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A Modified Picard's Method for Virus Transport in Ground Water

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ABSTRACT: Solution of transport equation by conventional numerical methods such as finite difference and finite element analysis exhibit either excessive diffusion and/or oscillations near the concentration front. This is due to the presence of advection term in the solute transport equation. In the present work, a computationally simple, numerical algorithm is developed to solve the solute transport equation in groundwater. The governing equation is solved using finite differences employing the modified Picard iteration scheme to determine the temporal derivative of the solute concentration. The total solute concentration is expanded in a Taylor series with respect to the solution concentration to linearize the transport equation, which then solved with conventional finite difference method. The algorithm avoids mass-balance errors and is numerically stable. The numerical solution is compared with analytical solution. The model is further being used for virus transport in ground water.

INTRODUCTION

Management of a ground water system involves assuring quality and quantity of water being provided for different purposes. It is necessary to develop the appropriate ground water quality management plan with proper understanding of physical phenomena of contaminants movement. Pollution of ground water occurs due to mixing of physical, chemical and bacteriological contaminants from different sources. It is viruses in drinking water that are an important source of human enteric diseases. Viruses from sewage sludges, septic tanks and other sources can transport with ground water to drinking water wells. So it is required to find out the source of pollutants which pollute the aquifers and take appropriate measures to prevent pollution.

Mathematical modeling has been used as an effective tool to evaluate the fate of contaminants in ground water. Many studies have been conducted both in the laboratory and field to investigate sorption, inactivation and transport of various viruses in different porous media. Udoyara and Mostaghimi (1991) have developed a numerical model, VIROTRANS, for simulating the vertical movement of water and virus through soils treated with waste-water effluents and sewage sludge. Yates and Ouyang (1992) have developed a model that can be used to predict virus movement from a contamination source through unsaturated soil to groundwater. Sim and Chrysikopoulos (1996) introduced a model for one dimensional virus transport in homogeneous, saturated porous media accounting for virus sorption and inactivation with time dependent rate coefficients. Runkel (1996) solved the analytical solution of the advection-dispersion equation for continuous load of both finite and infinite durations. Jin *et al.* (2000) has done the column flow experiment in both saturated and unsaturated condition and found that the difference in virus removal and transport behavior between saturated and unsaturated condition was likely caused by additional sorption at solid surfaces and the presence of air water interface in the unsaturated system. Jin *et al.* (2003) investigated the effect of soil properties on saturated and unsaturated virus transport through columns by laboratory experiment. The main difficulty in obtaining accurate solutions of the solute transport equation is the presence of advective term which introduces artificial diffusion in the conventional numerical scheme. The objective of this study is to develop a simple and accurate numerical model for the analysis of virus transport through unsaturated soil. The governing equation is solved using finite differences employing the modified Picard iteration scheme to determine the temporal derivative of the virus concentration. The total concentration is expanded in a Taylor series with respect to the solution concentration to linearize the transport equation, which then is solved with a conventional finite difference method. The algorithm avoids mass-balance errors and is numerically stable. The accuracy of the model prediction is tested by comparing the model prediction with the analytical solution.

GOVERNING EQUATIONS

The mass conservation equations for the simultaneous transport of water and suspended virus particles through variably saturated media under transient flow condition can be written as,

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial z}[K_\theta\{\frac{\partial h}{\partial z}+1\}] \quad \dots (1)$$

$$\frac{\partial(\theta c)}{\partial t}+\frac{\partial \rho s}{\partial t}=\frac{\partial}{\partial z}\left(\theta D\frac{\partial c}{\partial z}\right)-\frac{\partial qc}{\partial z}-\lambda_w\theta c-\lambda_s\rho s \quad \dots (2)$$

Where h = Pressure head; θ = volumetric moisture content; K_θ = hydraulic conductivity; $\partial h/\partial z$ = hydraulic gradient; c = mass per unit volume of the virus species residing in the liquid (suspended phase); ρ = soil bulk density; s = mass of adsorbed constituents of the virus species per unit mass of adsorbent; D = hydrodynamic dispersion coefficient; q = Darcian flux density; λ_w and λ_s = first order decay coefficient in liquid phase and solid phase respectively; t = time; z = vertical coordinate taken positive upwards.

