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Simulation of Water and Contaminant Transport Through Vadose Zone - Redistribution System

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1. Introduction

Movement of water in vadose zone, mainly focusing on infiltration and percolation that involves percolation of water under gravity from soil surface and redistribution which is the capillary rise of water movement upwards, is presented. In the global hydrologic cycle, 76% of the precipitating water enters the soil via percolation-infiltration, which leads to the downward movement of water (L'vovich 1974). The water used by natural processes, can move downwards due to infiltration and lift from groundwater table during natural redistribution process. The forecasting of water movement in unsaturated infiltration-redistribution system is linked between soil hydraulic properties and hydrologic condition of natural surface water system. The understanding of water movement processes associated with infiltration and redistribution has a number of practical applications. One such application is to predict the fate and transport of materials through soil including nutrients, organic carbon and microbes under natural processes, which in turn will help in developing appropriate management plans for irrigation, fertiliser application and waste disposal on land.

2. Infiltration and redistribution system

The prevailing weather condition can potentially affect the amount of water input to soil. The infiltration rate consists of (1) water input rate, which is the rate of water that arrives at soil surface due to rain, natural and artificial applications and (2) infiltration capacity, which is the maximum rate at which percolating water migrates through the soil pore. In general, water input rate responds to seasonal climatic variations and to any recharge from natural or artificial conditions. The infiltration capacity rate depends on the soil texture and soil hydraulic properties. The infiltration process can be separated into three categories (1) no ponding (2) saturation from above and (3) saturation from below. The "no ponding" refers to the condition, when water input rate is less than or equals to the infiltration capacity. The "saturation from above" presents the condition, when water input rate exceeds the

infiltration capacity rate. The “saturated from below” reveals the condition, when groundwater table has risen above the original saturation layer resulting in saturated soil, hence the infiltration rate becomes zero (Iwata et al. 1995, Dingman 2002).

The redistribution rate can be determined by the upward flow rate of water, which involves both the exfiltration and capillary rise. The exfiltration deals with evaporation or evapotranspiration. The exfiltration can reduce the soil pore water at the upper layer. The exfiltration rate of soil also depends on relative humidity of air and solar radiation. Furthermore, soil is a porous material and can behave as a series of capillary tubes. The surface tension force can abstract the water from aquifer into pore space above the water table. The capillary rise refers to the water movement from saturated zone to unsaturated zone owing to surface tension. The capillary rise acts opposite to the direction of gravitational force. The height of capillary rise relates to pore size and soil moisture content. Consequently, the height of capillary rise in fine grained soil is higher than in the case of coarse grained soil and the height of capillary rise into dry soil is lower than that of relatively wet soil. The water movement in unsaturated zone near the region of saturated zone or capillary fringe is mentioned because the water in the saturated and unsaturated zones is connected together and oscillates with fluctuations of groundwater table. The fluctuation of groundwater level during wet-to-dry season, causes the movement of capillary fringe region that causes of smearing of contaminants to soil above groundwater table. The critical point of predicting the water movement in the capillary fringe is the non-uniform capillary flow. In order to simplify this infiltration-redistribution system that occurs in the capillary fringe, it can be assumed that the redistribution rate is associated with the capillary height, which is normally considered under the equilibrium of capillary force (Fredlund & Rahardjo 1993, Dingman 2002).

The vadose zone is the entire zone of negative water pressure above the water table, so the pressure head at the deepest level of this zone is saturated or nearly saturated as a result of capillary rise. Almost all water in the vadose zone is available for plants and exfiltration (drainage). The plant available water is observed at pressure head ranged from -150 to -3.4 m H₂O and the drainable water will be at pressure head ranged from -3.4 m H₂O to saturation (Dingman 2002). The water infiltrating into vadose zone is influenced by both capillary and gravitational forces, and these are associated with upward and downward-directed pressure gradients, respectively. The movement of water due to infiltration capacity is described by the Richards equation and the movement of drainage is satisfactorily modeled with Darcy's law. The capillary gradient is determined by static capillarity equilibrium height using the capillary models (Bunsri et al. 2009).

3. Governing equation for unsaturated flow

Movement of water due to infiltration is assumed that water percolates under gravitational force. The vertical flow through interconnected intergrain pores, which are randomly distributed in a mix grained soil. The movement of water through the effective soil pores can be simplified so that water moves only in the liquid state (excluding, soil-water freezing or thawing) and there is no impact of airflow in soil pores. The 1D-vertical unsaturated flow in porous media can be described using Richards equation (Richards 1931).

The pressure head based equation is expressed as:

$$\frac{\partial}{\partial z} \left[K_z k_{rw} \left(\frac{\partial \psi}{\partial z} + 1 \right) \right] = S \frac{\partial \psi}{\partial t} \quad (1)$$

The volumetric moisture content based equation (Warrick, Islas & Lomen 1991) is:

$$\frac{\partial}{\partial z} \left(D_z \frac{\partial \theta}{\partial z} \right) - \frac{\partial K_z k_{rw}}{\partial z} = \frac{\partial \theta}{\partial t} \quad (2)$$

where k_{rw} is the relative hydraulic conductivity [unitless], K_z is the fully saturated hydraulic conductivity [$L \ T^{-1}$], S is the specific moisture capacity ($= \partial \theta / \partial \psi$), θ is the volumetric moisture content [unitless], ψ is the pressure head [L] and D_z is the soil water diffusivity ($= \partial K_z k_{rw} / \partial S$). Equations (1) and (2) contains Darcy's velocity, q_z , which is given by (the negative sign means downward flow) (Huyakorn et al. 1984):

$$q_z = -K_z k_{rw} \left(\frac{\partial [\psi + z]}{\partial z} \right) \text{ or } \frac{\partial \theta}{\partial t} = -\frac{\partial q_z}{\partial z} \quad (3)$$

where q_z is Darcy's velocity in vertical direction [LT^{-1}].

By inserting a series of tensiometers in different parts of a drainage field, the profiles of pressure head can be observed as shown in Figure 1. The negative pressure head determined in the unsaturated soil layer is due to suction head, zero pressure head occurred at the interface of groundwater table and the positive pressure head in the saturated soil layer is due to hydraulic head (gravitational head plus pore-water pressure head) (Fredlund and Rahardjo 1993).

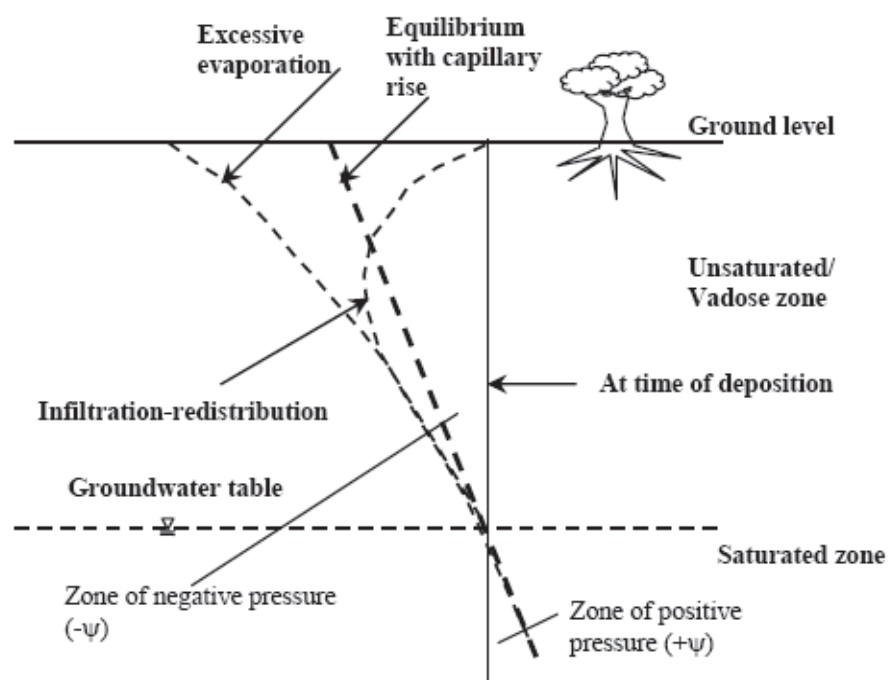


Fig. 1. Profiles of pore pressure under a steady state condition (Adapted from Fredlund & Rahardjo 1993)

Figure 2 presents possible pressure head profiles at varying Darcy’s velocities (q_z). If the velocity is constant ($\partial \psi / \partial z = 0$), the simplest pressure head profiles (case 1) are obtained. When $\partial \psi / \partial z$ is negative with $-K_z k_{rw} < q_z < 0$, this will lead to vertical downward flow (case 2). If $\partial \psi / \partial z$ is positive with $q_z < -K_z k_{rw}$, water moves downward with suction head (case 3). The upward flow is yielded (case 4), if Darcy’s velocity is greater than zero. However, in most unsaturated zone cases, the water will experience a downward flow, these are either case 2 for evaporation or case 3 for irrigation (Warrick et al. 1991).

