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MODELLING OF LEACHATE MIGRATION UNDER UNSATURATED-SATURATED CONDITION

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by

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ABSTRACT

A mathematical model to predict the migration of leachate from ground surface through surface soil to the groundwater table and then along with the regional groundwater flow is developed. The model couples the groundwater flow and solute transport equations in a two-dimensional, unsteady, integrated unsaturated-saturated porous media. The finite difference approximation is used to solve simultaneously the partial differential equations describing the groundwater flow and solute transport processes. The transport mechanisms considered in the model are advection, hydrodynamic dispersion, sorption, and degradation.

Validity of the model is tested by comparing its results to those obtained from existing numerical and analytical solutions.

A hypothetical problem of leachate migration from a surface impoundment in a vertical cross-section of an unconfined aquifer is solved to illustrate the applicability of the model.

1 INTRODUCTION

1.1 Groundwater Pollution

Recently, solute transport phenomena in soils and aquifers and their modeling have become of great interest in groundwater studies. Originally, the application of the solute transport theory was directed mainly towards the reclamation of saline soils (VAN DER MOLLEN anda VAN OMMEN, 1988). Later, as the pollution to the groundwater increases, while the role pf the groundwater in human life become vital, more attention is being given to the other sources of groundwater pollution pollution.

Groundwater pollution refers to the situation where the concentration of the solute, or contaminant, in the groundwater environment attains levels that are considered to be objectible (FREEZE and CHERRY, 1979). Groundwater pollution occurs in a number of ways either of natural origin or due to industrial or domestic activities. Chlorides, stemming from recent or former marine transgressions, boron, natural soda or nitrate, sulphates generated by the oxidation of natural pyrates with a high slenites anda selenates derived from shales containing pyrates with a high slenite content are among the natural pollutants. The vast growth in industrial activities nowadays has also affected the quality of groundwater. Polluted rivers due to industrial wated, liquid and solid disposal sites, and tailings from mining operations are recognized as causes of groundwater pollution. The intensive agriculture also contributes to the degradation of the groundwater quality. The extensive use of pesticides, herbicides, and fertilizers does help in increasing the crop productions but, on the other hand, causes groundwater pollution.

The disposal of refuse waste from industrial or domestic activities is commonly done by landfilling or dumping since it is the least expensive management option. The buride or dumped waste subject to leaching by percolating water derived from precipitation. The liquid derived from this process is known as leachate (FREEZE and CHERRY, 1979). This leachate may go further to the groundwater environment through the unsaturated surface soil by seepage water. Understanding these phenomena, it is clear that major sources of groundwater pollution originate from the ground surface which eventually percolate through unsaturated surface soil before reaching and spreading further to the groundwater environment.

During the migration, leachate, or solute in general term, suffers many attenuation effects. tHe transport mechanisms involved are advection, hydrodynamic dispersion, sorption and degradation. Since the leachate migration in soil matrix is governed by the flow velocity, mathematical model must detrmine the field velocity and corresponding the state of solute in the

Process of time and space. The distance that can be covered within a certain time depends on the velocity of flow and the persistence of solute. Since all of those processes are important in detecting the degree of pollution in the groundwater, it is essential to study the migration of leachate in an integrated unsaturated-saturated environment from its source in the ground surface to the groundwater flow system.

1.2 Objectives of the Study

The present study is a continuation of the previous study of a thesis undertaken by UPRETI (1987). Upreti's study dealt with modeling of one-dimesnional (vertical) solute transport from ground surface to the groundwater table through the unsaturated surface soil considering different transport mechanisms such as advection, dispersion, degradation and inter-phase mass transfer. In this study the solute transport in the unsaturated environment is analyze further by coupling it with the regional groundwater flow. Of particular concern is the coupled numerical finite difference solutions of an integrated unsaturated-saturated transient flow and solute transport in porous media.

The objective of the study is to develop a coupled unsaturated-saturated transport model to predict the migration of leachate from the ground surface through surface soil to the groundwater table and then along with the regional groundwater flow. A finite difference method is used to solve the partial differential equations governing groundwater flow and solute transport. In particular, the model developed is able to compute the following.

a) The time-dependent pressure head distributions in the vertical cross-section of unsaturated and saturated zones.
b) The time-dependet solute concentration distributions in the vertical cross-section of unsaturated and saturated zones.