The dispersion term D, in equation (2) represents the combined effects of molecular diffusion and mechanical dispersion,

$$D=D_m+\alpha\left|\frac{q}{\theta}\right| \quad \dots (3)$$

In which,

$$q=\theta V=-K_\theta(\frac{\partial h}{\partial z}+1) \quad \dots (4)$$

Where D_m = molecular diffusion coefficient; V = interstitial pore water velocity; and α = dispersivity of the medium which varies according to the scale of experiment ($0.01 < \alpha < 1.0$ cm for laboratory experiments and $10 < \alpha < 100$ m for field experiments) and depends on the heterogeneity of the medium.

The solution of equation (2) requires expressions for the distribution of viruses between the adsorbed and liquid (suspended) phases and the inactivation rate of viruses in the soil.

Virus Adsorption in Soil

The Langmuir-Freundlich model is used to describe the adsorption isotherm,

$$s=\frac{Q(kc)^\beta}{1+(kc)^\beta} \quad \dots (5)$$

Where Q = maximum sorption capacity, k = overall affinity coefficient; β = dimensionless fitting parameter. For $\beta = 1$, Eqn. (5) reduces to Langmuir sorption isotherm. The Freundlich isotherm is,

$$S=k_d c^\beta \quad \dots (6)$$

$$\text{Where } k_d=Qk^\beta \quad \dots (7)$$

At equilibrium, K_d is the distribution coefficient defined as the mass of adsorbed virus per unit mass of the absorbent per unit concentration of viruses in the liquid phase.

Virus Inactivation

Inactivation of microorganisms plays an important role in their survival and transport in the subsurface, especially under unsaturated flow conditions. Several factors may influence the inactivation of viruses after their release into the environment. These factors include pH, temperature, type of virus, and microbial antagonism. Virus inactivation in the subsurface environment can be described by a first order reaction of the following form,

$$S=k_d c\text{, taking } \beta=1 \quad \dots (8)$$

Substituting Eqn. (8) into Eqn. (2) and consider $\lambda_w = \lambda_s = \lambda$, further simplification yields,

$$R\frac{\partial c}{\partial t}=\frac{\partial}{\partial z}\left(D\frac{\partial c}{\partial z}\right)-v\frac{\partial c}{\partial z}-\lambda Rc \quad \dots (9)$$

Where R is the retardation factor which accounts for the apparent decrease in the propagation of a concentration front due to sorption and can be adequately defined by,

$$R=1+\frac{\rho K_D}{\theta} \quad \dots (10)$$

It should be noted that inactivation coefficients are often expressed in units of ln10 per day.

NUMERICAL SOLUTION OF RICHARDS EQUATION

A backward Euler approximation, coupled with a Picard iteration scheme, is used to discretize the left hand side of Eqn. (1), containing the time derivative of water content as,

$$\frac{\partial\theta}{\partial t}\approx\left[\frac{\theta^{n+1,m+1}-\theta^n}{\Delta t}\right] \quad \dots (11)$$

where m denotes the Picard's iteration and n denotes the time level.

Using a fully implicit (backward Euler) time approximation and representing the water content, $\theta^{n+1,m+1}$, by the first order approximation,

$$\theta^{n+1,m+1} \approx \theta^{n+1,m} + \left(\frac{d\theta}{dh}\right)^{n+1,m} \left[h^{n+1,m+1} - h^{n+1,m}\right] \quad \ldots (12)$$

The specific water capacity of a soil is defined as follows,

$$C(h) = \frac{d\theta}{dh} \quad \ldots (13)$$

The time derivative of water content of Eqn. (1) is approximated as follows,

$$\frac{\partial\theta}{\partial t} \approx \left[\frac{\theta^{n+1,m} - \theta^{n}}{\Delta t}\right] + C^{n+1,m}\left[\frac{h^{n+1,m+1} - h^{n+1,m}}{\Delta t}\right] \quad \ldots (14)$$

