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Modelling of Pollutant Transport Through Unsaturated Zone by the Method of Characteristics

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Abstract : *The transport of pollutants through the unsaturated zone is goverened by Richard's and mass transport equations. Thus, the distribution of pollutant in space and time for given initial and boundary conditions, can be estimated by the solution of the two coupled differential equations. However, the conventional numerical techniques may lead to siginificant errors due to 'numerical dispersion' especially when the convective and the diffusive transports are of the same order of magnitude. A numerical algorithm for the solution by the method of characteristics is described. The resulting model has been tested using reported data.*

Introduction

Waste disposal on land and application of fertilizers and pesticides to croplands has become a common practice universally. Water infiltrating at the ground, dissolves such matter and carries it downward through the unsaturated zone. Many types of waste material (e.g., heavy metals, radioactive material) do not decompose easily. Such pollutants travelling through the unsaturated zone join the water table and may affect the water quality adversely. Further, fertilizers which are not utilized by crops are transported below the root zone by the percolating water and pose a potential threat to the groundwater quality.

In order to prevent or minimize such a water quality hazard, a thorough understanding of the flow process combined with the mechanism of transport is essential. In recent years many research workers have turned their attention to the problem. Unsteady state solutions have been given by Warrick et. al., 1971 (analytical solutlon); Bresler, 1973; Russo 1988 (finite differences); Van Genuchten, 1988 (finite elements); Smajstrla et. al, 1975; Khaleel et. al., 1985 (method of characteristics) and many others.

A model for numerical simulation of transport of dissolved Inert pollutant through the unsaturated zone is presented. The model involves solution of Richard's equation to arrive at the velocity distribution. This is followed by estimation of transport by the method of characteristics. The model has been tested using reportad data.

Governing Equations

The governing equation for one dimensional flow of a chemically inert solute through an unsaturated porous medium, can be written as follows,

$$\partial(C\theta)/\partial t = \partial/\partial z(\theta D.\ \partial C/\partial Z - qC(z,t)) \quad (1)$$

$$q = K.\ \partial(-h(z, t) + z)/\partial z \quad (2)$$

whare, θ is volumretic moisture content, $h(=h(\theta))$ is the capillary pressure head, $K(=K(\theta))$ is the unsaturated hydraulic conductivity (known as capillaty conductivity), $h(\theta)$ and

(K (ϑ) are the soil characteristics, z is a co-ordinate along the vertical direction (+ve, upwards), t is time, C(=C(z,t)) is the solute concentration, D(=D(z,t)) is the hydrodynamic dispresion coefficient and q (=q(z,t) is the Darcy velocity in a vertically downward direction.

The dispersion coeffecient D represents the combined effect of both molecular diffusion and mechanical dispersion, and can be defined as follows, (Kemper and van, 1966; Bresler, 1973; Ogata, 1970; Van Genuchten, 1982; Russo, 1988).

$$D = D_o a e^{b\vartheta} + \lambda |v| \qquad (3)$$

where, a and b are empirical constants characteraizing the soil, λ is dispersivity, $v(=q/\vartheta)$ is seepage velocity and Do is the molecular diffusion cofficient in a free water system.

The head from of Richard's equation governing one-dimensional vertical flow (and hence the distribution of Darcy's velocity in z and t) in an unsaturated medium, can be written as follows,

$$Cu.\ \partial h(z,\ t)/\delta t = \partial/\partial z(K.\partial(-h(z,\ t) + z)/\partial z) \qquad (4)$$

where, $Cu(=d\vartheta/dh)$ is the specific moisture capacity.

The Model

The numerical model developed to obtain a solute concentration distributlon in space and time, essentially involves a coupled solution of equations (1) and (4).

