

## **CONTAMINANT TRANSPORT THROUGH INITIALLY DRY SOIL**

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### **ABSTRACT**

Horizontal contaminant transport through unsaturated soil been demonstrated both analytically and experimentally. The water and solute transport equations were solved using the Boltzman transformation, to convert the partial differential equations to ordinary differential equations. The resulted mathematical model was verified using experimental data. A laboratory scale column system was constructed and operated horizontally to monitor both the actual solute concentration profile and the development of the wetting front. Comparison between the predicted values and the experimental data has shown good agreement. Hence, the analytical solution can be used successfully to predict horizontal contaminant transport in initially dry soil.

### **1. Introduction**

Numerous human activities utilize subsurface as a receptor of various contaminant, which include hazardous waste landfills, ponds and lagoons bearing industrial or domestic wastewater and on land treatment applications of treated domestic and industrial wastewater. These activities have always resulted in the release of various pollutants into the terrestrial subsurface and consequently, to the nearby environment including groundwater resources. Thus, in recent years, great efforts have been directed towards establishing a better knowledge of the kinetics that govern the transport and fate of contaminants in the subsurface environment. Early investigation of the mechanisms of dispersion was confined to the saturated flow condition. Extensions of this work to the unsaturated flow region have somewhat inconclusive. Laboratory studies of contaminant transport in an unsaturated porous media have shown that the dispersion process during unsaturated flow is far more complicated than during saturated flow (Bigger and Nielsen 1960, 1962, 1967, Nielsen and Bigger 1961 and Kurtz and Melsted, 1973). Empirical and conceptual models developed for saturated flow conditions (such as Bear 1972) have not been easily adapted to the unsaturated case. Detailed studies have been carried out in recent years on understanding the nature of miscible displacement in porous media (Perkins and Johnston 1963, Bigger and Nielsen 1967 and Fried and Combarous 1971). The work of Wilson and Gelhar (1981) marked a significant advance in developing an understanding of the basic processes involved in dispersion in unsaturated porous media. In recent years several analytical methods were developed to simulate water movement and

solute transport in unsaturated zone (Warriek et al. 1991; Islas and IIIangasekare 1992; Barry et al. 1993). Simles et al. (1978) developed a quasi-analytical solution for non-reactive solute flow during unsteady horizontal absorption under constant concentration boundary conditions which has been discussed by Watson and Jones (1981) particularly in relation to assessing the performance of solute model. In recent study, horizontal contaminant transport through unsaturated soil has been demonstrated both analytically and experimentally. The quasi-analytical solution was applied, using an alternative integral solution. To predict contaminant transport profile and the results were verified using experimental values, to assist the adequacy of the proposed analytical solution.

## 2. Theoretical Study

### 2.1 Analytical Approach

The hydrodynamic dispersion of solute during horizontal transport can be represented by the following equation:

$$\frac{\partial(c\Theta)}{\partial t} = \frac{\partial}{\partial x} \left[ D_e (\Theta, \nu) \frac{\partial c}{\partial x} \right] - \frac{\partial}{\partial x} (qc) \quad (1)$$

where  $c$  is solute concentration in the water ( $\text{g/cm}^3$ ); the water content per bulk volume ( $\text{cc/cc}$ );  $q$  the flux of water  $\text{cm/min}$ ;  $D_e$  is the effective hydrodynamic ( $\text{cm}^2/\text{min}$ ), which depends upon the average velocity  $\nu = \frac{q}{\Theta}$ ;  $t$  the time in (min); and  $z$  the space coordinate (cm). Simles et al. (1978) showed that if the velocity dependence of  $D_e$  were neglected then the equation 1, with  $D_e(\Theta)$  replacing  $D_e(\Theta, \nu)$ , would lead to a convenient similarity solution using the

Boltzman transformation  $\lambda = xt^{\frac{1}{2}}$  where  $\lambda$  is the penetrated depth of solute front. The similarity solution is valid for the case of constant concentration boundary conditions.

These conditions for water and solute, together with initial conditions, may be written as follows:

$$\begin{aligned} \Theta &= \Theta_n & x &\geq 0 & t &= 0 \\ \Theta &= \Theta_0 & x &= 0 & t &\geq 0 \end{aligned} \quad (2)$$

and

$$c = c_n \quad x \geq 0 \quad t = 0$$

$$c = c_0 \qquad x = 0 \qquad t \geq 0 \qquad (3)$$

The flow of water in a rigid horizontal system may be described by the well known flow equation:

$$\frac{\partial \Theta}{\partial t} = \frac{\partial \Theta}{\partial t} \left[ D(\Theta) \frac{\partial \Theta}{\partial x} \right] \qquad (4)$$