1.3 Scope of Work

The scope of work of this study is as follows.

a) Developing an unsteady two-dimensional flow model representing water movement in unsaturated as well as saturated zones.
b) Developing a solute transport model representing leachate migration in a groundwater flow environment, from the ground surface to the ground water table and then along with the regional groundwater flow.
c) Applying the model developed to a hypothetical leachate migration problem.

2 LITERATURE REVIEW

2.1 Solute Transport and Groundwater Flow

Any solute transport model requires as an essential input the field velocity of flow (KINXELBACH, 1986). The flow field is either known a-priori or is modeled parallel to transport by a flow model, which is used in the present study. The flow model yields heads, from which specific flow-rates are calculated by means of the Darcy's law. The transport model requires pore velocities. These are obtained from specific flow-rates divided by effective porosity.

The transport mechanisms of solute in the unsaturated and saturated conditions are governed by the same natural processes, namely advection, dispersion, sorption and degradation. The major difference between unsaturated and aturated zones is that in the former the pores are partially filled with liquid and the rest filled with gas, whereas the pores are fully filled with liquid in the latter. There were studies dealt with the solute transport by different researchers. Some of them concerned with the transport mechanisms both in unsaturated or saturated condition. The transport processes in those studies were either all of the four processes or part of them. The present study is an integrated unsaturated-saturated solute transport using finite difference technique considering all of the transport mechanisms.

Previous studies relating to the solute transport problems in an unsaturated condition were ones conducted by BRESLER and HANKS (1969), WARRICK et al. (1971), BRESLER (1973), and WATSON (1987). For a saturated condition, there were studies of GUYMON (1970), GUYMEN et al. (1970), RUBIN and JAMES (1973), PICKENS and LENNOX (1976), GUPTA anda GREENKORN (1980), and LATINOPOULOS (1988). Studies considering both unsaturated and saturated conditions were ones with analytical solution (JINZHONG, 1988). The use of finite difference approximation was conducted by CHUNG (1987) but for vertical problem. There were limited number of studies in solute transport in integrated unsaturated and saturated flow conditions. Among these were one by KHALEEL and REDDELL (1985) using method of characteristics solution and by HUYAKORN et al. (1987) using semi-analytical solution.

Literatures pertaining to the present study are reviewed in the following sections.

2.2 Solute Transport in an Unsaturated Flow Condition

The main characteristic of unsaturated flow is the dependence of the hydraulic conductivity to the moisture content (and pressure head). It causes the non-linearity of the equation governing unsaturated flow. Thus the basic requirement of a solution of unsaturated flow is a known soil characteristics, that is the relationships between pressure head and moisture content, and hydraulic conductivity and moisture content, or hydraulic conductivity and pressure head.

2.2.1 Prediction of the unsaturated hydraulic conductivity

Closed-form analytical methods to predict the unsaturated hydarulic conductivity by the use of soil retention curve have been develeoped. Among them were ones proposed by BURDINE, CHILDS and COLLINS-GEORGE, MARSHALL, MILLINGTON and QUIRK, and BROOKS and COREY. JACKSON et al. (1965) compared the measured and calculated hydraulic conductivities of unsaturated soils for three different methods, that is ones proposed by Childs and Collis-George, by Marshall and by Millington and Quirk. They concluded that the latest method, when matched at the saturated value gave good results. On the other hand, GREEN and COREY (1971) found that the Marshall method gave the best results.

A simple analytical model was proposed by MUALEM (1976) for predicting the hydarulic conductivity of unsaturated soils by the use of the moisture content-capillary head curve and the measured value of the hydarulic conductivity at saturation. His relationship was similar to Child-and-Collins-George's. The method led to a simple integral equation for unsaturated hydraulic conductivity which enabled one to derived closed-form analytical expressions, provided suitable equation was proposed by VAN GENUCHTEN (1980). He found that four out of five soils with a wide range of hydraulic properties had good predicted unsaturated hydraulic conductivities using his equation. He also derived another closed-form equation based on Burdine's model.

A relatively complete test on various methods of predicting unsaturated hydarulic conductivity was conducted by ALEXANDER and SKAGGS (1987). A total of 14 methods were tested and their results were compared. It was found that the method proposed by McCuen et al. gave the best predictions (closest to the measuderd values), sepecially when the predicted value was matched with its corresponding measured value at saturation. They also found that for sandy soils substitution of the Ghosh's closed-form equation for soil moisture into the burdine's equation for hydraulic conductivity resulted in the best predictions for the unsaturated hydarulic conductivity (ALEXANDER an SKAGGS, 1987).

