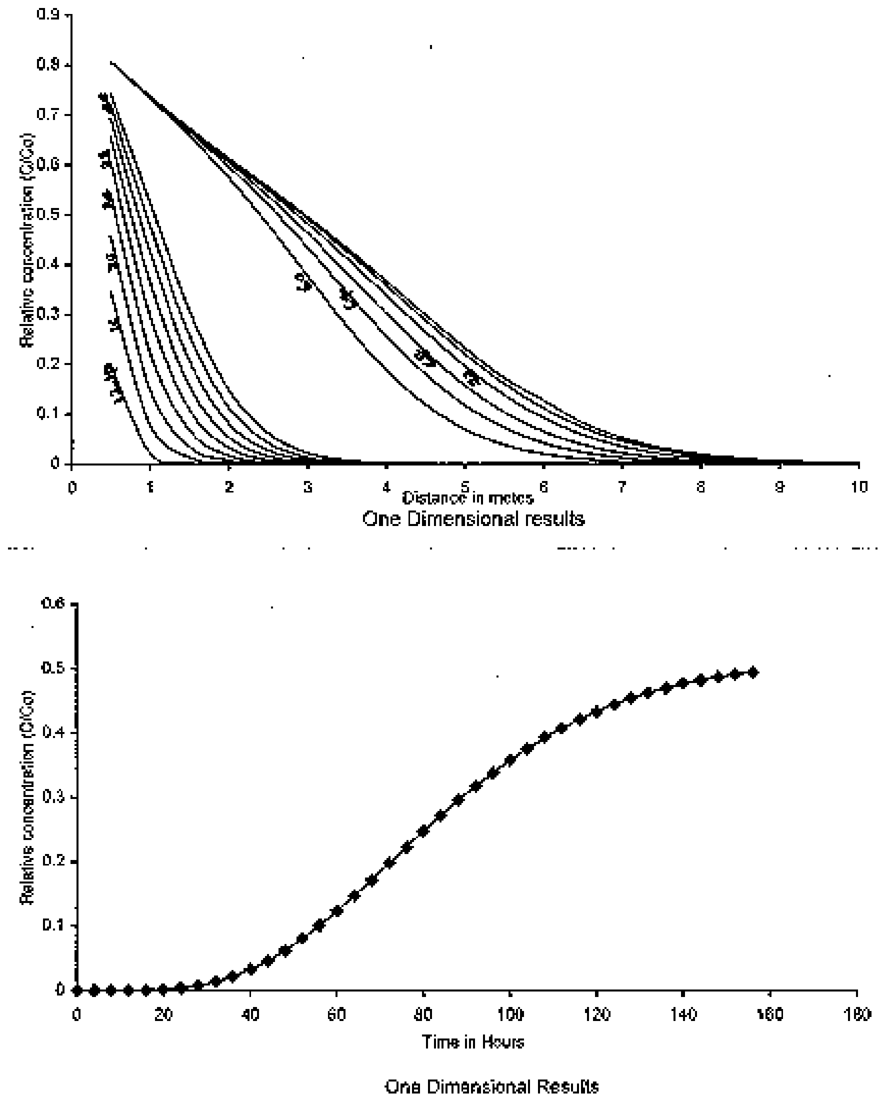

Figure 4. Finite difference solution of one-dimensional transport equation.

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