Contaminant Water Movement in Unsaturated Soil : Some Recent Studies

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ABSTRACT

The movement of water and solutes through the unsaturated zone has been of importance in traditional applications of ground water hydrology. In recent years, the need to understand the behavior of hazardous waste and toxic chemicals in soil has resulted in renewed interest in this subject. One of the primary concerns is the dissolved contaminant in ground water. The search for an analytical solution and numerical analysis to model water flow and solute transport continues to be of both scientific and practical interest. In this paper the numerical approach to water and solute movement in the unsaturated zone is summarized briefly including the model used to incorporate the effect of infiltration-redistribution on solute mass development. In addition an experimental work had been carried out in the field to understand the physical behavior of the system and to identify the parameters controlling solute movement is presented too.

The results obtained from the numerical simulation has been checked against experimental data. The comparison between the numerical and experimental results indicate the consistency of the numerical analysis in accurately representing hydrodynamic dispersion during infiltration-redistribution processes.

KEYWORDS

Unsaturated; moisture content, contaminant, infiltration, non-reactive solute, dispersion coefficient.

INTRODUCTION

The movement of water and solutes through the unsaturated zone has been of importance in traditional applications of groundwater hydrology, soil physics and agronomy. In recent years, the need to understand the behavior of hazardous waste and toxic chemicals in soils has resulted in a renewed interest in this subject. One of the primary concerns is that dissolved contaminant may migrate through the unsaturated zone, reach the saturated zone, and contaminate the ground water. The search for a numerical analysis to model water flow and solute transport continues to be of both scientific and practical interest. Typically, water flow and solute transport in unsaturated soils result in transient phenomena, making it a challenging problem. The nature of soil hydraulic conductivity properties like diffusivity and hydraulic conductivity renders the governing flow equation. The transport of soluble salts and pollutants in porous media, as a particular case of hydrodynamic dispersion phenomena, has been the subject of much research for more than forty years. Interest in this field has been from a wide range of disciplines: including petroleum engineers concerned with separation and transport of petroleum products, geophysicists concerned with mineral extraction; groundwater engineers concerned with water quality; chemists and public health engineers concerned with disposal of chemical, industrial, sanitary and radioactive wastes; and agriculturists concerned with managing soil-plant growth through salinity control as well as controlling the effective use of fertilizers and pesticides. Earlier research efforts were directed towards solute movement in saturated steady state flow fields. It is only recent years that attention has been focused on the more complex case where the soil is unsaturated and subject to unsteady state flow conditions. The unsaturated zone is the medium through which soluble salts and pollutants which originate at or near the soil surface are conveyed to the groundwater system. In this zone, the transport of solutes is subject to a complex system with several interrelated physical processes including: molecular diffusion, mechanical dispersion, ion exchange and anion exclusion or absorption and oxidation-reduction. Various theoretical models have been developed over the years to describe chemical transport in soils. The success of these models depends to a large degree on our ability to quantify the transport parameters that enter into the models. Important parameters are the fluid flux, the dispersion coefficient, and the adsorption or exchange coefficients in the case of interactions between the chemical and the solid phase.

NUMERICAL ANALYSIS OF WATER MOVEMENT

Mathematically the convection-diffusion equation is a second order parabolic partial differential equation. This is a particularly difficult equation to solve numerically because its character varies from being parabolic to virtually hyperbolic, depending upon the ratio of convection to dispersion. The most common approaches to solve this equation numerically have used finite difference approximations (Chaudhari 1971, Davidson et. al. 1975a). Reviews and comparisons of those methods to solve the convection-diffusion equation have been given by Chatwal et al. 1973; Gray and Pinder, 1976; Lam, 1977; Ehlig, 1977; Van Genuchten, 1977; Mercer and Faust, 1977; and Smith, 1977. These reviews showed that although most numerical methods were satisfactory when the flow was dominated by dispersion, they all demonstrated unstable characteristics when convection was the dominant mechanism. These instabilities are characterized by oscillations, overshooting and negative concentrations in the vicinity of the sharp solute front, and by numerical dispersion (smearing) of the front. Significantly, neither higher order integration schemes in time (Smith 1977) nor higher order finite element schemes (Van Genuchten 1977) eliminate oscillations or overshooting in convection dominated dispersion problems.

Methods which use central difference approximations for the convection terms result in oscillations, and Price et al. (1966) showed that this behavior could be removed only by using small spatial increments. If upstream difference approximations were used, no oscillation was evident, but large truncation errors were introduced which acted as an artificial dispersion term. Lantz (1971) showed that reducing this smearing to acceptable levels usually required an impractically small grid. Many improvements have been suggested, such as: transfer of overshoot (Peaceman and Rechford, 1962), two point upstream approximations (Price et al., 1966) and truncation error cancellation (Chaudhari, 1971; Laumbach, 1975) but none of these is entirely satisfactory for general usage.