BROOKS and COREY (1964) developed a soil characteristic relationship based on observation from a large number of experimental data. Their relationship was well known and have been used by researchers. HUYAKORN et al. (1984, 1985, 1987) and RAO et al. (1989) used similar relationship in their studies.

In recent years attempts have been made to take into account the effect of soil water hysteresis in the analysis of the soil retention curve. WATSON (1987) incorporated this effect on the water and solute movement in the hysterisis model based on the Brooks and Corey equation for the relationship between soil water content and matric potential. The method requires a knowledge of a drying curve (boundary or primary) to predict the wetting boundary and all scanning curves. Using this method one can derive scanning curves from a single curve.

2.2.2 Unsaturated flow model

Due to its non-linearity, the partial differential equation governing unsaturated flow in porous media is not readily amenable to accurate analytical solutions. The finite difference technique has been extensively used instead.

HANKS and BOWERES (1962) developed a numerical computer-based solution for infiltration into a loam and a silt-loam soin in vertical upward and downward directions. Solutions were also obtained for horizontal infiltration into two soils. The method rquired, in addition to a knowledge of the initial and boundary conditions of the specific problem, a known realtions between moisture content and pressure head, and moisture content and moisture diffusivity. A high speed computer for computation was also needed.

BESLER and HANKS (1969) developed a numerical model for non-interacting salt flow simultaneously with water in unsaturated soil. Solutions were obtained for ilfiltration, redistribution and evaporation under different wetting and boundary conditions. The effect of diffusion on salt distribution was neglected in their study.

WARRICK et al. (1971) carried out a study on a simultaneous solute and water transfer for an unsaturated soil both in the field and numerically. Their study provided an examination of the influence of soil moisture on solute transfer during inflitration. They stated that solute movement was nearly independent of the initial moisture content but varied with the infiltration rate. Another method for analyzing simultaneous transfer of non-interacting solute and water in unsaturated soils was developed by BRESLER (1973). The solute transport equation considering diffusion and convection was solved numerically by an approach that eliminated the effect of numerical dispersion.

VAN GENUCHTEN and WIERENGA (1976) presented an analytical solution for the movement of chemicals through a sorbing porous medium with lateral or intra-aggregate diffusion. The phase in the porous medium was devided into mobile and immobile liquids.

HUYAKORN et al. (1984 and 1985) developed a solution to the solute transport in unsaturated, which they called varaibly saturated, porous media using finite element method. They used an influence coefficient scheme for element matrix evaluation and a mass balance computation scheme. Their solution was named SATURN model.

A study on water an solute movement in unsaturated zone incorporating the effect of soil water hyteresis was conducted by WATSON (1987). The partial differential equations representing the movement of water and solute in unsaturated porous media were solved numerically with the aid of a computer program. The method was then applied to several unsaturated flow regimes including intermittent recharge to an unconfined aquifer, the modelling of vertical water movement under moving water table conditions and the effect of hysteresis on intermittent leaching.

UPRETI (1987) developed a one-dimensional (vertical) solute transport model in unsaturated flow condition considering advection, dispersion, degradation and interphrase mass transfer. The partial differential equation govering flow and solute transport were solved numerically using finite difference technique.

2.3 Solute Transport in a Saturated Flow Condition

HARLEMAN and RUMER (1963) described a method to measure lateral dispersion in an isotropic porous medium. They presented the relation between longitudinal and lateral dispersions. A numerical solution for the solute transport in porous media considering dispersion was introduced by REDDELL and SUNADA in 1970. They used method of characteristic tos olve the convective-dispersive solute transport equation.

The finite element technique has been extensively used to solve solute transport equations in saturated porous media (GUYMON, 1970; GUYMON et al. 1970; RUBIN and JAMES, 1973; PICKENS and LENNOX, 1976). GUYMON (1970) presented an equivalent principle to the govering partial differential for one-dimensional diffusion-convection problem. His solution was applicable to a wide variety of baoundary conditions and was not dependentupon constant parameters of motion over the entire domain of interest. But the existence of sources or sinks was not considered. A more general solution compared to this one where a two-dimensional case was considered was also presented (GUYMON et al., 1970).