Solution of Richard's Equation

Richard's equation is a non linear second order partial differential equation. The non-linearity arises due to the dependence of Cu and K on ϑ (and h). In order to solve this equation the domain of flow extending from ground to water table is descretized by a number of nodes. Simalarly the time domain is discretized by a finite number of discrete times. Thus h(z,t) at the j^{th} node and k^{th} discrete time is represented as $h_{j,k}$ Eqn (4) is rewritten expresing the spatial and temporal derivatives of h by central finite differences. The resulting equation for an interior node j and time step $\triangle t$ from k^{th} to $(k+1)^{th}$ discrete time is as follows.

$$Cu_{j,k+1}\frac{h_{j,\,k+1}-h_{j,\,k}}{\triangle t} = \frac{1}{2}\left[\left\{K_{j-1,k}\frac{h_{j,\,k}-h_{j-1,\,k}}{\triangle z_{j-1}}+\frac{\triangle z_{j-1}}{2}+K_{j,\,k+1}\frac{h_{j,\,k+i}-h_{j-1,\,k+1}+\triangle z_{j1}}{\Delta z_{j-i}}\right\}-\left\{K_{j,\,k}\frac{h_{j+1,\,k}-h_{j,\,k}+\triangle z_j}{\triangle z_j}+K_{j,\,k+1}\frac{h_{j+1,\,k+1}-h_{j,\,k}+\Delta z_j}{\triangle z_j}\right\}\right]\frac{2}{\triangle z_j+\triangle z_{j-1}} \qquad (5)$$

$j = 2, 3, 4, \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots n-i$

where, n is the total number of nodes.

This provides (n-2) non-linear simultaneous equations. Two additional equations are obtained by assigning boundary conditions at the ground (i.e,, j=1) and at the water table (i,e., j=h). The boundary condition at the ground may be either of Neuman type (when tha entire input infilters) or Dlrichiet type (when ponding occurs or just saturation is maintained at the ground). At the water tabie the boundary condition is of Dirichiet type ($\vartheta = \phi$ or h=D), This leads to a determinate system of equations.

The system of non-linear simultaneous equations is solved using Picard's iteration method (Remson et al, 1971). Accordlng to this method the system of equatious is linearized and solved successively by evaluating K and Cu in accordance with the known values of h arrived at in the previous iteration. Thus. for the m^{th} iteration eqn. (5) is rewritten with the following substitutions,

$$h_{j-1,\,k+1} = h^{(m)}_{j-1,\,k+1};\quad h_{j,\,k+1} = h^{(m)}_{1,\,k+1};$$

$$h_{j+1,\,k+1} = h^{(m)}_{j+1,\,k+1}$$

$$Cu_{j,\,k+1} = \overset{(1-m)}{Cu}_{j,\,k+1}\ ;\ K_{j-1,\,k+1} = \overset{(m-1)}{K}_{j-1,\,k+1}\ ;$$

$$K_{j,\,k+1} = \overset{(m-1)}{K}_{j,\,k+1}\ ;$$

$$\overset{(o)}{K}_{j,\,k+1} = K_{j,\,k} \text{ and } \overset{(o)}{Cu}_{j,\,k+1} = Cu_{j,\,k}.$$

The resulting system of equations is tridiagonal and can be solved for $(\overset{(m)}{h}_{j,\,k+1,\ j=1,\ \ n})$ using the thomas algorithm (Remson et al, 1971). As the itertion index approaches infinty, $(\overset{(m)}{h}_{j,\,k+1})$ converges to the unknown true solution $(\hat{h}_{j,\,k+1})$ of non-linear equations

$$\left| \overset{(m)}{h}_{j,\,k+1} - \hat{h}_{j,\,k+1} \right| \to o \qquad (6)$$

Limit m $\to$ ∞

To avoid to large a number of intertations, are stopped when the following check is satisfied,

$$\left| \overset{(m)}{h}_{j,\,k+1} - \overset{(m-1)}{h}_{j,\,k+1} \right| \geq \epsilon_o \qquad (7)$$

where θ is a small +ve value.

Thus the distribution of h in space and time is obtained.