The first term on the right side of Eqn. (14) is an explicit estimate for time derivative of water content, based on the m^{th} Picard level estimates of pressure head. In the second term of the right side of Eqn. (14), the numerator of the bracketed fraction is an estimate of the error in the pressure head at node j between two successive Picard iterations. Its value diminishes as the Picard iteration process converges. As a result, as the Picard process proceeds, the contribution of the specific water capacity is diminished,

$$\frac{\partial}{\partial z}\left\{K(\theta)\left(\frac{\partial h}{\partial z}+1\right)\right\} = \frac{1}{\Delta z}\left[\left(\frac{K_j^{n+1,m} + K_{j+1}^{n+1,m}}{2}\right)\left(\frac{h_{j+1}^{n+1,m+1} - h_j^{n+1,m+1}}{\Delta z}\right) - \left(\frac{K_j^{n+1,m} + K_{j-1}^{n+1,m}}{2}\right)\left(\frac{h_j^{n+1,m+1} - h_{j-1}^{n+1,m+1}}{\Delta z}\right)\right] + \frac{1}{\Delta z}\left[\left(\frac{K_j^{n+1,m} + K_{j+1}^{n+1,m}}{2}\right) - \left(\frac{K_j^{n+1,m} + K_{j-1}^{n+1,m}}{2}\right)\right] \quad \ldots (15)$$

The finite difference expressions for the spatial and temporal derivatives are rearranged by collecting all the unknowns on the left side and all the known on the right. Using the above implicit finite difference approximation, the pressure heads at the $n+1^{\text{th}}$ time level and $m+1^{\text{th}}$ Picard level are obtained from solution of the following system of simultaneous linear algebraic equations,

$$a h_{j-1}^{n+1,m+1} + b h_j^{n+1,m+1} + c h_{j+1}^{n+1,m+1} = d + e - f h_j^{n+1,m} \quad \ldots (16)$$

Where coefficients a, b, c, d, e, f are defined as,

$$a = \left(\frac{K_j^{n+1,m} + K_{j-1}^{n+1,m}}{2\Delta z^2}\right) \qquad b = -[a + c + f]$$

$$c = \left(\frac{K_j^{n+1,m} + K_{j+1}^{n+1,m}}{2\Delta z^2}\right) \qquad d = \left[\frac{\theta^{n+1,m} - \theta^{n}}{\Delta t}\right]$$

$$e = \frac{K_{j-1}^{n+1,m} - K_{j+1}^{n+1,m}}{2\Delta z} \qquad f = \frac{c_j^{n+1,m}}{\Delta t} \quad \ldots (17)$$

Equation (16) applies to all interior nodes; at boundary nodes this equation is modified to reflect the appropriate boundary conditions. The resulting set of consistent linear algebraic equations, for the unknown pressure-head values, is written in a matrix notation,

$$Ah = b \quad \ldots (18)$$

Where A = coefficient matrix, h = vector of unknown pressure heads and b = known right hand side vector.

The relationship given by Van Genuchten (1980) are used for θ–h and K–θ relationships which are given as,

θ–h Relationship

$$\Theta = \left\{\frac{1}{1 + \left(\alpha|h|\right)^n}\right\}^m \quad \ldots (19)$$

Where α and n are unsaturated soil parameters with,

$$m = 1 - \frac{1}{n} \quad \ldots (20)$$

Θ is the effective saturation defined as,

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad \ldots (21)$$

Where θ_s = saturated water content and θ_r = residual water content of the soil.

K–θ Relationship

$$K(\Theta) = K_s\left\{1 - \left\{1 - \Theta^{(1/m)}\right\}^m\right\}^2 \Theta^{(1/2)} \quad \ldots (22)$$

Where K_s = saturated hydraulic conductivity.

Numerical Solution of Transport Equation

The governing Eqn. (2) can be written in a mixed form as,

$$\frac{\partial M}{\partial t} = \frac{\partial}{\partial z}\left(\theta D\frac{\partial c}{\partial z}\right) - \frac{\partial qc}{\partial z} - \lambda\theta c \quad \ldots (23)$$

Where

M = Total concentration of solute per unit volume of soil

$$M = \theta c + \rho f(c) \quad \dots (24)$$

The procedures for implementing the Picard iteration scheme is basically same as that used for water flow equation. First, the implicit backward time scheme is applied to Eqn. (23), i.e.,

$$\frac{M^{n+1,m+1} - M^n}{\Delta t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial c^{n+1,m+1}}{\partial z}\right) - \frac{\partial q c^{n+1,m+1}}{\partial z} - (\lambda \theta c)^{n+1,m} \quad \dots (25)$$