Besides the variational principle, the Galerkin technique has also been used (RUBIN and JAMES, 1973; PICKENS and LENNOX, 1976). RUBIN and JAMES (1973) used Galerkin technique to solve equations describing dispersion and ion exchange affected one-dimensional transport of solutes in saturated porous media. PICKENS and LENNOX (1976) used Galerkin technique to formulate the problem of simulating a two-dimensional transient movement of conservative

Wastes in a steady state saturated groundwater flow system. The convection-dispersion equation was solved in two ways, in the conventional Cartesian coordinate system and in a transformed coordinate system equivalent to the orthogonal curvilinear coordinate system of streamlines and normals to those lines. The results of these two formulations were identical.

Numerical methods using finite difference approximation in solving dispersion equations were also used (SHAMIR and HARLEMAN, 1967; GUPTA and GREENKORN, 1973). SHAMIR and HARLEMAN (!967) presented a numerical method for the solution of dispersion equation in steady three-dimensional potential flow field in porous medium, in which the miscible fluids have the same density and viscosity. The numerical scheme was shown to be independent of the geometry of the flow field. GUPTA and GREENKORN (1973) formulated the equations for the dispersion and bilinear adsorption of various chemicals in porous media to calculate pollution movement.

LATINOPOULOS et al. (1988) presented a method of obtaining analytical solutions for chemicals transport in two-dimensional aquifers assuming a constant velocity field, linear adsorption and first-order decay. The solution was obtained by integrating the solution of a modified one-dimensional differential equation. VALOCCHI (1988) presented the theoretical analysis of deviations from local equilibrium during sorbing solute transport through idealized stratified aquifers.

2.4 Solute Transport in an Unsaturated-Saturated Flow Condition

GUVANASEN and VOLKER (1982) presented two analytical solutions for a problem of solute transport in a transient flow in unconfined aquifers. They considered a hypothetical unconfined aquifer with a strip of solute source, infinitely long and symmetrically placed in the middle of the aquifer. The major assumption used in their solution was that the rise of the free surface above the initial saturated depth was much smaller than the initial saturated depth. In their study the flow domain became a fully saturated flow after a certain transformation.

KHALEEL and REDDELL (1985) revised the method of characteristics (MOC) to solve convective-dispersion equations in a two-dimensional, integrated saturated-unsaturated porous medium. Instead of usual bilinear schemes, the revised procedure utilized a three-way linear interpolation scheme to assign seepage velocities to moving points in a two-dimensional grid system. The method was applied to a typical non-homogeneous two-dimensional drainage problem.

A model for the transient one-dimensional water movement in the saturated-unsaturated zone using a finite difference method with stochastic inputs was developed by CHUNG and AUSTIN (1987). They used an implicit finite difference scheme with the Douglas-Jones predictor-corrector method to solve the partial differential equation governing the one-dimensional saturated-unsaturated vertical flow. The effect of hysteresis in the soil water retention and hydraulic conductivity-versus-moisture content relationship was incorporated. Monte Carlo simulation, together with the nearest neighbor model, was used to incorporate the stochastic nature of hydraulic conductivity into the flow model. The model was applied to predict a long-term water-table fluctuation, and the results agreed well with the observed values.

HUYAKORN et al. (1987) developed a semi-analytical model to analyze leachate migration in unconfined aquifers. The model considered all the transport mechanisms, that is advection, dsipersion, adsorption and first-order decay. It consisted of three component, namely a simplified one-dimensional simulator describing steady-state vertical infiltration, a one-dimensional multilayered analytical solution describing vertical transport from the base of the land disposal unit to the water table and a three-dimensional analytical solution describing subsequent transport in a steady groundwater field. The results of the model were verified using those of SATURN model. SATURN model (HUYAKORN et al., 1984 and 1985) was a two-dimensional Galerkin finite element solute transport model having general flexibility but requiring much grater computational effort than the analytical model. They conclude that the simplified semi-analytical modeling approach was far more computationally efficient and easier to use than the numerical model.

JINZHONG (1988) conducted an empirical and numerical studies of solute transport in a two-dimensional saturated-unsaturated soil. The experiment conducted in a soil tank under infiltration and drainage conditions while Galerkin finite element model was designed to solve the transient movement of water and solute. The results given by the numerical model were then compared with the experimental data.

3 THEORITICAL CONSIDERATION

3.1 Groundwater Flow Equation

The present study dealt with flow in confined aquifers. The flow, both in the unsaturated and saturated zones, is an unsteady two-dimensional flow. The governing equation for flow was derived under the following assumptions.

a) Water is incompressible.
b) Viscosity and density of the water remain constant.
c) Temperature remains constant through out the medium.
d) The bed layer of the aquifer is horizontal.