Where  $D(\Theta)$  is the soil diffusivity. Since

$$q = -D(\Theta) \frac{\partial \Theta}{\partial x} \qquad (5)$$

Following Smiles et al. (1978) equation (1) may be written in terms of  $D_e(\Theta)$  as

$$\Theta \frac{\partial c}{\partial x} = \frac{\partial}{\partial t} \left[ D_e \frac{\partial c}{\partial x} \right] + D(\Theta) \frac{\partial \Theta}{\partial x} \frac{\partial c}{\partial x} \qquad (6)$$

Substitution  $\lambda = xt^{1/2}$  in Equations (2)-(6) and rearranging, the following equations are obtained:

$$\frac{d}{d\lambda} \left[ D(\Theta) \frac{d\Theta}{d\lambda} \right] + \frac{\lambda}{2} \frac{d\Theta}{d\lambda} = 0 \qquad (7)$$

$$\frac{d}{d\lambda} \left[ D_e(\Theta) \frac{g}{2} \frac{dc}{d\lambda} \right] = 0 \qquad (8)$$

For the following boundary conditions:

$$\begin{aligned} \Theta &= \Theta_n & \lambda &\rightarrow \infty \\ \Theta &= \Theta_0 & \lambda &= 0 \end{aligned} \qquad (9)$$

and

$$\begin{aligned}
 c &= c_n & \lambda &\rightarrow \infty \\
 c &= c_0 & \lambda &= 0
 \end{aligned}
 \tag{10}$$

Where  $g$  is penetrated depth of solute front and defined by:

$$g = \Theta\lambda + 2D(\Theta)\frac{\partial c}{\partial \lambda} = \Theta\lambda - \int_{\Theta_n}^{\Theta} \lambda d\Theta \tag{11}$$

Since the relationship between  $\Theta$  and  $\lambda$  is unique, Equation (8) may be written as an ordinary differential equation:

$$\frac{d}{d\lambda} \left[ D_e(\lambda) \frac{dc}{d\lambda} \right] + \frac{g}{2} \frac{dc}{d\lambda} = 0 \tag{12}$$

Using the same boundary conditions, described by Equations (9) and (10), Smiles et al. (1978) reported the following solution:

$$\frac{c - c_0}{c_n - c_0} = \frac{M(\lambda)}{M(\infty)} \quad \text{When } c_n \geq c_0 \tag{13}$$

$$\text{Where } M(\lambda) = \int_0^\lambda \left[ \frac{1}{D_e} \exp(-1/2) \int_0^\lambda \frac{g(\lambda)}{D_e(\lambda)} d\lambda \right] d\lambda \tag{14}$$

## 2.2 An Alternative Integral Solution

Defining  $\lambda_*$  as the value of  $\lambda$  at which  $g(\lambda) = 0$ , and assuming  $D_e$  to be constant in the region of the solute front, Equation (12) may be written as :

$$\frac{d^2 c}{d\lambda^2} = -\frac{g(\lambda)}{2D_e} \frac{dc}{d\lambda} \tag{15}$$

The  $\Theta(\lambda)$  relationship for sandy clay soil in the region of interest is shown in Fig. 1. Defining  $\lambda_0$  as the value  $\lambda$  where  $c \rightarrow c_0$ ,  $\lambda_n$  as the value where

$c \rightarrow c_n$  and  $c_*$  as the  $c$  value at  $\lambda_*$ , then the integration of Equation (15) for  $\lambda_0 \geq \lambda \geq \lambda_*$  gives

$$(c - c_*) = \left(\frac{dc}{d\lambda}\right)_* \int_{\lambda_*}^{\lambda} \exp\left\{-\frac{\tan \alpha_0}{4D_e} (\lambda - \lambda_*)^2\right\} d\lambda \quad (16)$$

Similarly for  $\lambda_n \leq \lambda \leq \lambda_*$

$$(c - c_*) = \left(\frac{dc}{d\lambda}\right)_* \int_{\lambda_*}^{\lambda} \exp\left\{-\frac{\tan \alpha_0}{4D_e} (\lambda - \lambda_*)^2\right\} d\lambda \quad (17)$$

From Equations (15) and (17), the following equation can be obtained:

$$\begin{aligned} \left(\frac{dc}{d\lambda}\right)_* &= (c_n - c_*) / \int_{\lambda_*}^{\lambda_0} \exp\left\{\frac{\tan \alpha}{4D_e} (\lambda_* - \lambda)^2\right\} d\lambda \\ &= (c_* - c_0) / \int_{\lambda_n}^{\lambda_0} \exp\left\{-\frac{\tan \alpha (\lambda_* - \lambda)^2}{4D_e}\right\} d\lambda \end{aligned} \quad (18)$$

When  $c_0$  and  $c_n$  are known in Equation (18),  $c_*$  can be determined and hence, the value of  $\left(\frac{dc}{d\lambda}\right)_*$  can be found and substituted in Equations (16) and (17) to find the two parts of  $c(\lambda)$ . The integration can be carried out for any value of  $D_e$  once  $\tan \alpha$  is known from the solution of Equation (11).