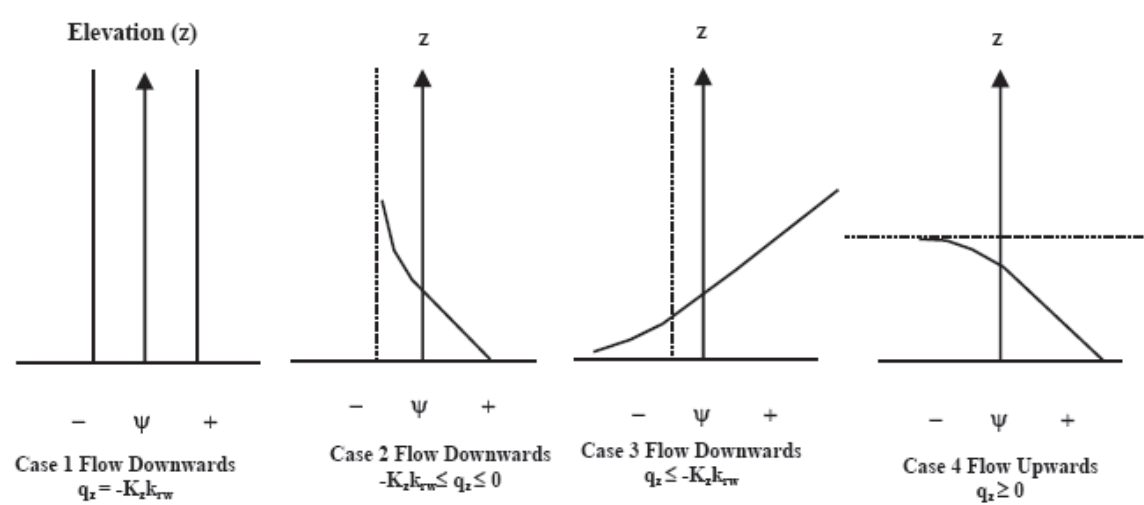


Fig. 2. Pressure head profiles at varying Darcy’s velocities (Adapted from Warrick et al. 1991)

The relationship between relative hydraulic conductivity ($k_{rw} K_z$), pressure head (ψ) and volumetric moisture content (θ) is defined as the hydraulic properties function, which is highly nonlinear. Typically used hydraulic properties equations in this research include those of Brooks and Corey (1964), Haverkamp et al. (1977), van Genuchten (1980) and Saxton et al. (1986). Brooks & Corey (1964) hydraulic properties function was firstly derived by modifying the statistical porewater interaction models of Childs and Collis-George (1950) (cited in Fredlund & Rahadjo 1993). The Brooks & Corey (1964) model is:

$$\theta = \left[\left(\frac{\psi_a}{\psi} \right)^{\tilde{N}} (\theta_s - \theta_r) \right] + \theta_r \tag{4a}$$

$$K_z k_{rw}(\psi) = K_z \left(\frac{\psi_a}{\psi} \right)^{\tilde{M}} \tag{4b}$$

$$K_z k_{rw}(\theta) = K_z \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{\tilde{M}/\tilde{N}} \tag{4c}$$

where ψ_a is the air entry suction pressure head [L], θ_s and θ_r are the saturated and residual volumetric water content, respectively [unitless]. \tilde{M} and \tilde{N} are empirical constants.

Haverkamp et al. (1977) fitted the properties of homogeneous soil in unsaturated conditions by the least square method and proposed the following empirical equations (HV equations):

$$\theta = \frac{\alpha(\theta_s - \theta_r)}{\alpha + |\psi|^\beta} + \theta_r \tag{5a}$$

$$K_z k_{rw} = K_z \left(\frac{A}{A + |\psi|^\gamma} \right) \tag{5b}$$

where A , α , β and γ are the curve fitting coefficients [unitless].
van Genuchten (1980) derived the hydraulic properties equations based on the equation of Brooks & Coley (1964) and proposed the following empirical equations for hydraulic properties (VG equations):

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + a|\psi|^p \right]^q} \tag{6a}$$

$$K_z k_{rw} = K_z \frac{\left[1 - \left(a|\psi|^{p-1} \right) \left(1 + \left(a|\psi|^p \right) \right)^{-q} \right]^2}{\left[1 + a|\psi|^p \right]^{q/2}} \tag{6b}$$

where a is the soil water retention function [L⁻¹], q and p are the empirical parameters, ($q = 1 - [1 / p]$) [unitless].
The possible values for the coefficients presented in VG equations are given in Table 1. The coefficients are sorted by soil textures in accordance with USDA textural classes (Carsel et al. 1988).

Soil Type	θ_s	θ_r	a (cm ⁻¹)	p
Clay*	0.38	0.068	0.008	1.09
Clay loam	0.41	0.095	0.019	1.31
Loam	0.43	0.078	0.036	1.56
Loam sand	0.41	0.057	0.124	2.28
Silt	0.46	0.034	0.106	1.37
Silt loam	0.45	0.067	0.020	1.41
Silty clay	0.36	0.070	0.005	1.09
Silty clay loam	0.43	0.089	0.010	1.23
Sand	0.43	0.045	0.145	2.68
Sandy clay	0.38	0.100	0.027	1.23
Sandy clay loam	0.39	0.100	0.059	1.48
Sandy loam	0.41	0.065	0.075	1.89

Note: *Agricultural soil, less than 60% clay.

Table 1. Recommended empirical coefficients for VG equations (Carsel et al. 1988).

The hydraulic properties are estimated from the soil texture using a method generalised by Saxton et al. (1986). The textural class is assessed according to the USDA system. The water retention curve is fitted with linear regression and the formulations are in S.I. unit as follows:

1) When the hydraulic pressure is between 10 and 1500 kPa (or 1.02 to 15.3 m H₂O), then the expression for ψ is given by:

$$\psi = \psi_a \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^H \quad (7a)$$

By assuming $\theta_r = 0$; will give

$$\psi = J\theta^H \quad (7b)$$

with $J = \psi_a \theta_s^{-H}$

where ψ and ψ_a are the hydraulic pressure and the air entry pressure, respectively [kPa]. H and J are obtained by the statistical curve fitting of 44 soil samples with an $R^2 = 0.99$.

$$H = -3.140 - 0.00222 \cdot [\% \text{ clay}]^2 - 3.484 \times 10^{-5} [\% \text{ sand}]^2 [\% \text{ clay}] \quad (8a)$$

$$J = \exp \left(\frac{-4.396 - 0.0715 \cdot [\% \text{ clay}] - 4.880 \times 10^{-4} \cdot [\% \text{ sand}]^2}{-4.285 \times 10^{-5} \cdot [\% \text{ sand}]^2 \cdot [\% \text{ clay}]} \right) \times 100 \quad (8b)$$

2) When the hydraulic pressure is between ψ_a and 10 kPa (or 1.02 H₂O), then:

$$\psi = 10.0 + \left(\frac{(\theta - \theta_{10})(10.0 - \psi_a)}{\theta_s - \theta_{10}} \right) \quad (9)$$

where θ_{10} is the volumetric moisture content at 10 kPa, $(= \exp[(2.303 - \ln J) / H])$ [cm³/cm³]. $\psi_a = 100.0(-0.108 + 0.341\theta_s)$ and $\theta_s = 0.332 - 7.251 \times 10^{-4} [\% \text{ sand}] + 0.1276(\text{Log}[\% \text{ clay}])$

3) when the hydraulic pressure is between 0.0 kPa and ψ_a (or 0.0 cm H₂O to ψ_a), then:

$$\theta = \theta_s \quad (10a)$$

Variable $K_z k_{rw}$ is estimated as follows:

$$K_z k_{rw} = 2.778 \times 10^{-6} \left(\exp \left(\frac{12.012 - 0.0755 \cdot [\% \text{ sand}]}{(1/\theta)(-3.8950 + 0.0364 \cdot [\% \text{ sand}] - 0.113 \cdot [\% \text{ clay}] + 8.7546 \times 10^{-4} \cdot [\% \text{ clay}]^2)} \right) \right) \quad (10b)$$

where $K_z k_{rw}$ is the unsaturated hydraulic conductivity [m s⁻¹].

Kunze et al. (1968) established a relative permeability function based on Poiseuille's equation. An example of estimating relative permeability using Kunze's equation is illustrated in Figure 3.