3.1.1 Govering equation

The flow of water in porous media is governed by Darcy's law.

$$q = -K(h)\frac{\partial H}{\partial l} \qquad 3.1$$

Where,

q = volume water flux [LT^{-1}]

$K(h)$ = hydraulic conductivity of the medium, a function of capillary pressure h .[LT^{-1}]

$\frac{\partial H}{\partial l}$ = hydraulic gradient

Figure 3.2 shows an elemental control volume for flow through porous media. The law of conservation of mass for transient flow in a porous medium states that the net rate of fluid mass flow into any elemental control volume is equal to the time rate of change of fluid mass storage within the element. For unsaturated flow, the rate of change of fluid mass storage is due to change in density, aquifer compressiblity, and saturation. With reference to Fig. 3.1 the equation of continuity that translates this law into mathematical expression can be written as follows (FREEZE and CHERRY, 1979).

$$-\frac{\partial}{\partial x}(\rho q_x)-\frac{\partial}{\partial y}(\rho q_y)-\frac{\partial}{\partial z}(\rho q_z)=\frac{\partial}{\partial t}(\rho\phi S_w)$$

Where,

q_x, q_y, q_z = volumetric water flux in $-x, -y, and - z$- directions, respectively [LT^{-1}]

ρ = water density [ML^{-3}]

ϕ	= porosity
S_w	= water saturation
	= V_v / V_w
V_v, V_w	= columes of void and water, respectively [L^3]
x, y, z	= sapce coordinates [L]
t	= time [T]

Expanding the right-hand side of Eq. 3.2 yields

$$-\frac{\partial}{\partial x}(\rho q_x)-\frac{\partial}{\partial y}(\rho q_y)-\frac{\partial}{\partial z}(\rho q_z)=\phi S_w\frac{\partial \rho}{\partial t}+\rho\frac{\partial \phi}{\partial t}+\rho\phi\frac{\partial S_w}{\partial t} \qquad 3.3$$

For unsaturated flow, the first two terms on the right-hand side of Eq. 3.3 are much smaller than the third one. Discarding those two terms and introducing volumetric water content $\theta = \phi S_w$, one gets

$$-\frac{\partial}{\partial x}(\rho q_x)-\frac{\partial}{\partial y}(\rho q_y)-\frac{\partial}{\partial z}(\rho q_z)=\rho\frac{\partial \theta}{\partial t} \qquad 3.4$$

Substituting Darcy's law into Eq. 3.4 and applying it for constant density water yield

$$\frac{\partial}{\partial x}\left[K(h)\frac{\partial H}{\partial x}\right]+\frac{\partial}{\partial y}\left[K(h)\frac{\partial H}{\partial y}\right]+\frac{\partial}{\partial z}\left[K(h)\frac{\partial H}{\partial z}\right]=\frac{\partial \theta}{\partial h}\frac{\partial h}{\partial t} \qquad 3.5$$

For unsaturated porous media, changes in water content, θ, are accompanied by changes in pressure head, h, through the θ-h relationship displayed on the retention curve. The slope of this retention curve represents the unsaturated storage property of the media. It is called the specific water capacity, SC, and is defined as follows (FREEZE and CHERRY, 1979).

$$Sc=\frac{d\theta}{dh} \qquad 3.6$$

Substituting Eq. 3.6 into Eq. 3.5 yields

$$\frac{\partial}{\partial x}\left[K(h)\frac{\partial H}{\partial x}\right]+\frac{\partial}{\partial y}\left[K(h)\frac{\partial H}{\partial y}\right]+\frac{\partial}{\partial z}\left[K(h)\frac{\partial H}{\partial z}\right]=SC\frac{\partial h}{\partial t} \qquad 3.7$$

The two-dimensional form of Eq. 3.7 is

$$\frac{\partial}{\partial x}\left[K(h)\frac{\partial H}{\partial x}\right]+\frac{\partial}{\partial z}\left[K(h)\frac{\partial H}{\partial z}\right]=SC\frac{\partial h}{\partial t} \qquad 3.8$$

Expanding Eq. 3.8 to include both the unsaturated and saturated conditions and noting that the hydraulic head, H, is the sum of pressure head, h, and elevation, z, one obtains (JINZHONG, 1987)

$$\frac{\partial}{\partial x}\left[K(h)\frac{\partial H}{\partial x}\right]+\frac{\partial}{\partial z}\left[K(h)\frac{\partial H}{\partial z}\right]=\left[\beta S_s+SC(h)\right]\frac{\partial h}{\partial t} \qquad 3.9$$