Gray and Pinder (1976) examined the behavior of common finite difference and finite element schemes using a similar approach to that used by Stone and Brian (1963) to determine their relative merits in terms of overshooting and frontal smearing. The general solution to the dispersion equation was represented by the Fourier series, and the analytically and numerically determined amplitude and rate of propagation of the Fourier components. They found that the overshooting of the concentration pulse resulted from the failure of the numerical schemes to propagate the small wavelengths, which are significant in describing the solute front. The frontal smearing resulted from the dissipation of these small wavelengths. They concluded that the finite element methods were consistently better than the finite difference methods on both counts.

Pandy,S.; Huyakorn, P.S.; Therrien, R. and Nicholos, R.L. (1993) developed a three dimensional Galerkin finite element model to simulate the saturated-unsaturated groundwater flow and contaminant transport in highly heterogeneous porous media. They overcame the challenge encountered in solving such complex problems. To do so they employed the upstream-weighting residual procedure. The model treated the highly nonlinear flow problems by using chord-slope Newton-Raphson linearization and upstream weighing of the relative permeabilities. For computational time savings the model uses the less robust Picard scheme. And to overcome convergence difficulties in solving the nonlinear equation, they used the under-relaxation formulas. They used hexahedral, orthogonal, curvilinear elements which accurately and efficiently discretize domains with irregular formation. Finer mesh was used in regions of high gradients. Influence coefficient formulas were used to generate element matrices in an effort to avoid costly numerical integration. To increase the accuracy of the solution, or enhance computational speed and storage requirements a 7-, 11-, and 17 point lattice connectivity structure was employed. They used the model for assessment of moisture movement and contaminant migration from a shallow waste-disposal site above a multilayer unconfined aquifer system.

Xiang, J. and Elsworth, D. (1992) developed two methods using finite element to identify the spatial distribution of parameters of contaminant transport in a two-dimensional potential groundwater flow system. The velocity and transmissivity distribution was determined by inverting the groundwater flow equation. The computed Darcyian velocity components were used to estimate aquifer dispersivities. An integration based method was employed and found to perform well in both noise free and relatively high noise level environments. Additional parameters of dispersivity and velocity components were evaluated for the cases where the head distribution is not available using equations based on the dispersivity variation with position.

Ewing, R.E. and Lin, T. (1991) developed less time-consuming methods which can be used to solve some parameter estimation inverse problems of fluid flow in porous media without iteratively solving the related forward problems many times. Hyperbolic perturbation was used to enforce stability during the estimation of spatially-dependent parameters. The temporally-dependent parameters were computed via a nonclassical partial differential equation. Finally, they conducted several numerical experiments in an effort to show the stability, convergence, and dependence of the solution upon the error in the data. Weber, W. J. , McGinley, P.M. and Kartz, L.E. (1991) presented a review which covers current levels of understanding of the reactions and processes comprising sorption phenomena, and the forms and utilities of different models used to describe them. They placed an emphasis on concept development on the translation of these concepts and models into functional models for characterizing sorption rates and equilibria, as well as the application of these concepts and models for explaining contaminant behavior in subsurface systems.

THEORETICAL BACKGROUND

One dimensional vertical water movement in a rigid, homogeneous porous material may be described by equation

$$C_s(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[k(h)\frac{\partial h}{\partial z} \right] + \frac{\partial k(h)}{\partial z} \tag{1}$$

Where	h	soil water potential (expressed on a weight basis) relative to atmospheric pressure	L
	k(h)	hydraulic conductivity	LT
	t	time	T
	z	vertical ordinate, positive upwards	L
	$C_s(h)$	specific water capacity,	L^{-1}
	θ	volumetric water content	$L^3 L^{-3}$

Eq.(1) is a convenient form of the unsaturated flow equation and has been used in solving a wide range of problems involving the hydrology of the unsaturated zone. A computer based numerical solution of eq.(1) was developed using an implicit finite difference forward method to solve the governing equation This computer program has been continually updated by research students and staff of the Hydrology and Water Resources management Department, KAAU, Jeddah. The program is able to handle all types of constant and time dependent boundary conditions, material variations including spatial heterogeneity, and intermittency in the application of water. The program has also been extended for this report to allow the study of horizontal flow systems. For the latter development, eq.(1) was modified to remove the gravity flow component, giving

$$C_s(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[k(h)\frac{\partial h}{\partial z} \right] \tag{2}$$

So that essentially the same computer program could be used in solving eq.(1) and (2), the sign convention has not been changed.

APPLICATION OF THE WATER FLOW MODEL

As indicated earlier the computer program based on the implicit finite difference model outlined above has been successfully applied to a wide range of unsaturated one dimensional flow problems. The applications involve various boundary conditions including surface ponding (or constant concentration), steady and time dependent precipitation at the soil surface, redistribution and drainage, a stationary or moving water table and controlled flux from the profile. Other systems studied include scale heterogeneous media, intermittent surface involving soil hysteresis, air compression effects in bounded profiles and stratified profiles. The model has also been linked with a steady state drainage equation to analyze tile drainage system.