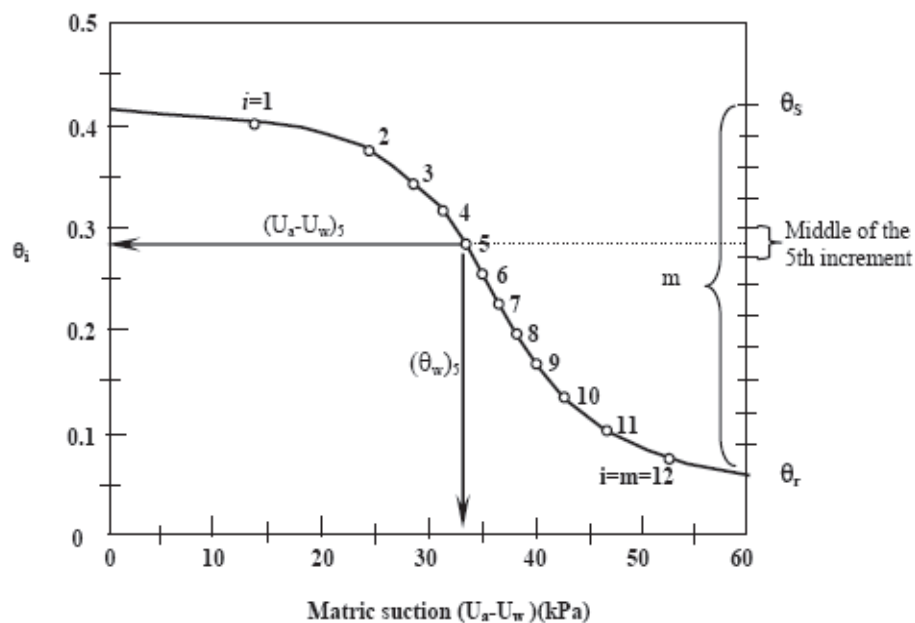


Fig. 3. Graphical estimation of relative permeability (Adapted from Fredlund & Rahardjo 1993)

The coefficient of relative permeability was obtained from the relationship between the matrix suction and volumetric moisture content. The equation was given as follows:

$$k_{rw}(\theta_i) = \frac{(K_z)_{mea}}{(K_z)_{cal}} \frac{\sigma_s^2 \rho_w g \theta_s^P}{2 \mu_w N^2} \sum_{j=1}^m \left[(2j+1-2i) |\psi_j|^{-2} \right] \quad i = 1, 2, \dots, m \quad (11)$$

where $k_{rw}(\theta)_i$ is the calculated coefficient of permeability for a specified volumetric moisture content; θ_i , corresponding to the i^{th} interval [unitless]. i is the interval on the water retention curve [unitless] and j is the counter number from i to m [unitless]. $(K_z)_{mea}$ and $(K_z)_{cal}$ are the measured saturated coefficient of permeability and the calculated coefficient of permeability, respectively [L T^{-1}]. σ_s is the surface tension of water [M T^{-2}], ρ_w is the water density [M L^{-3}] and μ_w is the absolute viscosity of water [M T^{-1}]. P is a constant which accounts for the interaction of pores of various sizes, usually assumed to be 2.0 (Green & Corey 1971 cited in Fredlund & Rahardjo 1993) [unitless]. m is the total number of intervals between the saturation volumetric water content and the residual volumetric water content [unitless] and N is the total number of intervals ($N = m\theta_s / [\theta_s - \theta_r]$) [unitless].

4. Numerical solution for the unsaturated flow equation

The finite discretionary scheme is given in Figure 4. The number of nodes in the system is assigned sequentially to the flow direction.

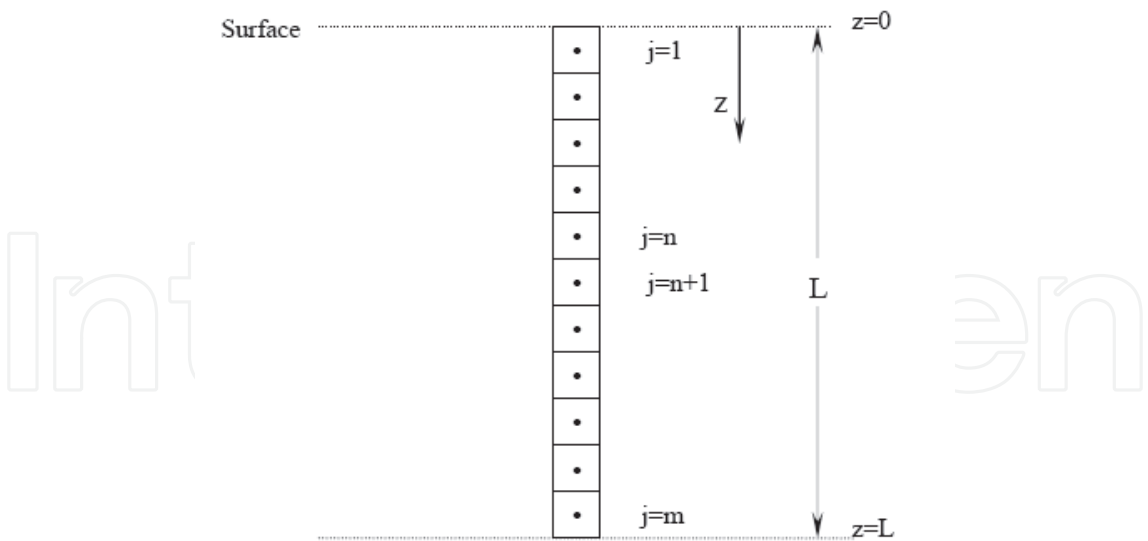


Fig. 4. Scheme of finite discretisation.

As the hydraulic properties model can be applied to modify Richards’ equation between the θ based to ψ based formulations. Generally, ψ based Richards’ equation is preferred over θ based equation as it is possible to accurately measure the pressure head using tensiometers. Several previous works (Wang & Anderson 1982, Coley 1983, Segerlind 1984, Paniconi et al.1991) have assumed the approximate solution to Richards’ equation as:

$$\psi(z,t)=\sum_{j=1}^mN_j(z)\psi_j(t) \tag{12}$$

where $N_j(z)$ is the shape function [unitless], $\psi_j(t)$ is the unknown coefficient with corresponding to the value of nodal pressure head [L] and the subscript “j” is defined to denote a nodal sequence.
Richards’ equation (Eq. 1) is now written in the form of $L[\psi]=0$ as follows.

$$L[\psi]=S\frac{\partial \psi}{\partial t}-\frac{\partial}{\partial z}\left[K_zk_{rw}\left(\frac{\partial \psi}{\partial z}+1\right)\right] \tag{13}$$

The weighting function, N_i was assigned the same value as N_j . Applying Galerkin’s finite element method yields (Bunsri et al. 2009):

$$\int_{z=0}^{z=L}L[\psi]N_idz=0 \tag{14}$$

Substituting Eq. 13 into Eq. 14, yields:

$$\int_{z=0}^{z=L}N_iS\frac{\partial \psi}{\partial t}dz-\int_{z=0}^{z=L}N_i\left[K_zk_{rw}\left(\frac{\partial \psi}{\partial z}+1\right)\right]dz=0 \tag{15}$$

The numerical solution of Richards’ equation is (Bunsri et al. 2009):

$$\int_{z=0}^{z=L} N_i S \frac{\partial \psi}{\partial t} dz - N_i K_z k_{rw} \left(\frac{\partial \psi}{\partial z} + 1 \right) \bigg|_{z=0}^{z=L} + \int_{z=0}^{z=L} K_z k_{rw} \psi_j \left(\frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right) dz + \int_{z=0}^{z=L} K_z k_{rw} \frac{\partial N_i}{\partial z} dz = 0 \quad (16)$$

The algebraic matrix systems were defined as follows (Bunsri et al. 2009):

$$[A_{ij}] \cdot \psi_j + [B_{ij}] \cdot \frac{\partial \psi_j}{\partial t} = \{E_{ij}\} \quad (17)$$

where

$$[A_{ij}] = \sum_e \int_{z=0}^{z=L} K_z k_{rw} \left(\frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right) dz, \quad [B_{ij}] = \sum_e \int_{z=0}^{z=L} N_i S dz, \text{ and}$$

$$\{E_i\} = N_i K_z k_{rw} \left(\frac{\partial \psi}{\partial z} + 1 \right) \bigg|_{z=0}^{z=L} - \sum_e \int_{z=0}^{z=L} K_z k_{rw} \frac{\partial N_i}{\partial z} dz$$

Using Eq. 3, the vector matrix $\{E_i\}$ could be written in the form of Darcy's flux boundary condition as:

$$\{E_i\} = N_i q_z \big|_{z=0}^{z=L} - \sum_e \int_{z=0}^{z=L} K_z k_{rw} \frac{\partial N_i}{\partial z} dz \quad (18)$$

The time derivative approximation at a particular node "j" can be explained by (Wang & Anderson 1982, Paniconi et al. 1991, Ségol 1993):

$$\frac{\partial \psi_j}{\partial t} = \frac{\psi_j^{t+\Delta t} - \psi_j^t}{\Delta t} \quad (19)$$

where $\{\partial \psi / \partial t\}$ is a column matrix, which refers to time-dependent hydraulic pressure head $(\psi_j(t))$. The term " $\{\partial \psi / \partial t\}$ " can be simplified with the vector symbol " $\{\psi\}$ ". The iterative scheme obtained using a single Picard's method is given by (Wang & Anderson 1982, Paniconi et al. 1991, Ségol 1993):

$$\left(\frac{1}{2} [A_{ij}]^t + \frac{1}{\Delta t} [B_{ij}]^t \right) (\{\psi\}^{t+\Delta t} - \{\psi\}^t) = \{E_i\} - [A_{ij}]^t \{\psi\}^t \quad (20)$$

Celie et al. (1990) estimated the pressure head profiles using Richards' equation. The numerical model is developed using both finite difference model (FDM) and finite element method (FEM). The model developed using FEM has given an oscillation of pressure head that is near to infiltration front. This oscillation pressure head could be reduced by applying a diagonal time matrix (mass lumping technique). The net water balance between inflow and outflow of soil pore water at any node and time step t (MB) is defined based on a diagonal time matrix. This aspect is investigated to evaluate the existence of any errors within the calculation process if existed. The water balance equation for the finite element technique is presented as follows (Celie et al. 1992, Ségol 1993):

$$MB^{t+1} = \frac{\sum_{i=1}^{E-1} (\theta_i^{t+1} - \theta_i^0) \Delta z + (\theta_0^{t+1} - \theta_0^0) \frac{\Delta z}{2} + (\theta_E^{t+1} - \theta_E^0) \frac{\Delta z}{2}}{\sum_{t=1}^{t+1} (q_0^t - q_E^t) \Delta t} \quad (21)$$

where q_0 and q_E are the boundary fluxes associated with z_0 and z_L , respectively [$L T^{-1}$]. Symbols “ i ” and “ t ” count for the sequence of nodes and time steps, respectively. Subscripts “ 0 ”, “ E ” refer to the upper boundary of downward flow and the number of elements, respectively. Superscripts “ 0 ”, “ t ” and “ $t+1$ ” refer to the initial, previous and current iteration time step, respectively.