Where S, is the specific storage of the medium, and z is measured positive downward. Eq. 3.9 is known as Richard's Equation for transient two dimensional flow in porous media. Introducing source and sink terms yields

$$\frac{\partial}{\partial x}\left[K(h)\frac{\partial H}{\partial x}\right]+\frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial H}{\partial z}-1\right)\right]+S=\left[\beta S_s+SC(h)\right]\frac{\partial h}{\partial t} \qquad 3.10$$

Where S[T^{-1}] is positive for source and is negative for sink. Eq. 3.10 is a general form of equation for flow in unsaturated and saturated porous media. Coefficient β serves as a flow parameter which is equal to 1 for saturated flow condition, and 0 otherwise. For saturated flow condition, in addition, the specific water capacity, SC, is zero and the hydraulic conductivity, $K(h)$, becomes the saturated hydraulic conductivity, K_s, which is independent of the prssure head.

Parameters to be detrmined for solving Eq. 3.10 are specific storage, S_s, porosity, ϕ, volumetric water content, θ , and hydraulic conductivity, K. They are normally to be determined by experimentation, either in the field or in the laboratory on field samples. In this study S_s and ϕ are taken from data available, whereas K and θ are detrmined according to the equations as explained in the following sections.

3.1.2 Estimates of flow parameters

A functional relation for the pressure head and moisture content that can be adopted in the groundwater flow equation was presented by RAO et al. (1989). The relationship was derived based on Brooks-and-Corey's experimentally determined discrete point data. Their equation took the form.

$$\begin{aligned}\theta &= \phi-\frac{h}{h_b}\theta_r && h_b\le h\le 0\\ &=\exp\left[\frac{h}{h_b}\ln(\phi-2\theta_r)\right]+\theta_r && h\le h_b\end{aligned} \qquad 3.11$$

Where h_b is the air entry pressure and θ_r is the residual moisture content. The other parameters are the same as previously defined.

Eq. 3.11 was used in a study of estimation of recharge and pollutant transfer conducted by KASHYAP et al. (1989). The equation relating the hydraulic conductivity and moisture content which was used in their study was also derived based on Brooks-and-Corey's equation. It took the form as follows.

$$K(\theta) = K_s\left(\frac{\theta-\theta_r}{\phi-\theta_r}\right)^4 \qquad \theta \geq \theta_r$$
$$= 0 \qquad \theta < \theta_r \qquad 3.12$$

The specific capacity could then be determined by differentiating Eq. 3.11. with respect to pressure head.

$$SC = \frac{d\theta}{dh} = \frac{\theta_r}{h_b} \qquad for \qquad h_b \leq h \geq 0$$
$$= \frac{1}{h_b}\ln(\phi - 2\theta_r)\exp\left[\ln(\phi-2\theta_r)\frac{h}{h_b}\right] \qquad for \qquad h \leq h_b \qquad 3.13$$

3.2 Solute Transport Equation

The equation governing solute transport in porous media were derived under the following assumptions.

a) Viscosity and density differences between two miscible fluids are neglible.

b) The disperive transport is governed by Fick's first law.

c) The sorption is according to linear isotherm.

3.2.1 Transport mechanisms

The transport mechanisms involved in leachate migration are advection, hydrodynamic dispersion, sorption, and degradation. They are discussed in the following sections.

a) Advection

A solute when injected into an aquifer travels with the same velocity as the liquid. Since the flow is laminar, the form of mass transport can be described by Darcy's law. Consequently.

$$M = qc \qquad 3.14$$

Where M is the mass of the solute transported per unit area per unit time [$ML^{-2}T^{-1}$] and C is concentration of the solute [ML^{-3}].

b) Hydrodynamic dispersion

As solute moves with the flow there is a tendency of the solute to spread out from the flow path expected to be followed. This phenomenon is called hydrodynamic dispersion. Due to the complex pore structure of the medium, the movement of a solute is characterized by numerous bifuractions, continual velocity variations and intricate deflection of flow. This causes some particles to move faster and some slower than the mean flow velocity; the result is a "S-shaped" distribution curve.