RELATIONSHIP BETWEEN WATER FLOW AND SOLUTE FLOW MODEL

The soil water program package provides all the external controls for the simulation (such as the maximum rate of progression of the solution, specification of initial and boundary conditions, flow direction, and all data input and output). Additionally, it provides the necessary data on soil water content and flux distributions at each time step as input for the solute movement analyses described in the next chapter.

NUMERICAL ANALYSIS OF NONREACTIVE SOLUTE MOVEMENT

Introduction

The differential equation describing solute under isothermal, unsteady state in one dimension in unsaturated porous media is written as

$$\frac{\partial(c\theta)}{\partial t} = \frac{\partial}{\partial z}(D_e(\theta,\nu)\frac{\partial c}{\partial z} - \frac{\partial(qc)}{\partial z} \qquad (3)$$

where

c	solute concentration of the soil solution
$D_e(\theta,v)$	combined dispersion coefficient (diffusion plus mechanical dispersion)
D_p	molecular dispersion coefficient
β	dispersive length
q	volumetric (Darcy) flux of water
v	pore water velocity q/θ

The combined hydrodynamic coefficient D has been taken with the molecular diffusion component as constant value. Thus

$$D_e(\theta,\nu) = D_p + \beta|\nu| \qquad (4)$$

In the above equation the solute is assumed to be nonreactive and sufficiently dilute so that density changes can be neglected. Other workers (e.g. Davidson et.al 1975) use a different form of equation 4 where D_e is replaced by θD_e. The chosen definition is particularly useful when comparing the numerical model performance with the analytical solution.

FIELD STUDY

Introduction

As mentioned before, the treated effluent from KAAU treatment plant will be used in field contaminant transport studies. Hence, it is important to have adequate knowledge on both the treatment plant and the influent wastewater to the plant. In this chapter of the report the collected data on the layout and performance of the treatment plant and the composition of the influent wastewater will be presented. In addition, all available geological and hydrological information related to the selected site will be presented.

Site investigation and instrumentation

Site investigation

An extensive field program supplemented by laboratory analyses was implemented in order to collect the information needed as a prerequisite for determining solute transport in unsaturated soil. Field and laboratory studies implemented in the site and consisted of equipment installation, soil sampling and effluent application experiment. The site has been instrumented by TDR equipment for measuring the moisture content, pressure transducer for measuring the pressure head and lysimeter suction for extracting the soil solution. Soil sampling was necessary to determine the physical and hydraulic properties of the soil profile.

Site Description and Characterization

The study site is comprised of two adjacent rooms. One is used as the instrumentation room (air conditioned) in which all monitoring instrument, accessories and computer system are installed. The adjacent 5 x 7m area has been fenced and provided with an entry door and used as the irrigation site for actual field experiments. The appropriate electric power supply needed for the operation of the computer system and pilot plant system has been connected to the instrumentation room and the irrigation site. Also, a pipe line carrying treated wastewater has been diverted from the treatment plant terminal to the study site where it will be used as the solute bearing water for field experiments. The pilot plant system within the irrigation site comprises a 500 liter water storage tank, centrifugal pump, flow meter, water distribution system and control valves. The desired water application rate was controlled using a recycle system and a control valve. An application area of about 20 m^2 has been used for controlled application of the influent water. Ten irrigation lines, each having eight emitters were connected to a header pipe that was connected to the bottom of the influent storage basin. A control valve and a flow meter were installed at the end of the header pipe to control water application rate. The influent water was applied continuously to provide an average surface flux of 2.89 cm/day. On the northern side of the irrigation are a 500 cm long by 150 cm wide strip that has been excavated to a depth of 400 cm for sampling and monitoring of the application area during solute transport experiments, as it provides horizontal access to the application area. The detailed layout of equipment installation and sampling location on the ditch face is shown in Fig.1. The water application is carried out through a system consisting of a water storage tank discharging flow through a flowmeter and regulated through valves and connected to a plastic pipe network with a diameter of 1/4 inch which is assembled as shown in Fig.2.

SOLUTE MOVEMENT DURING VERTICAL INFILTRATION

Introduction

The need to safely dispose of hazardous waste and the increased demand on our groundwater resources require the use of numerical models to forecast the potential migration and fate of contaminants introduced into the subsurface. The complexity of the soil system and its hydrologic, geochemical and biological interactions, make accurate and reliable predictions of field scale of contaminant migration difficult. The complexity of the processes controlling subsurface flow and transport is no where more evident than in the unsaturated zone.

The experiment consisted of a flux application of water with several tracers on an irrigated strip of initially dry soil. Water and solute movements were monitored in the subsurface using TDR equipment, solution sampler and by destructive soil sampling. In the course of this research efforts were made to establish a bilateral relation between the moisture content and dielectric constant as well as between pressure head and transducer signal.

The numerical model for non-reactive solute transport as presented in chapter three has been subjected to a comprehensive testing program using experimental and quasi-analytical results as mentioned in the original objectives of the research proposal. This chapter extends the study to vertical flow systems involving both infiltration and redistribution processes.