5. Boundary condition for infiltration system

The initial condition was defined as the starting condition of the system at $t=0$. The boundary conditions were classified into upper and lower boundaries that were located on the top and bottom of the considered system (Huyakorn & Pinder 1983). The upper boundary was the condition at the discharge point and the lower boundary was the condition at the water table or the column base. The boundary and initial conditions for the solute transport model and Richards’ equation included the known concentration of contaminant and pressure head, respectively (Bear 1979, Huyakorn & Pinder 1983). The change of infiltration is mainly controlled by intensity of infiltration and surface soil properties. The infiltration rates are determined by: (1) Rate of water approaching above soil surface via rainfall, snowmelt, irrigation, natural or artificial recharge and depth of ponding on the surface; (2) Fully saturated hydraulic conductivity at soil surface; (3) Degree of saturation at soil surface when the infiltration begins; (4) Inclination and roughness of topsoil; and (5) Chemical characteristics of top soil and physical and chemical properties of water.

The infiltration rate; $f(t)$ is computed as (Nassif & Wilson 1975):

$$f(t) = i - q(t) \quad (22)$$

where i is natural precipitation or application rate and $q(t)$ is the rate of surface runoff. The natural infiltration recharge can be technically determined using Green-Ampt approach (Green & Ampt 1911). In the case of infiltration coming from runoff or rainfall recharge, the percolation rate is based on top soil properties. It can be classified into 2 categories as:

1) Water input rate is less than saturated hydraulic conductivity ($i < K_z$). At initial stage ($t=0$), the hydraulic conductivity is defined as K_{z0} and it increases to K_z at the specified time; t_w . At this stage, water will percolate and it is stored until the soil pore is fully filled.

$$f(t) = i \quad 0 < t < t_w \quad \text{and} \quad f(t) = 0 \quad t >> t_w \quad (23)$$

2) Water input rate is greater than saturated hydraulic conductivity ($i > K_z$). This process is observed at an early stage of infiltration in which the excess water cannot be transmitted downwards. The maximum water content and the hydraulic conductivity are limited at θ_s and K_z , respectively. Therefore, when the soil surface reaches saturation, ponding will occur or in the case of a hilly area, overland flow will take place. However, the

corresponding equation for this case cannot give a valid value of $f(t)$ as there is no well developed relationship for ponding.

The percolation of water during infiltration process with no ponding can be expressed as:

$$f_p = \frac{K_z \psi_w}{z_s} + K_z \quad (24a)$$

$$I = (\theta_s - \theta_0) z_s \quad (24b)$$

$$t = \frac{\theta_s - \theta_0}{K_z} \left\{ z_s - \psi_w \ln \left(1 + \frac{z_s}{\psi_s} \right) \right\} \quad (24c)$$

where θ_0 is the initial soil moisture content [unitless], f_p is the percolation rate, ψ_w is the pressure head at the wetting front, I is the cumulative infiltration and z_s is the wetting front distance for Green-Ampt model.

Schmid (1990) has modified Green-Ampt approach with a Taylor series expansion, and obtained the explicit approximation for a function of the infiltration rate.

$$f(t) = w \left[1 + 2 \frac{(w - K_z)^2}{K_z |\psi_f| (\phi - \theta_0)^t} \right]^{-0.5} \quad (25)$$

where ψ_f is the effective tension at the wetting front ($= 0.76 |\psi_s|$) (Brakensiek 1977, Freyberg et al. 1980), ψ_s is the pressure head at saturation and term $(\phi - \theta_0)$ is the initial soil water deficit. The soil moisture content under infiltration process can be estimated using Wang et al. (2003) equation as follows.

$$\theta = \begin{cases} \left(1 - \frac{z}{z_f} \right)^\delta (\theta_s - \theta_0) + \theta_0, & z \leq z_f \\ \theta_0 & z > z_f \end{cases} \quad (26a)$$

$$I = \frac{(\theta_s - \theta_0) z_f}{1 + \delta} \quad (26b)$$

$$f_p = \frac{K_z}{\phi z_f} + K_z \quad (26c)$$

$$t = \frac{(\theta_s - \theta_0)}{(1 + \delta) K_z} \left(z_f - \frac{\ln[\phi z_f + 1]}{\phi} \right) \quad (26d)$$

where z_f is the wetting front distance that is located between soil surface and the bottom of the wetted soil layer. Variable δ is the shape coefficient of Brook and Corey (1964) hydraulic properties model, ($= \tilde{M} / \tilde{N}$). ϕ is the soil suction allocation coefficient ($= \tilde{M} / \xi$) and ξ is a constant.

6. Boundary condition for redistribution system

The boundary conditions for a redistribution system can be evaluated according to the physical model of capillary rise. The zone of negative pressure is observed within the depth of capillary height. The capillary height is the height of the water level inside the capillary tube. The capillary height could be estimated using (Fredlunde & Rahardjo):

$$U_w = -\rho_w h_c g \quad (27)$$

where U_w is the hydraulic pressure at the capillary height [$M L^{-1} T^{-2}$], ρ_w is water density [$M L^{-3}$], h_c is the capillary height [L] and g is the gravitational acceleration [$L T^{-2}$].

The physical model of capillary pressure force in unsaturated soil is presented in Figure 5. If matric suction ($U_a - U_w$) or capillary height (h_c) is plotted against pore radius (r) on a Log-Log plot, a linear relationship is expected. Further details can be found in Fredlunde & Rahardjo (1993). The variables " σ_s ", " r_s " and " α " refer to the surface tension, the radius of capillary tube and the contact angle, respectively. The variable " U_a " is the atmospheric pressure (guage) that is normally taken as 0 cm H_2O .

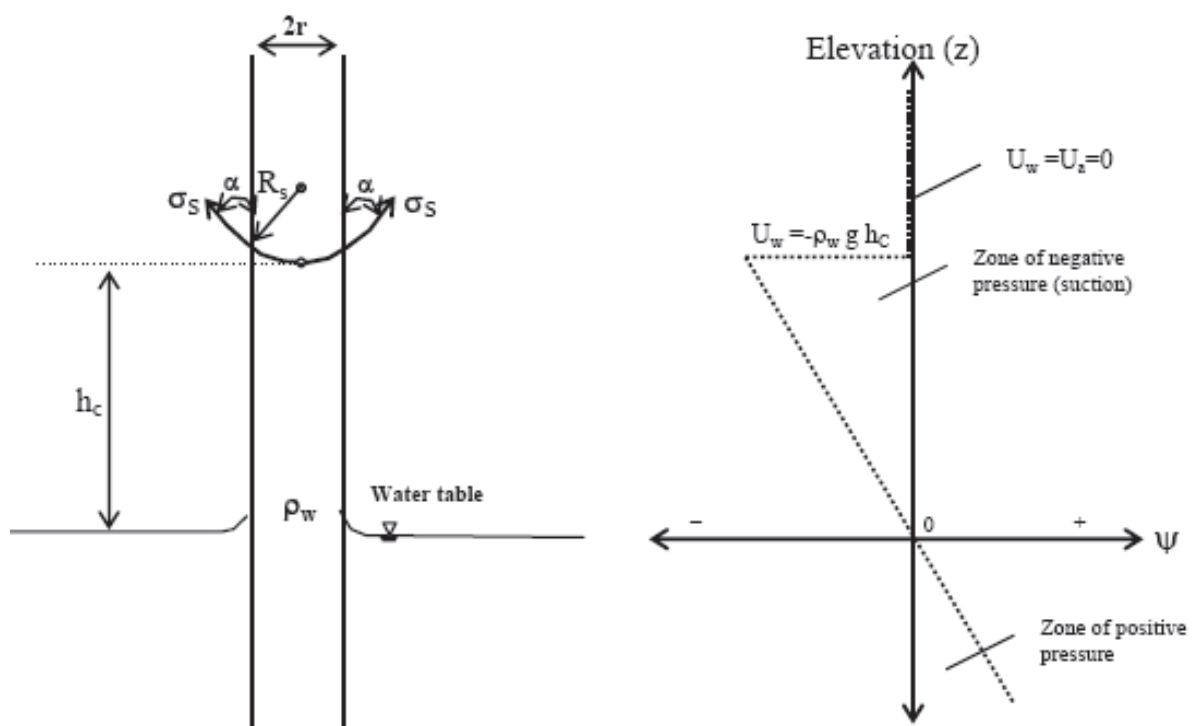


Fig. 5. Physical model of capillarity (Adapted from Fredlund & Rahardjo 1993)

7. Governing equation for solute transport

In practice, the objective is not only to predict the movement of water in the vadose zone, but also to determine the movement of reactive and non-reactive contaminants through the soil pores. The developed model can predict the fate and transport of reactive constituents such as phosphate, nitrate, organic carbon compounds and microbes.