The rate of mass transport by dispersion is described by the Fick's first law.

$$M = -D\frac{\partial c}{\partial t} \quad 3.15$$

Where M is the mass transported per unit area per unit time [$ML^{-2}T^{-1}$], D is hydrodynamic dispersion coefficient [L^2T^{-1}] and dc/dl is concentration gradient. The hydrodynamic dispersion coefficient can be expressed as

$$D = D_d + \alpha(\phi\upsilon)^b \quad 3.16$$

Where D_d is molecular dispersion [L^2T^{-1}], α and b are dimensionless constants, ø is representative particle size of the medium [L] and υ is seepage flow velocity [LT^{-1}]. In general,molecular dispersion is a few orders of magnitude less than hydrodynamic dispersion coefficeint and thus can be neglected. A more convenient from Eq. 3.16 is given by

$$D = \alpha\upsilon^b \quad 3.17$$

In which α is intrinsic dispersivity of the medium [L] and b is dimensionless empirical constant. For simplicity and practical purposes b may be taken to be unity. Hence,

$$D = \alpha\upsilon \quad 3.18$$

c) <u>Sorption</u>

Often termed as interphrase mass transfer, sorption refers to the transfer of a solute between the solid and liquid phases and includes both absorption and adsorption. Sorption can be described in the functional form, called an isotherm, as

$$\frac{dS_c}{dt} = f(c, S_c) \quad 3.19$$

Where S_c is the concentration of the solute in the solid phase [ML^{-3}]. A linear form of the Freundlich isotherm was used in the present study.

$$S_c = K_d c \quad 3.20$$

Where K_d is sorption distribution coefficient.

d) <u>Degradation</u>

Degradation refers to the decay of a solute with respect to time. In a first-order degradation the rate of decay is proportional to the concentrate presents.

$$\frac{dc}{dt} = \lambda c \quad 3.21$$

Where λ is decay constant [T^{-1}]

3.2.2 Governing Equation

An elemental control volume for solute transport through porous media was considered as shown in Fig. 3.2. total mass inflow in $x-$direction considering advection and hydrodynamic dispersion is

$$I_x = q_x c(\Delta y \Delta z) + D_x\left(-\frac{\partial c}{\partial x}\right)(\theta \Delta y \Delta z) \qquad 3.22$$

Mass outflow in $x-$ direction is

$$\mathrm{O}_x = I_x + \frac{\partial I_x}{\partial x}\Delta x \qquad 3.23$$

Net mass flux in $x-$direction is obtained by subtracting Eq. 3.23 to Eq. 3.22.

$$\left[-\frac{\partial}{\partial x}(q_x c) + \frac{\partial}{\partial x}\left(\theta D_x \frac{\partial c}{\partial x}\right)\right]\Delta x \Delta y \Delta z \qquad 3.24$$

Similarly, for $y-and\, z-$direction.

$$\left[-\frac{\partial}{\partial y}(q_y c) + \frac{\partial}{\partial y}\left(\theta D_y \frac{\partial c}{\partial y}\right)\right]\Delta x \Delta y \Delta z \qquad 3.25$$

$$\left[-\frac{\partial}{\partial z}(q_z c) + \frac{\partial}{\partial z}\left(\theta D_z \frac{\partial c}{\partial z}\right)\right]\Delta x \Delta y \Delta z \qquad 3.26$$

The time rate of change of solute concentration within the emental control volume is

$$\frac{\partial}{\partial t}(\theta c)\Delta x \Delta y \Delta z \qquad 3.27$$

The law of conservation of mass states that the net rate of mass flux is equal to the time rate of change of solute concentration within the element. Hence, combining Eqs. 3.24, 3.26 and 3.27 results in

$$-\frac{\partial}{\partial x}(q_x c) + \frac{\partial}{\partial x}\left(\theta D_x \frac{\partial c}{\partial x}\right) - \frac{\partial}{\partial y}(q_y c) + \frac{\partial}{\partial y}\left(\theta D_y \frac{\partial c}{\partial y}\right) - \frac{\partial}{\partial z}(q_z c) + \frac{\partial}{\partial z}\left(\theta D_z \frac{\partial c}{\partial z}\right) = \frac{\partial}{\partial t}(\theta c) \qquad 3.28$$

Writing Eq. 3.28 in vectorial form, yields

$$-\vec{\nabla}(qc) + \vec{\nabla}\left(\theta \overline{D}\vec{\nabla} c\right) = \frac{\partial}{\partial t}(\theta c) \qquad 3.29$$