INFILTRATION- REDISTRIBUTION FIELD EXPERIMENT

A water flow and solute experiment was performed as part of a comprehensive field trench study located on King Abdulaziz University Campus to test the numerical model of vadose zone flow and transport. The study area was drip irrigated with water containing a chloride tracer. The advance of the water front during the two irrigation episodes was measured with pressure transducer and TDR equipments. Solute front positions were determined from soil solution sampling through suction samplers.

The experiment was conducted using a constant flux containing an initial concentration of KCL 100 meq/l with a uniform initial water content of approximately 0.1 cc/cc. A dilute KCL solution of concentration 100 meq/l was supplied at the surface at a constant rate of 0.063 cm/min for 60 min. Fig.3 shows the resultant experimental water constant profile at the end of the infiltration period and Fig.4 the normalized salt concentration profile. In both

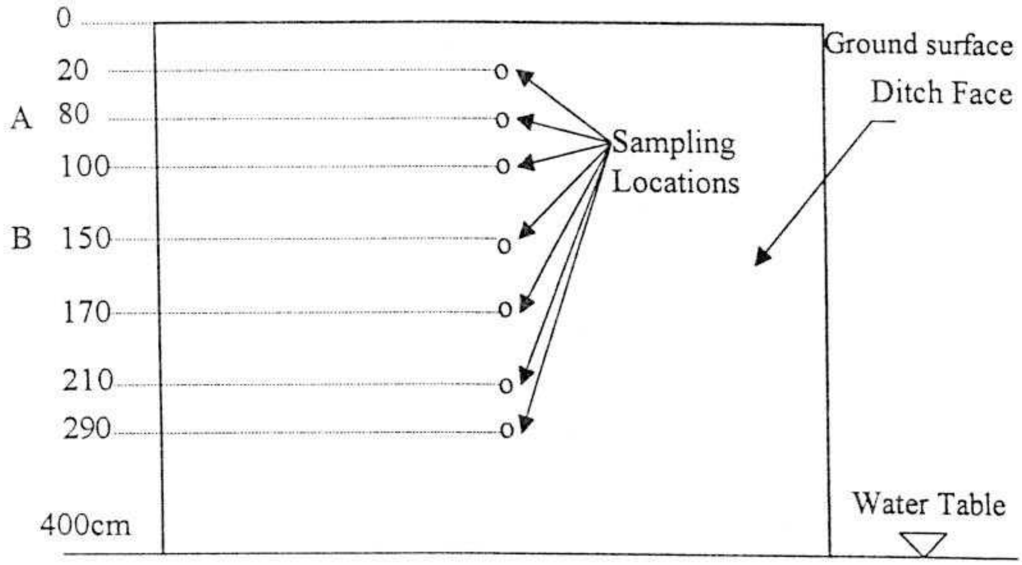

Fig. 1 Soil Sampling Location

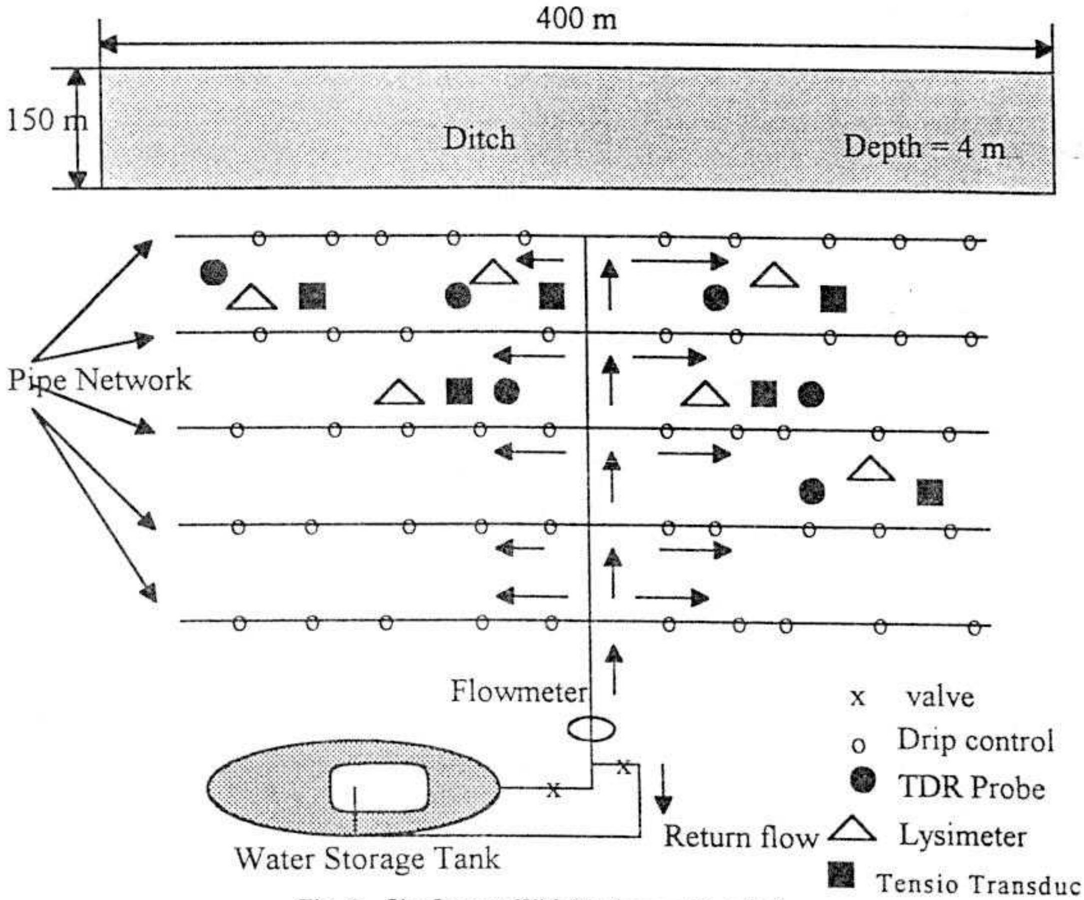

Fig. 2 Site Layout With Equipment Instulation

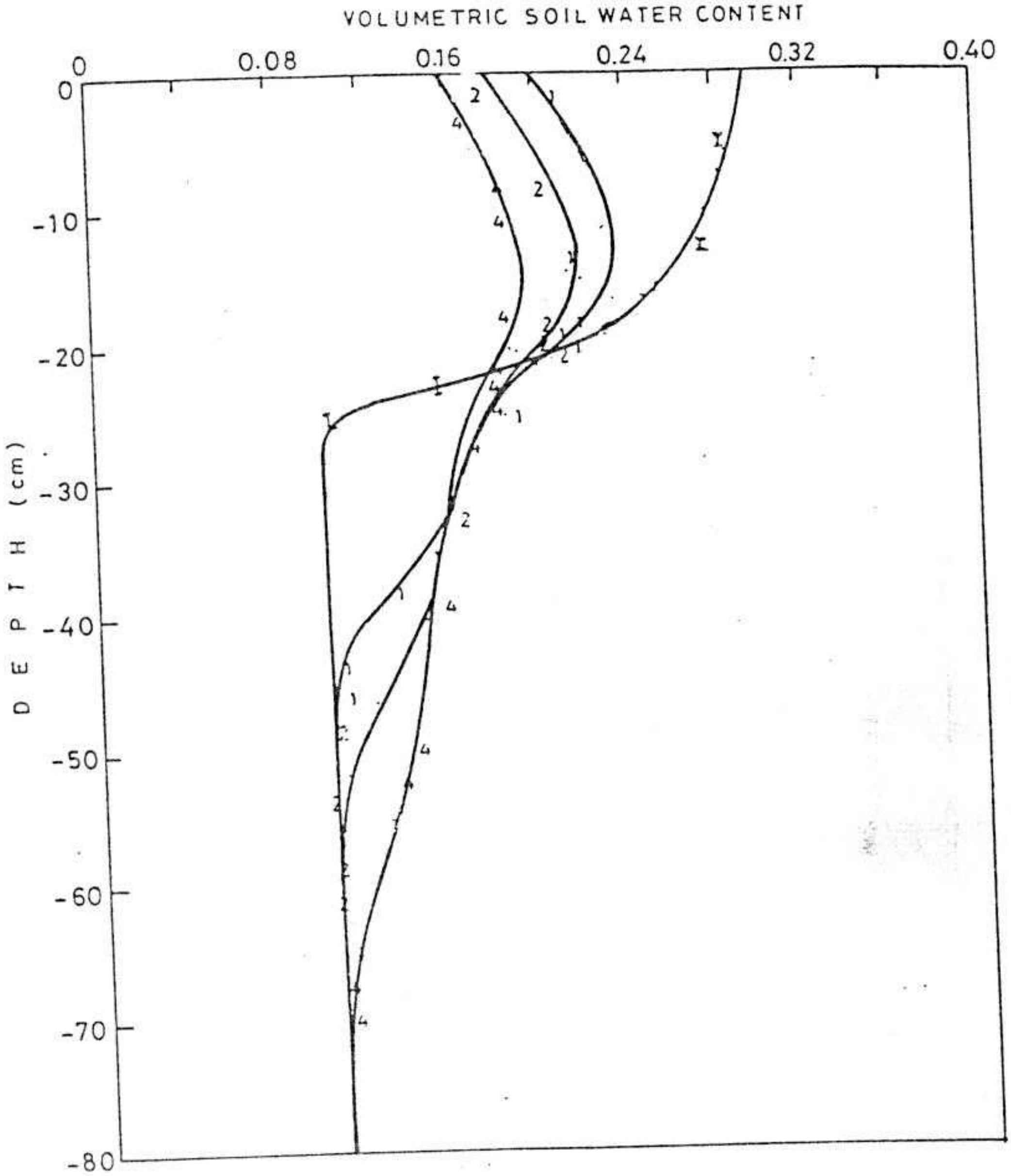

Fig. 3. Experimental and numerical θ (z) profiles for constant flux vertical infiltration followed by redistribution (symbols are defined in the text)