Computation of Velocities

Using the values of $h_{j,\,k}$, seepage velocities are computed as follows.

$$V_{j+1/2,k+1/2} = K_{j+1/2,k1/2} \cdot (\overline{h} + 2\triangle z_j \cdot \overline{\theta}_{j,k+1/2}) \qquad (8)$$

where,

$$\overline{h} = h_{j+1,k+1} - h_{j,k+1} - h_{j+1,k} - h_{j,k}$$

$$\overline{\theta}_{j,+k1/2} = (\theta_{j+1,k+1} + \theta_{j,k+1} + \theta_{j\ k+1,} + \theta_{j,\,k})/4$$

Solution of the Solute Transport Equation

The transport equation i.e. eqn(1) comprises of a convective and a diffusive component. In the proposed model, the convective component is simulated by the method of characteristics. The diffusive component is subsequently accounted for by an implicit finite difference scheme.

In the method of characteristics, instead of solving eqn(1) directly the characteristic equations are determined and solved. An equivalent set of ordinary differential equations for eqn(1) can be written as follows :

$$dz/d\theta = q/\theta \qquad (9)$$

$$d(C\theta)/dt = d/dz(\theta D.\ dC/dz) \qquad (10)$$

The solution of eqn(1), thus reduces to the solution of equations (9) and (10). The following steps are involved.

(i) The solute infilterating at the ground is represented by a small strip of uniform thickness, the bottom of which coincides with the initial interface (ground surface) between the solute and the unsaturated flow region. This has been termed as the off take point (refer Fig. 1) This off take point will move into the system with a velocity equal to the flow velocity at the ground. When the vertical distance moved by it equals (or exceeds) the thickness of the strip, the entire solute content represented by it, would have entered the flow domain. At this stage the off take point is assumed to have taken off and is termed as a moving point (refer fig. 1). The instant an off take point enters the flow domain it is replaced by a new one, to account for a continuous movement of flow.

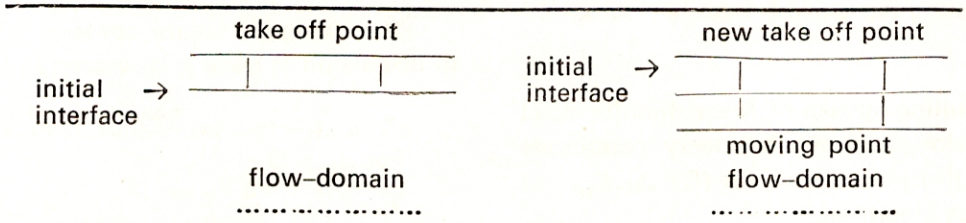

Fig. 1. Illustration of an off-take point and a moving point

(ii) Once a moving point has entered the flow domain, it's movement is goverened by the velocity distribution obtained by solving eqn(4) (as described previously). $U_{,k+1/2,}$ an average velocity of the p^{th} moving point during the period k to k+1 is assigned in accordance with the rollowing equation.

$$U_{p,k+1/2}=V_{j-1/2,k+1/2}+(V_{j+1/2,k+1/2}-V_{j+1/2,k+1/2}).\frac{\zeta_{p,k}-Z_{j-1/2}}{Z_{j+1/2}-_{j-1/2}} \quad (11)$$

where, z_j is the depth co-ordinate of the j^{th} node and $\zeta_{p,k}$ is the depth co-ordinate of the p^{th} moving point at k^{th} discrete time.

The depth co-ordinate $\zeta_{p,k+1}$ of the p^{th} moving point at the discrete time k+1 can be quantified as follows,

$$\zeta_{p,k+1}=\zeta_{p,k}+U_{p,k+1/2}.\ \triangle t \quad (12)$$

where,

$\zeta_{p,k+1}$ is the co-ordinate at time level k+1.

(iii) Each node represents an area of influence and any moving point falls within the area of a certain node j, if

$$z_j - \triangle z_{j-1}/2 \leqslant \zeta_{p,k+1} \leqslant z_j + z_{j+1}/2 \quad (13)$$

All moving points lying in the area of influence of a certain node contribute towards the solute content of that node. Thus the solute concentration at any node j at time k+1, due to convection is assigned as follows,

$$\hat{C}_{j,k+1} = \frac{J_1 \Sigma V_p}{Vol_j.\ \theta_{i,k+1}} \quad (14)$$

where, J_1 comprises of all the moving points lying in the area of influence of the j^{th} node at the time level k+1, V_p is the solute content of the p^{th} moving point, Vol_j is the representative volume of node j and $\theta_{j,k+1}$ is the moisture content at node j at the time level k+1.