The governing equation for multi-component transportation of contaminants in porous media under variable saturation conditions could be expressed in a general form as follows (Schnoor 1996).

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z} \left(D_z \frac{\partial C}{\partial z} \right) - \frac{\partial}{\partial z} (q_z C) - \frac{\rho_B}{\theta} \left(\frac{\partial C^*}{\partial t} \right) \pm \sum_{x=1}^n r_x \quad (28)$$

(accumulate) (dispersion) (advection) sorption (reaction)

where C^* is the concentration of a considered constituent in sorbed phase [$M L^{-3}$]; D_z is the dispersion coefficient; $(= D_m + D^*)$ [$L^2 T^{-1}$]; D_m and D^* are the mechanical and the molecular dispersion [$L^2 T^{-1}$], respectively; and r_x is the rates of reaction "x" with $x=1,2,\dots, n$ [$M L^{-3} T^{-1}$].

The dispersion can be obtained from Fick's Law (Fetter 1992) as follows.

$$D_z = \omega v_i + D^* \quad (29)$$

where D^* is an effective molecular diffusion coefficient [$L^2 T^{-1}$], ω is a coefficient relating to tortuosity [unitless] and v_i is the average linear velocity in the vertical direction; $(= q_z / \theta)$ [$L T^{-1}$].

7.1 Nitrogen and organic carbon compounds

The total rate of organic carbon compounds (substrate) utilisation, r_s was a combination of the substrate utilisation rate due to aerobic and nitrate respiration (Widdowson et al. 1988).

$$r_s = r_{SO} + r_{SN} \quad (30)$$

where r_s , r_{SO} and r_{SN} are the total substrate utilisation, substrate utilisation under aerobic respiration and substrate utilisation under nitrate respiration, respectively [T^{-1}].

Using a modified Monod's equation, the substrate utilisation rates could be derived as follows (Widdowson et al. 1988):

$$r_{SO} = \frac{\mu_o}{Y_o} \left[\frac{C_s}{K_{SO} + C_s} \right] \left[\frac{C_o}{K_o + C_o} \right] \left[\frac{C_A}{K_{SA} + C_A} \right] \quad (31a)$$

$$r_{SN} = \frac{\mu_N}{Y_N} \left[\frac{C_s}{K_{SN} + C_s} \right] \left[\frac{C_o}{K_N + C_N} \right] \left[\frac{C_A}{K_{AN} + C_A} \right] I[C_o] \quad (31b)$$

where μ_o and μ_N are the maximum specific growth rate for aerobic and denitrifying bacteria, respectively [T^{-1}]. Y_o and Y_N are a heterotrophic yield coefficient for aerobic and denitrifying bacteria, respectively [unitless]. C_s, C_o and C_A are the concentration in aqueous of organic carbon, oxygen and ammonia, respectively [$M L^{-3}$]. K_{SO}, K_o and K_{AO} are half concentration of substrate, oxygen and ammonia nitrogen under aerobic respiration, respectively [$M L^{-3}$]. K_{SN}, K_N and K_{AN} are half concentration of substrate, nitrate and ammonia nitrogen under nitrate respiration, respectively [$M L^{-3}$]. $I[C_o]$ is the inhibition factor $I[C_o] = (1 + C_o / K_c)^{-1}$ [unitless] and K_c is the coefficient of inhibition [$M L^{-3}$].

By referring to the rate of kinetic reaction (Eq. 31a and 31b) for organic carbon compounds biodegradation, the equation for transport of organic carbon compounds is written as (Schnoor 1996):

$$\frac{\partial C_S}{\partial t} = -\frac{\partial}{\partial z}(q_z C_S) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C_S}{\partial z}\right) - r_{SO} C_S \theta \tag{32}$$

The nitrate transport equation can be formulated as follows (Schnoor 1996):

$$\frac{\partial C_N}{\partial t} = -\frac{\partial}{\partial z}(q_z C_N) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C_N}{\partial z}\right) - r_{SN} C_S C_N \theta \tag{33}$$

Harvey et al. (1984) determined the kinetic coefficients for nitrifying and denitrifying bacteria. These coefficients are given in Table 2.

Parameter	Value	Parameter	Value
M_b (mg/cm ³)	5.64x10 ⁻⁴	K_{SO} (mg/cm ³)	0.040
μ_o (1/day)	3.1	K_{SN} (mg/cm ³)	0.040
μ_N (1/day)	2.9	K_o (mg/cm ³)	0.00077
Y_o	0.45	K_N (mg/cm ³)	0.00260
Y_N	0.5	K_{AO} (mg/cm ³)	0.0010
k_o (1/day)	0.02	K_{AN} (mg/cm ³)	0.0010
k_N (1/day)	0.02		

Table 2. Kinetic parameters for organic carbon and nitrate retardation (Harvey et al. 1984 cited in Widdowson et al. 1988).

7.2 Phosphate phosphorus compounds

Phosphorus adsorption on soil was formulated as follows (Shah et al. 1975):

$$\rho_B \frac{\partial C_P^S}{\partial t} = K_t \left(C_P^w - C_P^{w*}\right) \tag{34}$$

where C_P^S is the concentration of adsorbed phosphorus [M M⁻¹] and K_t is the overall volumetric mass transfer coefficient [L T⁻¹]. C_P^{w*} is the concentration of phosphorus in liquid phase that is in equilibrium with the concentration of phosphorus in the solid phase [M M⁻¹] and $C_P^w - C_P^{w*}$ is a driving force for transferring phosphorus from liquid to solid phase [M L⁻³].
The Langmuir isotherm equation is the best fit for phosphorus adsorption (Shah et al. 1975). Variable C_P^{w*} is modified into Langmuir isotherm equation, yielding (Schnoor 1996, Watts 1997):

$$C_P^{w*} = \frac{k_L k_M C_P^w}{1 + k_M C_P^w} \tag{35}$$

where k_L and k_M are the coefficients (Langmuir rate constant) [unitless] and the maximum phosphate adsorption capacity on soil [L³ M⁻¹], respectively.
The soluble phosphate, C_P can be assumed as soil pore water, which can be presented as volumetric portion of moisture (Fetter 1992). The transport of soluble phosphate is obtained by:

$$\frac{\partial(\theta\kappa C_p)}{\partial t} = -\frac{\partial}{\partial z}(q_z C_p) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C_p}{\partial z}\right) \quad (36)$$

where κ is a retardation factor $(=1+[\rho_b K_d/\theta])$ and K_d is the distribution coefficient, $(=k_L k_M/(1+K_M C_p^w)^2)$.

7.3 *E. coli*

The overall reaction rates of microbial kinetics were the summation of production, maintenance, decay, adsorption and desorption. The retardation equation was given as (Zysset et al. 1994):

$$n \frac{d(C_b^f)}{dt} = n v_y \eta k_\mu C_s C_b^f - n k_d C_b^f + \theta k_c C_b^w - n k_s C_b^f \quad (37)$$

where n is the fraction of aqueous volume and biofilm in total volume (equals to porosity) [unitless]. C_b^f and C_b^w are the concentration of adhering microbes and free swimming microbes $[M L^{-3}]$, respectively. C_s is the concentration of limiting substrate in aqueous compartment $[N L^{-3}]$, v_y is the stoichiometric coefficient $[M N^{-1}]$, η is an effectiveness of biofilm [unitless]. k_μ and k_d are Monod's constant for substrate utilisation in biomass $[L^3 M^{-1} T^{-1}]$ and the constant of decay rate $[T^{-1}]$, respectively. k_s and k_c are the constant desorption (detachment) and adsorption (attachment) rate $[T^{-1}]$, respectively. The unit N is the quantity of microbes involved (cfu or MPN).

The concentration of *E. coli* relates to the substrates consumed. Substrate utilisation during metabolism processes is defined using the first order Monod's kinetics equation as follows (Zysset et al. 1994).

$$\frac{\partial C_s}{\partial t} = -k_\mu C_s C_b^t - k_m C_b^t \quad (38)$$

where $k_\mu = \mu_b / Y_b (K_{sb} + C_s)$, but $C_s \ll K_{sb}$, so $k_\mu = \mu_b / Y_b K_{sb}$. C_s and C_b^t are the carbonaceous substrate concentration $[M L^{-3}]$ and the total microbial concentration $[M L^{-3}]$, respectively. μ_b and Y_b are the microbial maximum specific growth rate $[T^{-1}]$ and a heterotrophic microbial yield coefficient [unitless], respectively. K_{sb} and k_m are the substrate concentration when the rate of utilisation of half of the maximum rate under aerobic condition $[M L^{-3}]$ and a biomass maintenance rate $[T^{-1}]$, respectively.

The *E. coli* transport equation was governed as follows (Zysset et al. 1994):

$$\frac{\partial(\kappa\theta C_b)}{\partial t} = \frac{\partial}{\partial z}\left(D_z \frac{\partial C_b}{\partial z}\right) - \frac{\partial}{\partial z}(q_z C_b) - \lambda_b \theta \kappa C_b \quad (39)$$

where $\lambda_b = (k_\mu - k_m) \cdot C_b^t$, which involves assimilation and dissimilation of microbes and $C_b^t = \kappa C_b$.