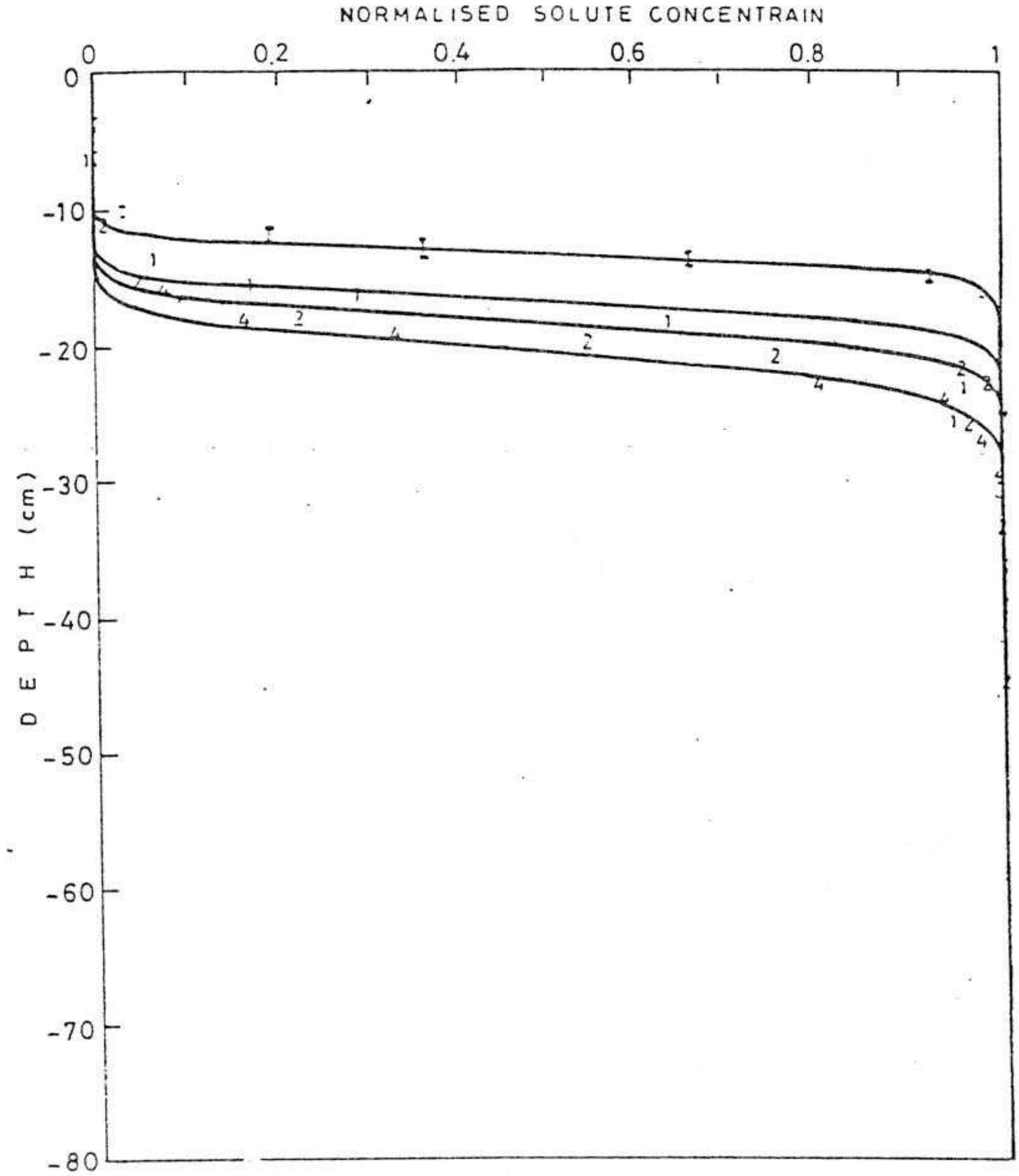

Fig. 4. Experimental and numerical $\overline{c}(z)$ profiles for constant flux vertical infiltration followed by redistribution (symbols are defined in the text)

figures the continuous lines represent the results of the numerical analysis and the points denoted "i" represent the experimental data.

COMPARISON BETWEEN NUMERICAL ANALYSIS AND EXPERIMENTAL DATA DURING VERTICAL REDISTRIBUTION

Computer models are increasingly used to properly understand fluid flow and water transport through unsaturated soils. Before such models can be used for prediction purposes, they need to be validated with field data. A critical component of the field validation is the availability of high quality data from carefully controlled field experiments.

The experiment described earlier was extended to study the disposition of solute during the redistribution phase. The experimentally determined water content and solute concentration profiles for three redistribution times are shown in Fig.4. and 5. The experimental data is represented by numerals, with "1" representing 100 min, "2" representing 200 min, and "4" representing 400 min of redistribution respectively.