### 3. Experimental Study

To compare the analytical prediction of solute transport in initially dry soil with observed values, solute flow experiments were conducted using a 48 cm long plexi-glass column filled with sandy clay soil. Four sampling ports are located at 9 cm interval. The inlet part of the column was equipped with a porous plate and cloth to insure well distribution of the influent flow. The size of the soil grains were in the range 0.4-1.5 mm, having a density of 1.58 g/cm<sup>3</sup> and composed of 83.0% sand and 17.0% clay. The column was operated at a flow rate of 32 ml/min using 90 mg/l chloride solution ( $c_0$ ). Flow through the

column was facilitated with use of Cole-Parmer pump with Master-Flex pump head. Unsaturation conditions in the column was maintained by operating at a flow rate less than the measured saturated hydraulic conductivity ( $K_{sat}$ ). The background solute concentration was 2200 mg/l ( $c_n$ ). Solute concentration, wetting front location and moisture content were monitored, with time, along the length of the column. The saturated hydraulic conductivity was determined using the constant head test. The chemical analysis was performed according to Standard Method for Examination of Water and Wastewater (1985).

#### 4. Results and Discussion

The integration in the above equation is carried out from zero to  $\lambda$ . The quasi-analytical approach first determine  $\Theta(\lambda)$  (Philip, 1955) from which, the value of  $g(\lambda)$  can be calculated. This is used in Equations (13) and (16) to find the normalized relationship  $c(\lambda)$ . Smiles and Philip (1978) and Smiles et al. (1978) describe a comprehensive set of experiment using a fine sand-kaolinite mixture as the porous material and show the uniqueness of  $c(\lambda)$  for a range of initial water contents and for different solute concentration conditions.

Figure 1 shows the mean  $\Theta(\lambda)$  relationship obtained using Bruce and Klute method (1965). The value of the saturated hydraulic conductivity was determined as 0.238cm/min, and the saturated volumetric water content as 0.331 cc/cc. Using the following functions that correlate the moisture content ( $\Theta$ ) with hydraulic conductivity ( $k$ ) and water diffusivity ( $D$ ), the relationships between water, hydraulic conductivity and water diffusivity were obtained.

$$k(\Theta) = k_{sat} \left( \frac{\Theta}{\Theta_{sat}} \right)^{4.35} \quad (19)$$

$$D(\Theta) = k(\Theta) \frac{\partial h}{\partial \Theta} \quad (20)$$

Using the above expressions [Equations (19) and (20)] and substituting the experimental values of  $k_{sat}$ ,  $\Theta_{sat}$  and  $\Theta_i$ , the  $h(\Theta)$ ,  $k(\Theta)$  and  $D(\Theta)$  relationships are determined. Figure 2 shows the relationship between the moisture content and diffusivity.

The  $\Theta(\lambda)$  relationship was determined experimentally by monitoring the speed of the wetting front and the corresponding moisture content. Similarity was

shown to be preserved exactly, with the  $\Theta(x,t)$  profiles collapsing onto the one  $\Theta(\lambda)$  relationship, and gave  $\lambda_* = 3.46 \times 10^{-3} \text{ ms}_{-1/2}$ ,  $\tan \alpha_0 = .4$  and  $\tan \alpha_n = .42$ .

Figure 3 shows the observed solute concentration (c) profile along the length of the column (x). The observed solute concentration were transformed to the normalized solute concentration  $\bar{c}$  and plotted against the penetrated depth of the solute front ( $\lambda$ ) for a simulation time of 40 minutes, as shown in Figure 4. The predicted solute concentration profile along the length of the column, using the analytical solution, are used and plotted on the same figure as a solid line. As shown in the figure there is a good agreement between the observed experimental values and the predicted values. Hence, the demonstrated analytical method can be used to correctly simulate horizontal transport of non-reactive contaminant through initially dry soils.

#### 4. Conclusion

The horizontal transport of non-reactive solute through sandy clay soil has been demonstrated both analytically and experimentally. A quasi-analytical solution was used, under constant concentration boundary condition and constant dispersion coefficient, to predict solute concentration profile along the length of the column. The predicted solute concentration profile was compared with that obtained experimentally. Good agreement was found between the analytical predictions and experimental observations. Hence, the demonstrated analytical method is found adequate to simulate horizontal transport of non-reactive contaminant through initially dry soils.