(iv) The change in solute concentration due to dispersion is computed for each node using an implicit centered in space finite difference scheme. A finite difference form of eqn (10), including the convective term can be written as follows,

$$\frac{\theta_{j,k+1}+\theta_{j,k}}{2}.\ \frac{C_{j,k+1}+C_{j,k}}{\triangle t} = \left\{\frac{C_{j+1,k+1}-C_{j,k+1}}{\triangle z_j}\ \bar{\theta}_{j,k+1/2}D_{j+1/2,k+1/2} - \frac{C_{j,k+1}-C_{j-1,k+1}}{\triangle z_{j-1}}\ \bar{\theta}_{j-1,k+1/2}D_{j-1/2,k+1/2}\right\}\frac{2}{\triangle z_j+\triangle z_{j-1}} - C_{j,k}\frac{\theta_{j,k+1}-\theta_{j,k}}{\triangle t} - (qC)_{j,k+1} \quad (15)$$

$$j = 2,3,4 \ldots\ldots\ldots\ldots n-1$$

where,

$\bar{\theta}_{j-1,k+1/2}=(\theta_{j,k+1}+\theta_{j-1,k+1}+\theta_{j,k}+\theta_{j-1,k})/4$

$C_{j,k+1}$ is the solute concentration at node j, at the end of $k+1^{th}$ discrete time.

$(qc)_{j,k+1}$ is computed as follows.

$$(qc)_{j,k+1} = \frac{\left[\begin{array}{l}\text{incoming solute content}\\ \text{at node j}\end{array}\right] - \left[\begin{array}{l}\text{outgoing solute content}\\ \text{at node j}\end{array}\right]}{\triangle t.\ Vol_i}$$

The incoming and outgoing solute contents are computed by keeping a track of the moving points entering and leaving the area of influence of node j during the period from k^{th} to $k+1^{th}$ time level.

The resulting system of linear simultaneous equations (along with the boundary conditions at j=1 and j=n) is solved for $(C_{j,\ k+1,j=1,2\ \ n})$ using thomas algorithm.

(v) Change in solute content of each moving point due to dispersion is taken care of in the following manner.

The change in solute content $\Delta V_{j,\ k+1}$ due to dispersion at node j, is written as follows,

$$\Delta V_{i,\ k+1}=(C_{j,\ k+1}-\hat{C}_{j,\ k+1}).\ \theta_{j,\ k+1}\ Vol_j$$

For $J_1 > 0$

$$V_p = V_p + \frac{\Delta V_{j,\ k+1}}{J_1} \qquad \text{if } \Delta V_{j,\ k+1} \geqslant 0$$

$$V_p = V_p = \frac{V_p}{J_1 \Sigma V_p} \cdot \Delta V_{j,k+1} \qquad \text{if } \Delta_{j,k+1} < 0$$

For $J_1 = 0$ (i.e. no moving point is preasnt in the area of influence of the node), a new moving point is created as follows.

$$np = np + 1$$

where, np is the total number of moving points present in the flow domain at time k+1.

$$V_{np+1} = V \Delta V_{j,k+1}$$

The depth co-ordinate of the new moving point is assigned as follows,

$$\zeta_{np+1,k+1} = Z_i$$

(vi) The solute content V_{k+1} leached into the water table till the discrete time k+1, is computed as follows,

$$V_{k+1} = {}_{jz}\Sigma V_p$$

where, J_z comprises of all the moving points which have entered the water table (i e., satisfying the inequality $\zeta_{p,k+1} \geqslant D$, D being the depth to water tale).

MODEL TESTING

A field experiment of calcium chloride and water has been reported by Warrick et al (1971). The reported data have been used to test the model.