Then using the Taylor expansion for $M^{n+1,\, m+1}$ with respect to c at $c^{n+1,\, m}$

$$M^{n+1,m+1} \approx M^{n+1,m} + \left(\frac{\partial M}{\partial c}\right)^{n+1,m} \times \left(c^{n+1,m+1} - c^{n+1,m}\right) \quad \dots (26)$$

Substituting Eqn. (26) into Eqn. (25) yields the modified Picard iteration formulation for the mixed form of transport equation as,

$$C_s^{\,n+1,m} \frac{c^{n+1,m+1} - c^{n+1,m}}{\Delta t} + \frac{M^{n+1,m} - M^n}{\Delta t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial c^{n+1,m+1}}{\partial z.}\right) - \frac{\partial q c^{n+1,m+1}}{\partial z} - (\lambda \theta c)^{n+1,m} \quad \dots (27)$$

Where

C_s = specific solute capacity,

$$c_s = \frac{\partial M}{\partial c} = \theta + \rho \frac{\partial f(c)}{\partial c} \quad \dots (28)$$

Equation (27) describes the proposed modified Picard iteration method for the nonlinear transport equation.

Initial and Boundary Conditions

For Flow Equation

The initial and boundary condition for Richards equation is,

$h(z, 0) = -100$ cm, $0 \le z \le 100$ cm

$h(0, t) = h_{bottom} = -100$ cm

$h(100, t) = h_{top} = -10$ cm

For Transport Equation

The initial condition is,

$$c(x,0) = 0 \quad \dots (29)$$

Here, a constant concentration boundary condition is used i.e.,

$$c(0,t) = C_0 \quad \dots (30)$$

In Eqn. (30), C_0 denotes the source concentration.

The downstream boundary condition,

$$\frac{\partial c(\infty,t)}{\partial x} = 0 \quad \dots (31)$$

RESULTS AND DISCUSSIONS

Virus Transport in Saturated Soil

Analytical and numerical solutions are compared to validate the numerical scheme for the solution of one dimensional virus transport equation in a saturated soil.

In this problem, a continuous source of virus is imposed such that the concentration at the upstream boundary is 100 concentration units (C_0 = 100). The pore water velocity is taken as 34 cm/day. Bulk density of soil ρ is taken as = 1.11 gm/cm^3. Distribution coefficient k_d is taken as 0.02 ml/gm. Inactivation coefficient λ is taken as 0.58 /day. The water content θ is taken as 0.4. The domain is discretized into 100 grids so that spacing between the grids Δx is equal to 1.0 cm. The governing equation 9 is solved numerically subject to initial and boundary conditions given in Eqns. (29, 30 & 31). The numerical model is simulated for Peclet number equal to 1.0 situation.

Figure 1 shows the comparison of concentration profile predicted the present scheme and those obtained by the analytical solution given by Ogata and Banks (1961). It is clearly seen from Figure1 that the numerical solution matches excellently with the analytical solution.

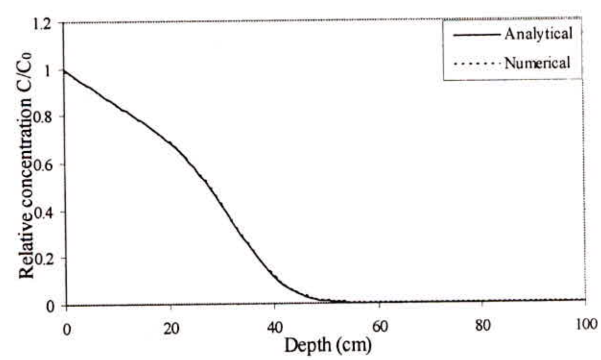

Fig. 1: Comparison of analytical and numerical solution of virus transport in saturated soil

Virus Transport in Unsaturated Soil

The following flow parameters are used in simulations for the solution of one dimensional virus transport equation in an unsaturated soil.

Saturated moisture content = 0.368
Residual moisture content = 0.102
van genucheten parameter $\alpha = 0.0335$ /cm, $n = 2.0$
Saturated hydraulic conductivity = 796.608 cm/day.