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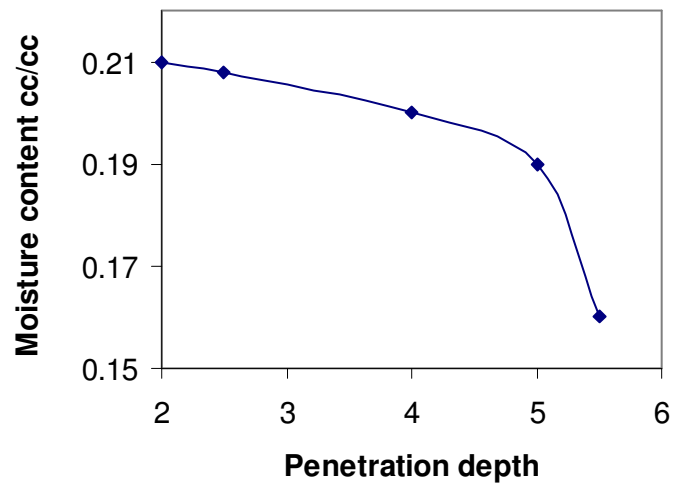
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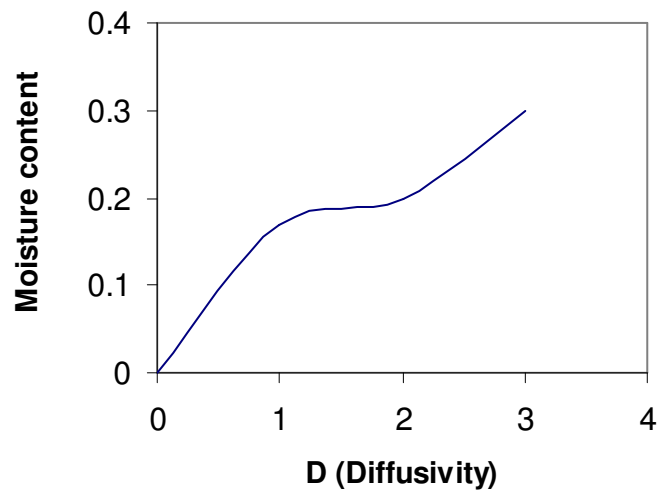
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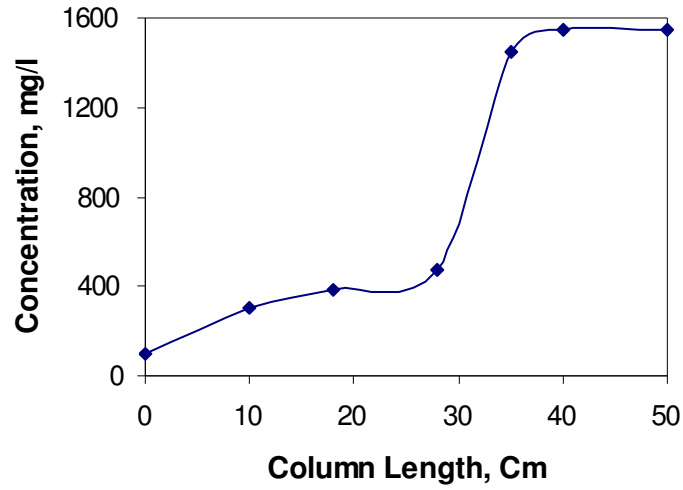




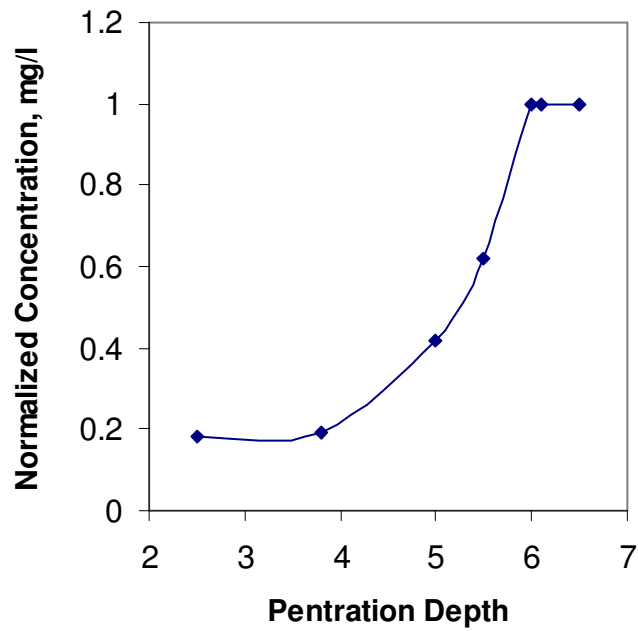
**Fig. 1 Relationship between the penetration depth and moisture content**



**Fig.2 Relationship between the diffusivity and moisture**



**Fig. 3 Observed solute concentration along the soil column**



**Fig. 4 Normalized solute concentration at a simulation time of 40 minutes**