The reported hydraulic properties and initial and boundary conditions are stated below,

$$h(\theta) = \left\{ \begin{matrix} 0\ 6829 - 0\ 09524in & (\ |\ h\ |\ ) \\ 0.4531 - 0.02732in & (\ |\ h\ |\ ) \end{matrix} \right\}$$

$$h > 29.5$$

$$29.5 > h > 14.495$$

$$K(\theta) = 3.24 \times 10^{-8} \exp(35.8)$$

where, K is in cm/min.
For the solution of eqn(4),

$$\theta(z,O) = f(z) \qquad O \leqslant z \leqslant Z$$

$$h(O,t) = hs$$

$$h(Z,t) = hi$$

where, Z is the total depth of simulation, hs is the capillary head at saturation value and hi is the initial capillary head at depth Z.

For the solution of eqn(1),

$$C(z,O) = O \qquad O \leqslant z \leqslant Z$$

$$C(O,t) = 0.209 \qquad d < 7.62$$

$$C(O,t) = O \qquad d > 7.62$$

where, d is the cumulative depth of infilteration in cm.

$$\partial C / \partial z(Z,t) = 0$$

where, z is in cm, θ is in cm^3/cm^3, C is in meq/1 and t is in minutes. To compute the hydrodynamic dispersion co-efficient, parameters a and b were taken as 0.002 and 10 (Olsen and Kemper, 1968; Russo, 1988). For the dispersivity λ a range of 0.7—1.2 was taken to demonstrate it's effect on the concentration distribution with time. The computer code was written in FORTRAN IV and was run on a DEC 2050 mainframe.

RESULTS AND DISCUSSIONS

The measured and computed soil moisture profiles at 2,9,11 and 17 hrs of infilteration are presented in fig. 2. An examination of the profiles reveals that there is a close agreement between the observed and computed distribution of moisture in space and time. According to the reported data, the infilteration of the solute (7.62 cm) and water (22.9 cm). required a time period of 1050 minutes (17.5 hrs). The model simulated period of infiltration is 1044 ninutes (17.4 hrs).

The reported and computed solute concen-tration profiles at 2,9,11 and 17 hrs are plotted in fig. 3. It is revealed that at 9 hrs. $\lambda = 0.7$ yields a close match. However, at subsequent times higher λ values ($\lambda = 1.0$ at 11 hrs, $\lambda = 1\ 2$ at 17 hrs) are necessary for matching the reported and computed profiles. The corroborates the time (or depth) variability of λ reported by Corey et al (1970).

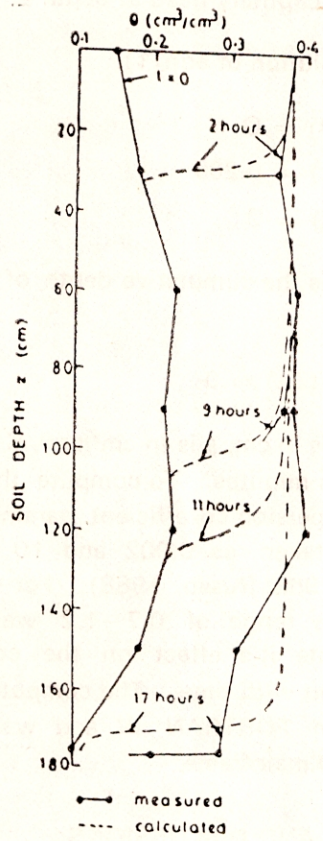

Fig. 2 Measured and simulated soil moisture profiles

An apparent lag between the simulated and measured solute concentration profiles is observed at all time levels (2,9.11 and 17 hrs). Attributing this lag to an incomplete mixing of solute within the soil pores (i.e. most of the water moves through the larger water filled pore sequences), the velocity computation (Gaudet et al, 1977) was modified as follows,

$$V_{j+1/2,k+1/2} = q_{j+1/2,k+1/2}/(\overline{\theta}/-\theta_{jm})$$

where θim is an immobile water content.
For $\theta \leqslant \theta$im, the capillary conductivity is taken as zero.

Neglecting the transfer of solute from the mobile phase to the immobile phase and taking a value of θim=0.08 the runs were repeated.

The modified results are ploted in fig. 4. It can be seen that the lag between the two profiles has been considerably reduced.

CONCLUSION

The proposed model is capable of simulating the convective and dispersive solute transport through the unsaturated zone.