The problem is simulated for 1 day. The results of the simulation for unsaturated soil are shown in Figure 2 to Figure 4. Figure 2 shows the moisture content profile and Figure 3 shows the comparison of virus concentration obtained by the numerical solution and the corresponding analytical solution for one dimensional virus transport in unsaturated soil with $P_e = 0.25$. It can be seen again in Figure 3 that the numerical predictions match excellently with the analytical solution. Figure 4 shows the comparison of model predicted virus concentrations for different Peclet numbers. It is clearly evident from Figure 4 that the distance travelled by the Virus decreases with an increase in the Peclet number. This is due to the fact that with an increase in Peclet number the effect of advection decreases. As a result the virus moves at a slower rate resulting in lower concentrations at a given time. It can be seen from Figure 4 that for $P_e = 1$, the maximum distance covered by virus is about 10 cm while for $P_e = 0.25$, the maximum distance travelled by the virus is about 30 cm.

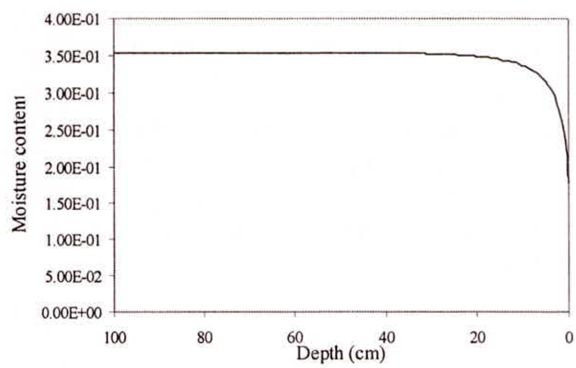

Fig. 2: Variation of moisture content with soil depth

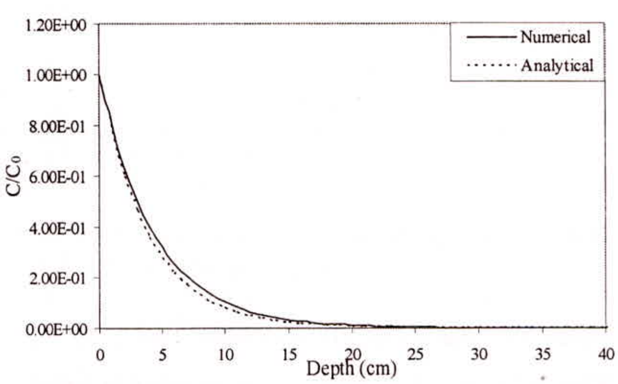

Fig. 3: Comparison of analytical and numerical solution of virus transport in unsaturated soil having *Pe* = 0.25

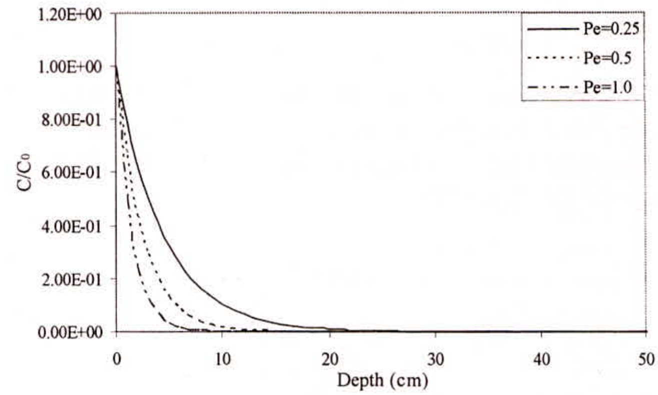

Fig. 4: Comparison of one dimensional virus transport in unsaturated soil for different Peclet numbers

CONCLUSIONS

In the present study, a numerical model is developed to analyse the virus transport in both saturated and unsaturated soils using modified Picard's method. The accuracy of the scheme is studied by comparing the numerical solution with the available analytical solution. Then the model is used to compare the virus movement for different peclet numbers. It is observed that the distance travelled by the virus decreases with an increase in the Peclet number. It is concluded that the modified Picard's method accurately predicts the virus movement in both saturated and unsaturated soils.

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