The corresponding solute profiles during redistribution are also shown in Fig.5. Although the paucity of experimental data does not allow any definitive statements to be made concerning solute distribution, there is general consistency. The comparisons for the redistribution times of 100 min and 200 min are more variable than 400 min; however discrepancies are consistent with the variation in the water content profiles at these intermediate times. The numerical model has been programmed to provide additional data on the transport processes involved. Fig.6 gives the solute mass profile for infiltration-distribution corresponding to the end of infiltration, and to 100 min, 200 min and 400 min redistribution. This figure is most instructive in indicating salt disposition within the profile. Fig.7 provides the h(z) relationship and is included for completeness. It can be concluded that the overall consistency between the numerical and experimental results is good, indicating that the numerical approach may be used with confidence in redistribution studies.

The 60 min profile of Fig.5 shows that during the first infiltration period, a bell shaped distribution is formed with a peak 250 meq/ l at a depth of approximately 15 cm. During the first redistribution period the mass peak is reduced to 200 meq /l at a depth in the vicinity of 20 cm with a distinctly skewed distribution becoming evident. By varying the length of the redistribution period relative to the infiltration period the rate of movement of the peaks down the profile can be regulated.

In the sphere of field management, it would appear that under appropriate conditions relating to soil type and depth to water table an intermittent leaching regime could be used both to control the movement from a pool sensitive area without necessarily purging it through to the groundwater system.

CONCLUSION

The comparison given indicates that the approximate analytical solute yields excellent prediction of solute concentration profiles for vertical infiltration. When the hydrodynamic

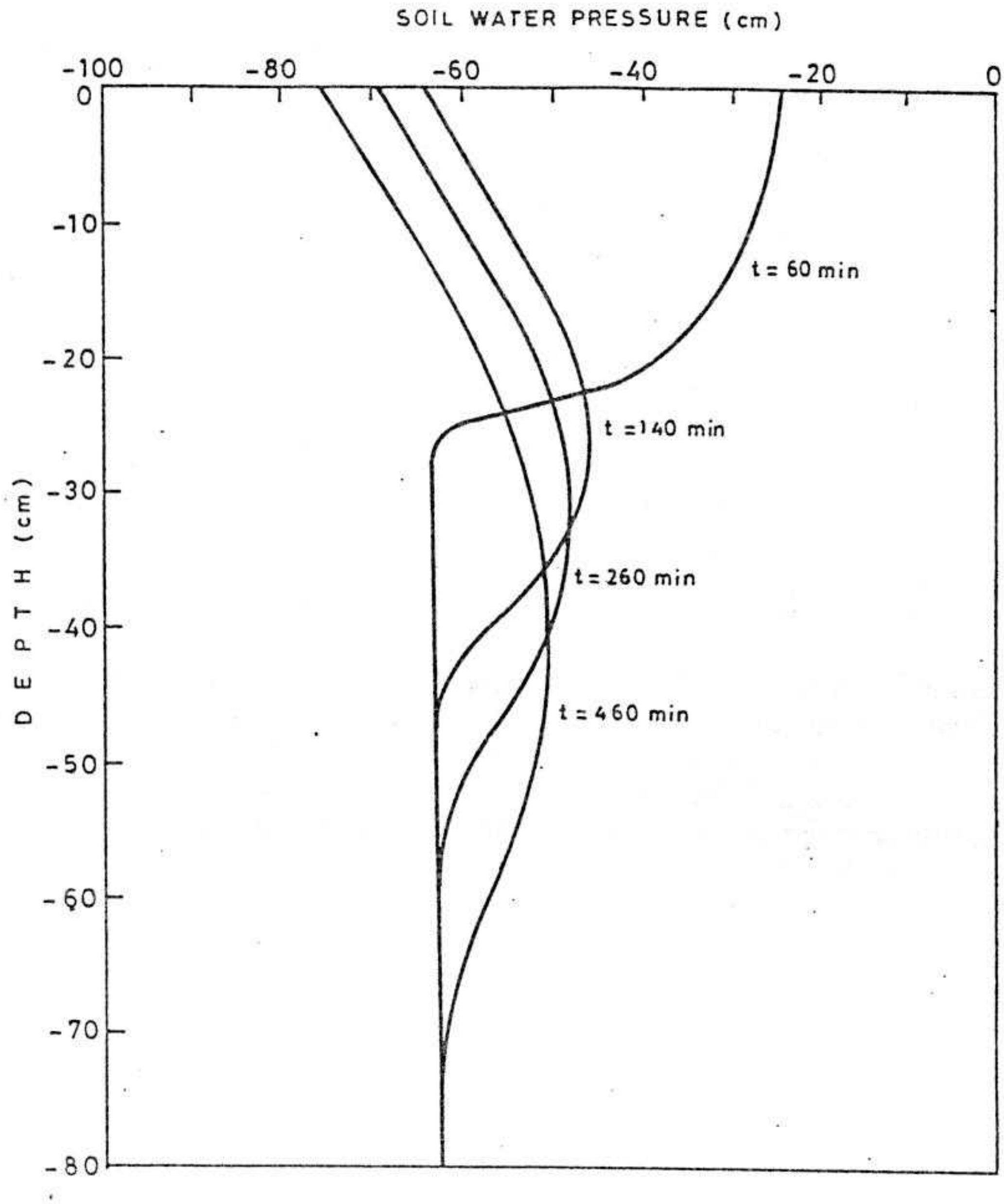

Fig. 5. Numerical h(z) profiles constant flux vertical infiltration followed by redistribution