A general form of the mathematical model for contaminant transport coupling retardations could be written as follows (Huyakorn et al. 1985):

$$\begin{array}{ccccccc}
 \frac{\partial}{\partial z} \left(D_z \frac{\partial C}{\partial z} \right) & - \frac{\partial}{\partial z} (q_z C) & = & \frac{\partial}{\partial t} (\theta \kappa C) & + & \lambda \theta \kappa C & (40) \\
 (dispersion) & (advection) & & (accumulation) & & (1^{st} \text{ order decay}) &
 \end{array}$$

The retardation factor, κ equals 1.0 for organic carbon and nitrate compound transport equations. The biodecay factor (involving growth of microbes), λ equals 0.0 for phosphate compounds transport equation. Only microbial transport contains all of these factors.

8. Numerical solution for solute transport equation

The approximate solution of contaminant concentration at any nodes and time “ t ” is defined as (Segerlind 1984, Huyakorn et al. 1985, Clement et al. 1998):

$$C(z, t) = \sum_{j=1}^m N_j(z) C_j(t) \quad (41)$$

where $N_j(z)$ is the shape function [unitless], $C_j(t)$ is the concentration of contaminant at time t [M L⁻³].

The mathematical model presented in Eq. 40 can be modified as follows:

$$L[C] = \frac{\partial}{\partial z} \left(D_z \frac{\partial C}{\partial z} \right) - q_z \frac{\partial C}{\partial z} - \theta \kappa \left[\frac{\partial C}{\partial t} + \lambda C \right] \quad (42)$$

The integral form of Eq. 42 is given as follows:

$$\int_{z=0}^{z=L} N_i L[C] dz = 0 \quad (43)$$

where $[0, L]$ is the extent of the vertical direction (one dimension) domain. The subscripts “ i ” and “ j ” denoted the sequence of elements in the domain as presented in Figure 4.

Substituting Eq. 42 into 43, gives:

$$\int_{z=0}^{z=L} N_i \frac{\partial}{\partial z} \left(D_z \frac{\partial C}{\partial z} \right) dz - \int_{z=0}^{z=L} N_i q_z \frac{\partial C}{\partial z} dz - \int_{z=0}^{z=L} N_i \theta \kappa \left[\frac{\partial C}{\partial t} + \lambda C \right] dz = 0 \quad (44)$$

The numerical solution of Eq. 44 is governed as:

$$\int_{z=0}^{z=L} \left(D_z \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} + N_i \frac{\partial N_j}{\partial z} q_z \right) C_j dz + \int_{z=0}^{z=L} N_i N_j \theta \kappa \left[\frac{\partial C_j}{\partial t} + \lambda C_j \right] dz - N_i D_z \left(\frac{\partial C}{\partial z} \right) \Big|_{z=0}^{z=L} = 0 \quad (45)$$

The algebraic matrix systems are defined as follows:

$$\left\{ [P_{ij}] + [R_{ij}] \right\} C_j + [Q_{ij}] \frac{\partial C_j}{\partial t} = \{S_i\} \quad (46)$$

where

$$\left[P_{ij} \right] = \sum_e \int_{z=0}^{z=L} \left(D \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} + N_i \frac{\partial N_j}{\partial z} q_z \right) dz, \quad \left[Q_{ij} \right] = \sum_e \int_{z=0}^{z=L} N_i N_j \theta \kappa dz$$

$$\left[R_{ij} \right] = \sum_e \int_{z=0}^{z=L} N_i N_j \theta \kappa \lambda dz \quad \text{and} \quad \{ S_i \} = N_i D_z \left(\frac{\partial C}{\partial z} \right) \bigg|_{z=0}^{z=L}$$

The initial concentration in the entire domain $[0, L]$ at time $t = 0$ is defined as follows (Bear 1979, Huyakorn & Pinder 1983, Huyakorn, et al. 1985, Ségol 1993, Clement et al. 1998):

$$C_j(z, 0) = C_0(z) \quad (47)$$

where $C_0(z)$ is the known distribution of solute concentration at time $t = 0$ $[\text{ML}^{-3}]$.

The boundary concentration on the edge of domain $[0, L]$ at time " t " is defined using the Dirichlet boundary condition (Bear 1979, Huyakorn & Pinder 1983, Huyakorn, et al. 1985, Ségol 1993, Clement et al. 1998).

$$C_j(z, t) = C(z, t) \quad \text{on} \quad z_1 < z < z_2 \quad (48)$$

The specific dispersive flux on the edge of domain $[0, L]$ at time " t " is employed using Neumann boundary condition. The dispersive flux was defined as $\partial C / \partial z$, (Bear 1979, Huyakorn & Pinder 1983, Huyakorn, et al. 1985, Ségol 1993, Clement et al. 1998).

$$\text{For rainfall infiltration} \quad D_z \frac{\partial C}{\partial z} = q_C^D \quad \text{on} \quad 0 \leq z \leq L \quad (49a)$$

$$\text{For seepage flow} \quad D_z \frac{\partial C}{\partial z} - q_z C = q_C^T \quad \text{on} \quad 0 \leq z \leq L \quad (49b)$$

where q_C^D and q_C^T are the portion of the boundary flux attributable to concentration due to dispersion $[\text{M L}^{-1} \text{T}^{-2}]$ and the portion attributable to total concentration $[\text{M L}^{-1} \text{T}^{-2}]$, respectively.

9. Model applications

The simulation results of solute transport in unsaturated infiltration-redistribution system is an active research area where a variety of attempts are being made to determine the dynamics of vadose zone in relation to water and contaminant movement and quality of soil. The model presented above is used to simulate the experimental data obtained by Paniconi et al. (1991). The input parameters for this case study are given in Table 3.

The Neumann and the Dirichlet conditions were applied to the upper and lower boundary, respectively. Both the experimentally observed and simulated pressure head and moisture content profiles are presented in Figures 6 and 7, respectively. The developed models predicted the experimental observations of Paniconi et al. (1991) very well. This implied that the developed model is robust, and that it could effectively predict the water movement in the infiltration-redistribution systems. On the other hand, the simulation results from the solute transport model could not be compared with experimental observations due to lack

of appropriate data. However, a series of simulations are carried out as shown in Figures 8 through 11. The kinetic rate constants of each contaminant are assumed based on the case study of contaminants movement in sandy soil near Perth (McArthur & Bettenay 1964, cited in Whelan & Barrow 1984). The input parameters used in model are presented in Table 4.

Parameters	Values
Domain	Column with depth of 10 m (saturation maintained at the base of the column).
Hydraulic properties model	van Genutchten model with saturated hydraulic conductivity; K_z is 5 m/h, Air entry pressure; ψ_a is -3.0 mH ₂ O. Saturated moisture content; θ_s is 0.45 and residual moisture content; θ_r is 0.08. q and p are 0.667 and 3.0, respectively.
Boundary and initial conditions	At the top, Darcy flux (q_z) is applied as a function of time, equalled to $t/64$ m/h. Constant head at the column base, ψ_{bot} of 0 m. Constant head at the initial, ψ_i of 0 m.
Number of element; $nelem$	100.
Increment time interval; dt	Time step varies between 0.1 to 0.5 hour.

Table 3. Input parameters for water movement model (Paniconi et al. 1991).

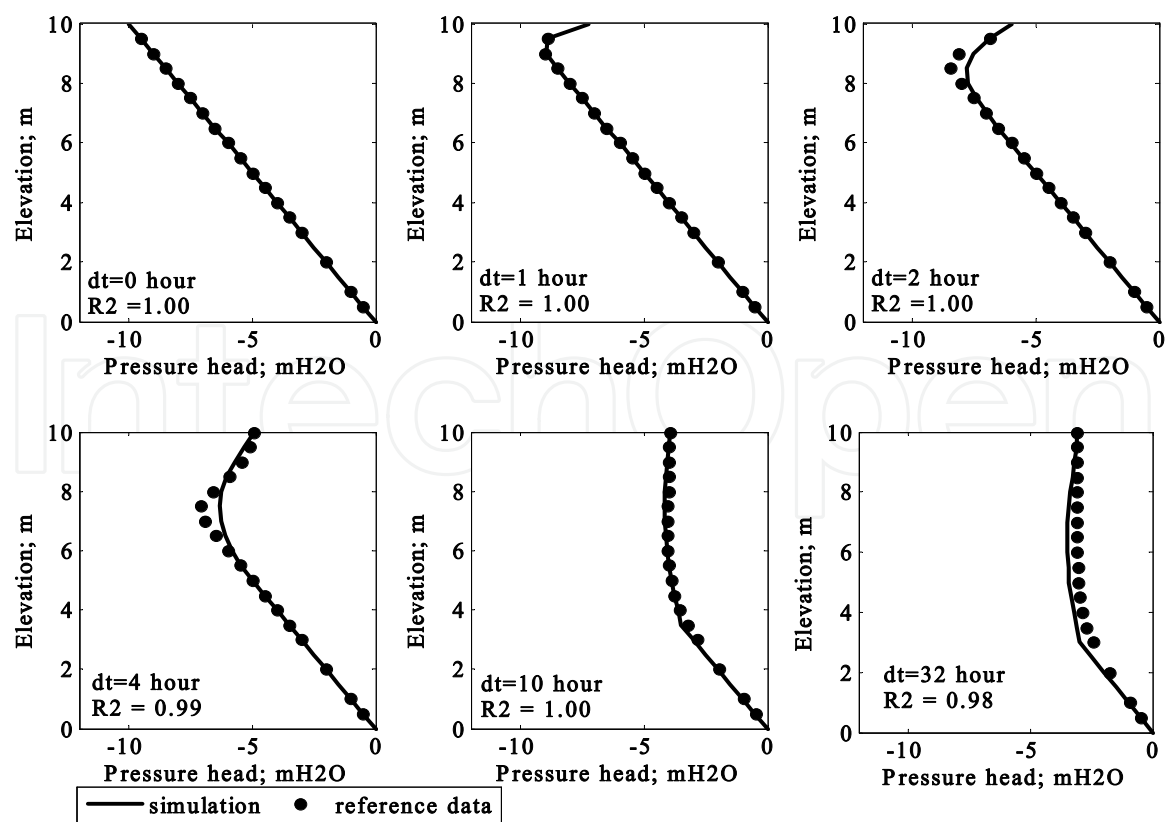


Fig. 6. Pressure head profiles (datum was at the groundwater table).