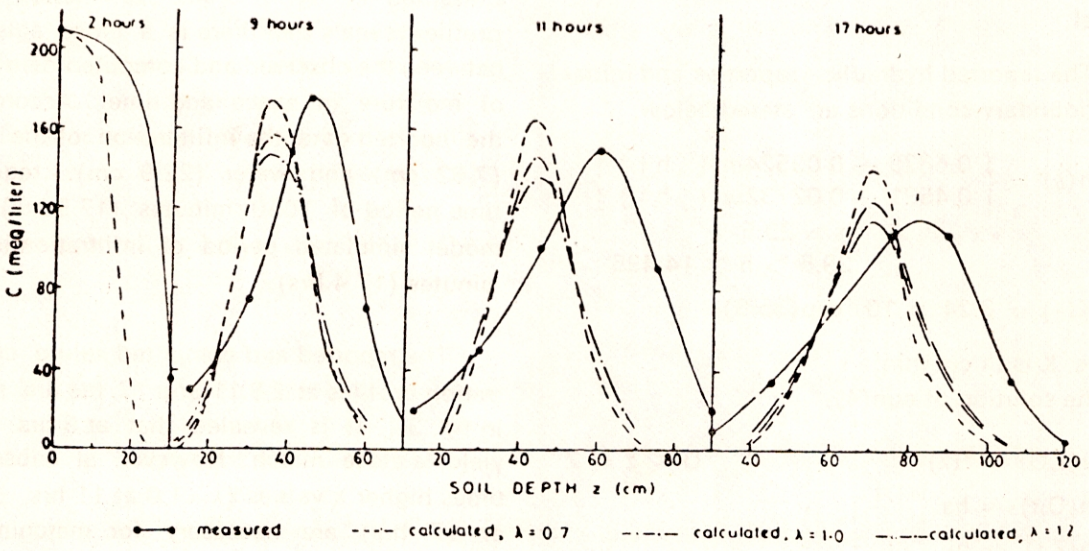

Fig. 3 Measured and simulated concentration profiles

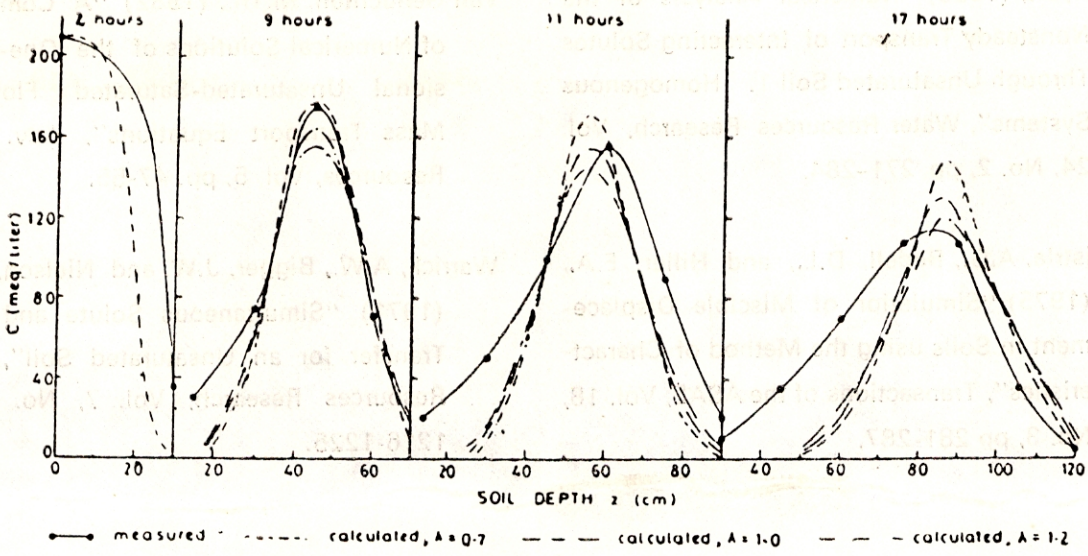

Fig. 4 Measured and simulated concentration profiles considering immobile pore water

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