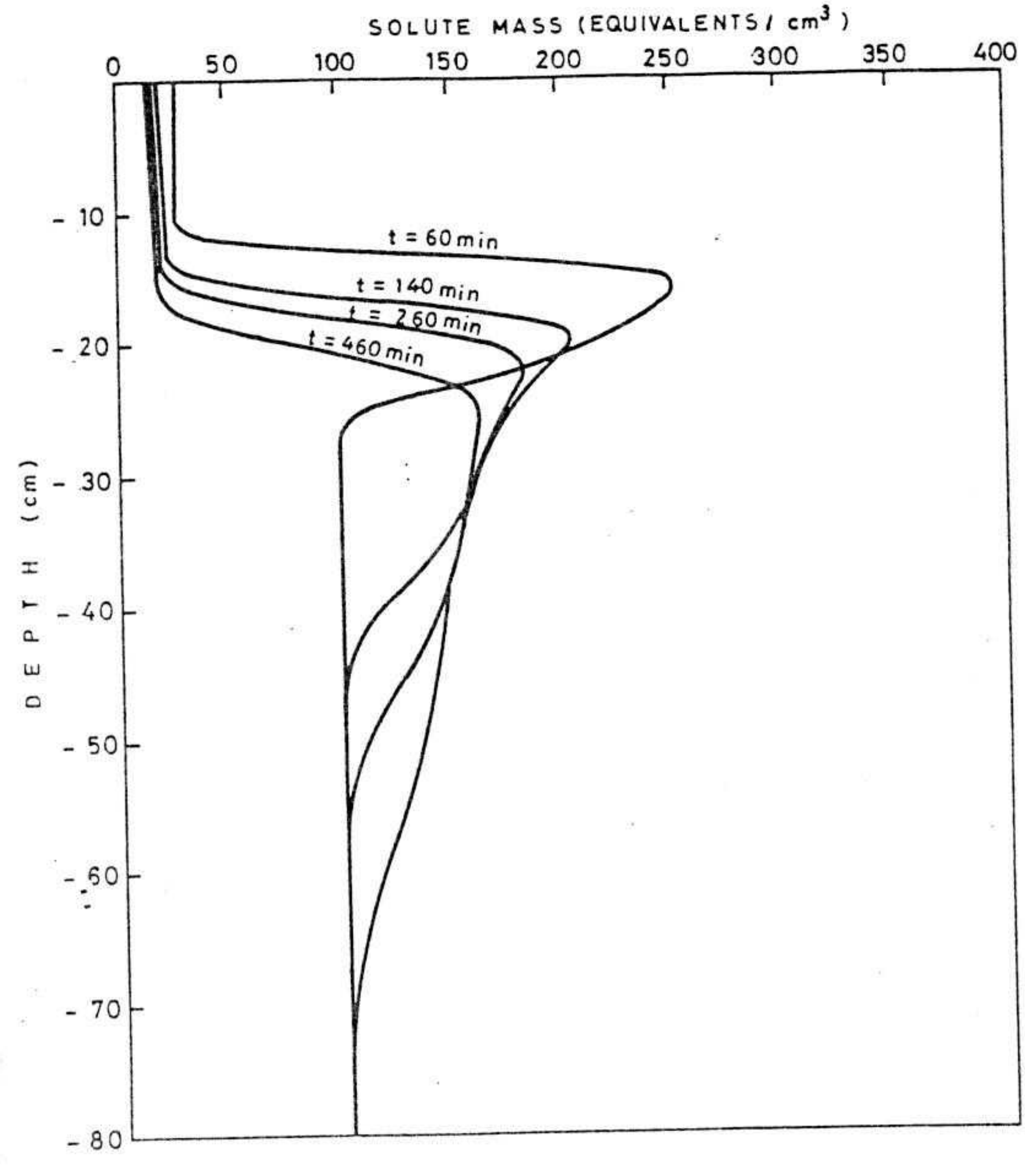

Fig. 6. Numerical solute mass profiles for constant flux vertical infiltration followed by redistribution

dispersion coefficient is velocity independent, it appears that the analytical solution could prove very useful as a predictive tool in solute movement studies. In addition the comparisons between the numerical predictions and experimental results indicate the consistency of numerical analysis in accurately representing hydrodynamic dispersion during infiltration-redistribution. However, the specification of the velocity independent of dispersion coefficient represent the experimental data satisfactorily with the normalized concentration as function of depth and time.

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