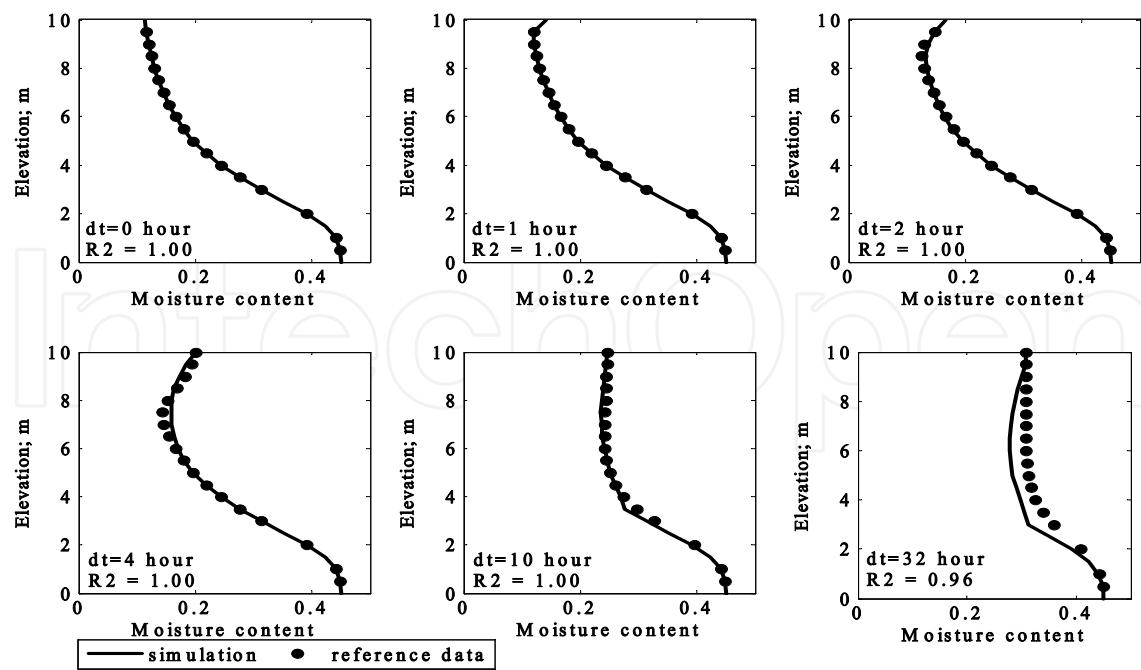


Fig. 7. Moisture content profiles (datum was at the groundwater table)

Parameters	Values
Contaminant transport	Organic carbon compounds: Constant concentration at the surface, C_{top} of 1250 mg/L and at the datum, C_{bot} of 39 mg/L. Initial concentration, C_{int} of 39 mg/L. Nitrate nitrogen compounds: Constant concentration at the surface, C_{top} of 2 mg/L and at the datum, C_{bot} of 83 mg/L. Initial concentration, C_{int} of 2 mg/L. Phosphate phosphorus compounds: Constant concentration at the surface, C_{top} of 15 mg/L and at the datum, C_{bot} of 0.72mg/L. Initial concentration, C_{int} of 0.72 mg/L. <i>E. coli</i> : The initial microbial concentration 1.03×10^9 cfu/L. The microbial concentration at the column surface and base were 2.14×10^{10} and 1.318×10^3 cfu/g (weight of <i>E.Coli</i> is 7×10^{-10} mg/cfu).
Dispersivity; α_T (cm)	3.25 (organic carbon), 7.54 (nitrate), 1.57 (phosphate) and 7.59 (<i>E.Coli</i>)
Molecular diffusion; D^* (cm ² /h)	0.03924 (Organic C), 0.06840 (Nitrate), 0.07055 (Ammonia), 0.02304 (Phosphate) and 0.0479 (<i>E.coli</i>) (Kemper 1986, Stevik 1999).
Kinetic rate constant	Organic C and Nitrate: μ_o =74.4 h ⁻¹ , Y_o =0.45, K_{so} =0.040 mg/cm ³ , K_o = 0.00077 mg/cm ³ , K_{AO} = 0.001 mg/cm ³ , C_A =50 mg/L, C_o = 2 mg/L, μ_N = 69.6 h ⁻¹ , Y_N =0.5, K_{SN} =0.040 mg/cm ³ , K_N =0.0026mg/cm ³ , K_{AN} =0.001 mg/cm ³ and $I[C_o]$ =0.0802 (Widdowson 1998). Phosphate: K_d = 1.22×10^{-9} cm ³ /g and ρ_B =1.7 kg/L. (McArthur & Bettenay 1964, cited in Whelan & Barrow 1984). <i>E.coli</i> : Adsorption rate= 0.015 h ⁻¹ , Growth-decay rate 56.8 h ⁻¹ , (Stevik et al 1999, Schnoor 1996).
Increment time interval; dt (hour)	Varies between 0.1-0.5.
Maximum simulation time; t (hour)	32

Table 4. Input parameters for solute transport model (adopted from McArthur & Bettenay 1964, cited in Whelan & Barrow 1984).

Figures 8, 9, 10 and 11 present the simulations of nitrate, organic carbon, phosphate and *E.coli* transport in infiltration-redistribution system. The simulation results reveal that the contaminants could reach the groundwater table over a longer period. Also, it appears that the top soil can remove substantial amount of contaminants. Particularly, the organic carbon and *E.coli*, are removed within the few centimetres of the top soil layer. On the other hand, phosphate can move downwards to a depth of 2 metres. This might relate to phosphate adsorption capacity, which is relatively low in the sandy soil. However, to make proper assessment of contaminant transport and its potential contamination of groundwater longer periods of simulation are required. At this stage it can be concluded that the contaminant transport model presented earlier could be used to predict the contaminant transport within the unsaturated (vadose) zone.

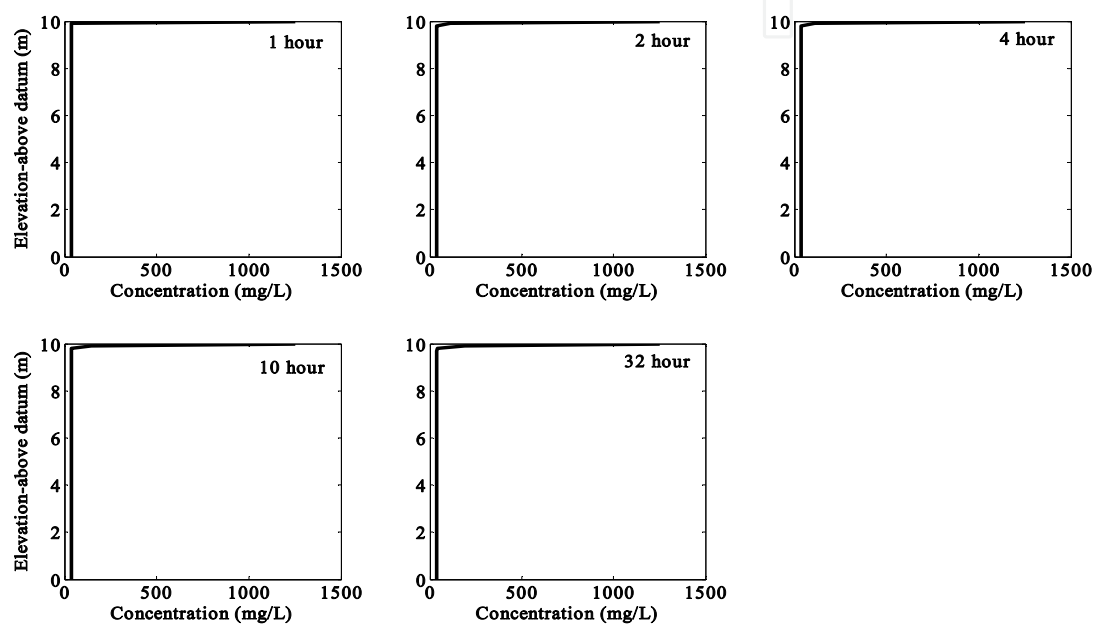


Fig. 8. Organic carbon concentration profile (datum was at the groundwater table).

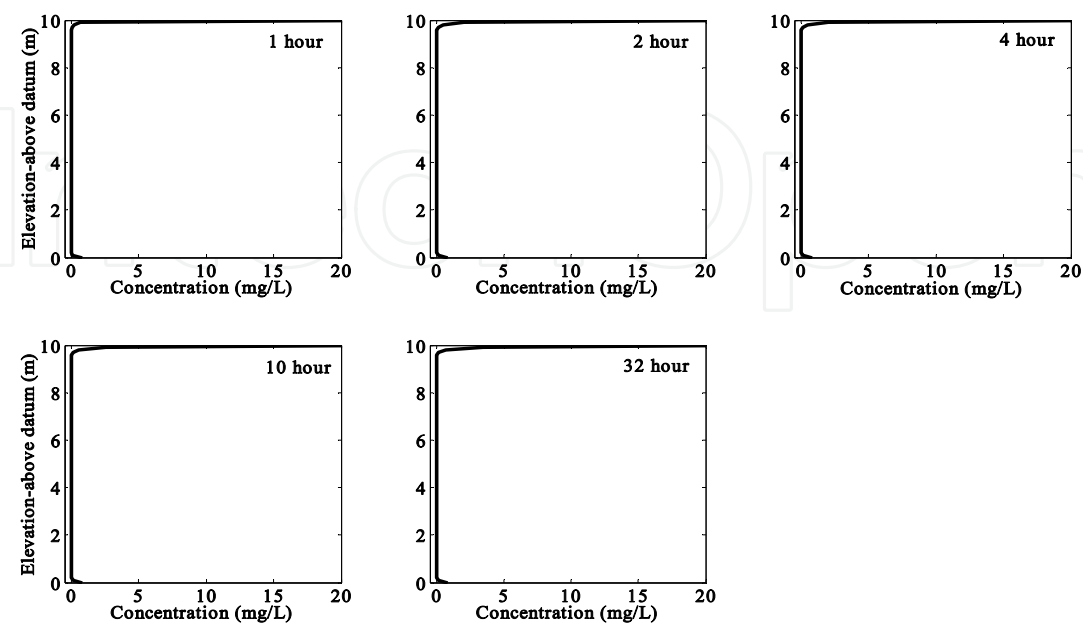


Fig. 9. Nitrate concentration profile (datum was at the groundwater table).

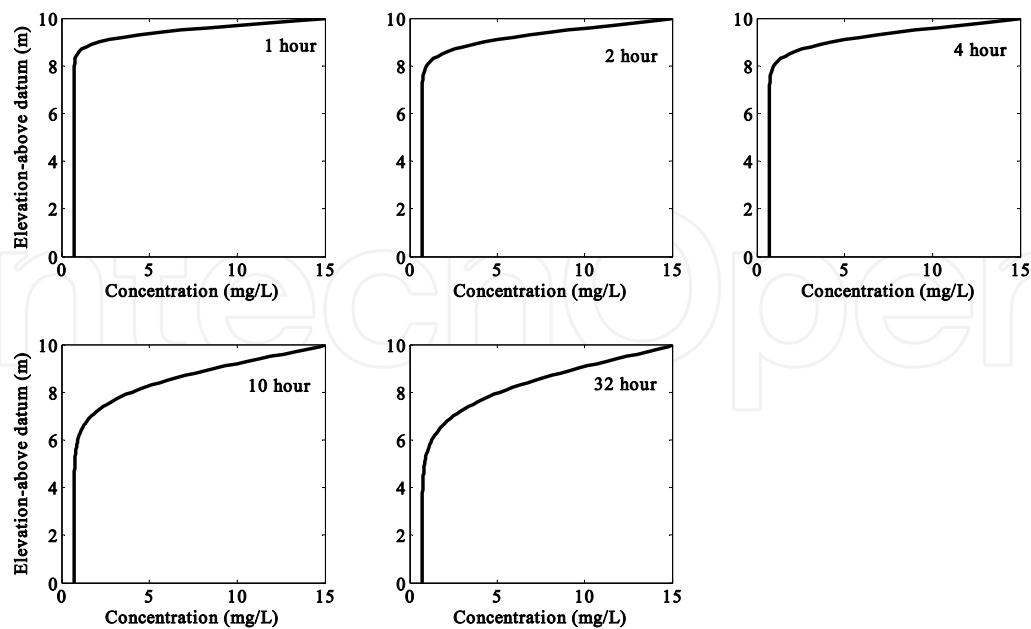


Fig. 10. Phosphate concentration profile (datum was at the groundwater table).

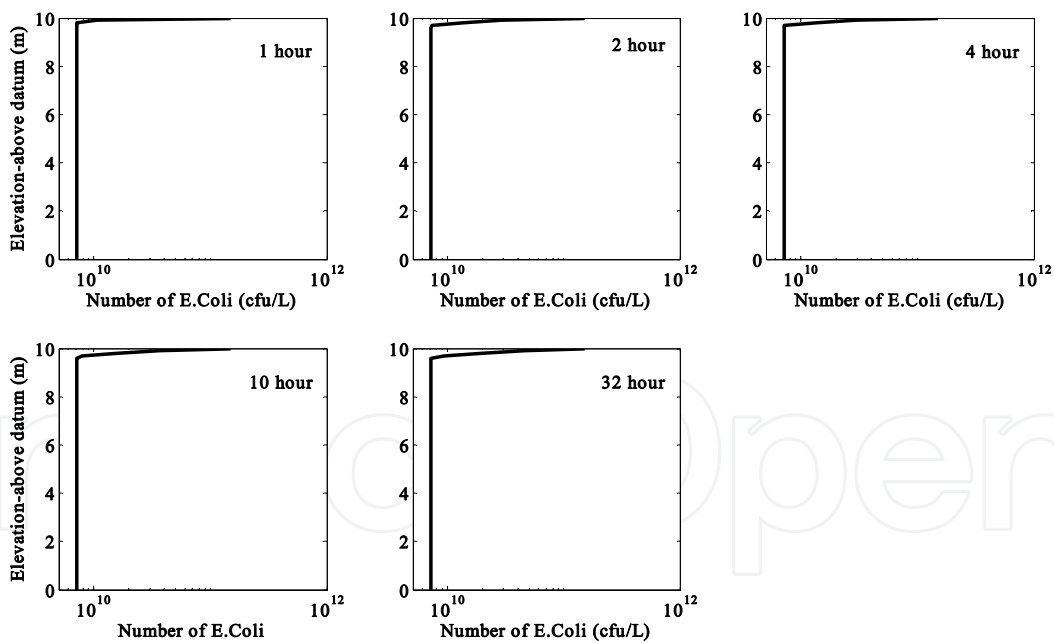


Fig. 11. *E.coli* distribution profile (datum was at the groundwater table).

10. Conclusion

A comprehensive model for predicting the movement of water and contaminants through unsaturated soil is presented. The models were developed based on Richards equation and mass balance relationships. Also, Finite Element Method (FEM) based solution techniques

were developed for obtaining numerical solution to the models developed. The water movement simulation model predicted fairly well the water movement observed through column studies. Thus, the water movement model can be used for predicting the water movement through unsaturated zone with confidence. However, it is important to use site specific input parameters for reliable results. In the case of contaminant transport model, it could not be tested with experimental observations due to lack of appropriate data. However, some of the simulation results for organic carbon, nitrate, phosphate and *E.coli* appear to indicate that the model is able to predict the contaminant transport through soil. It is recommended that the model is further tested with experimental and/or field data. The water can carry contaminants during percolation, however there are some chemical and biological mechanisms, which can retard the migration of contaminants. The capillary force can extract water from aquifer, which is important for redistribution system. With the infiltration-redistribution system, the pore velocity of water may be reduced. This can lead to self protection of groundwater from contamination. Further, it is apparent that the relative hydraulic conductivity $K_{z,k_{rw}}$ is one of the critical parameters that influence the water and contaminant transport through vadose zone. In this study the influence of relative hydraulic conductivity on the water and contaminant transport was not fully investigated. Evidently, further studies are required to fully understand the influence of relative hydraulic conductivity and hence identify critical soil types that may be readily affected by the on-site waste disposal systems.

11. Acknowledgement

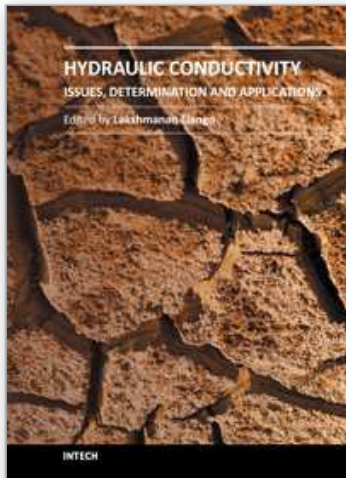
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There are several books on broad aspects of hydrogeology, groundwater hydrology and geohydrology, which do not discuss in detail on the intrigues of hydraulic conductivity elaborately. However, this book on Hydraulic Conductivity presents comprehensive reviews of new measurements and numerical techniques for estimating hydraulic conductivity. This is achieved by the chapters written by various experts in this field of research into a number of clustered themes covering different aspects of hydraulic conductivity. The sections in the book are: Hydraulic conductivity and its importance, Hydraulic conductivity and plant systems, Determination by mathematical and laboratory methods, Determination by field techniques and Modelling and hydraulic conductivity. Each of these sections of the book includes chapters highlighting the salient aspects and most of these chapters explain the facts with the help of some case studies. Thus this book has a good mix of chapters dealing with various and vital aspects of hydraulic conductivity from various authors of different countries.

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