Recalling the effect of sorption that the solute may be adsorbed (or desorbed) by the matrix of grains, the total mass of solute within the elemental control volume is equal to $\theta c + (1-\phi)S_c$ is the mass of solute adsorbed per unit volume of solid. Whereas the rate of decay of the solute is proportional to the concentrate present according to Eq. 3.21. it is noted that the adsorbed solute mass also decays. Thus, including sorption and degradation effects, Eq. 3.29 becomes

$$\frac{\partial}{\partial t}\left[\theta c + (1-\phi)S_c\right] + \lambda\left[\theta c + (1-\phi)S_c\right] + \nabla\left(\vec{q}c\right) - \nabla\left(\theta\vec{D}\nabla c\right) = 0 \qquad 3.30$$

Substituting linear isotherm of Eq. 3.20 into Eq. 3.30 and introducing source or sink term yield

$$\frac{\partial}{\partial t}\left[\theta c + (1-\phi)K_d c\right] + \lambda\left[\theta c + (1-\phi)K_d c\right] + \nabla\left(\vec{q}c\right) - \nabla\left(\theta\vec{D}\nabla c\right) + c^* S = 0 \qquad 3.31$$

Where c^* is solute concentration in source or sink fluid [ML-3] and S is volume flow rate per unit volume of the source sink. Putting $R = 1 + (1-\phi)K_d/\theta$, which is known as retardation factor, and noting that $q/\theta = \upsilon$,

$$R\frac{\partial c}{\partial t} + \lambda Rc + \vec{\nabla}\left(\vec{\upsilon}c\right) - \vec{\nabla}\left(\bar{D}\vec{\nabla}c\right) + \frac{c^* S}{\theta} = 0 \qquad 3.32$$

Eq. 3.32 is the general form of equation of solute transport in unsaturated flow condition. For two-dimensional problem Eq. 3.32 could be written in the following tensorial form, considering the components of its coefficients.

$$R\frac{\partial c}{\partial t} + \lambda Rc + \frac{\partial}{\partial x_t}\left(\ \right) - \vec{\nabla}\left(\bar{D}\vec{\nabla}c\right) + \frac{c^* S}{\theta} = 0 \qquad 3.33$$

For the case of saturated flow condition θ = ϕ

The dispersion coefficient for any arbitrary coordinate alignment has tensor for as follows.

$$\bar{D} = \begin{bmatrix} D_{xx} & D_{xz} \\ D_{xx} & D_{zz} \end{bmatrix} \qquad 3.34$$

The calculation of the dispersion coefficient in Eq. 3.34 requires representative celocities between two adjacent cells. KINZELBACH (1986) presented equations to compute the dispersion coefficient as follows.

$$D_{xx} = \alpha_L \frac{u_x^2}{|u|} + \alpha T \frac{u_z^2}{|u|}$$

$$D_{xz} = (\alpha_L - \alpha_T)\frac{u_x u_z}{|u|}$$

3.35

Where,

$$u_x = \upsilon_{t.j}$$

$$u_x = \frac{1}{4}\left(\upsilon_{x_{i.j-1}} + \upsilon_{x\,i+1.j-1} + \upsilon_{z_{i.j}} + \upsilon_{z_{i+1.j}}\right)$$

$$|u| = \sqrt{\left(u_x^2 + u_x^2\right)}$$

And

$$D_{zz} = \alpha_T \frac{u_x^2}{|u|} + \alpha_L \frac{u_z^2}{|u|}$$

$$D_{zx} = (\alpha_L - \alpha_T)\frac{u_x u_z}{|u|}$$

3.36

Where,

$$u_x = \frac{1}{4}\left(\upsilon_{x_{i-1.j}} + \upsilon_{x_{\,i.j}} + \upsilon_{x_{i-1.j+1}} + \upsilon_{x_{i.j+1}}\right)$$

$$u_z = u_z$$

$$|u| = \sqrt{\left(u_x^2 + u_x^2\right)}$$

In which α_L dan α_T are lateral and transverse instrinsci dispersivities [L], respectively. If one of the coordinate axis is aligned with the velocity vector, $D_{xz} = D_{zx} = 0$.

4 MODEL FORMULATION

4.1 Groundwater Flow Model

A semi-implicit finite difference scheme was adopted to solve the flow governing aquation. A block-centered grid system, as illustrated in Fig. 4.1., was adopted in this study to discretized the modeled domain. Even though there are two cases of flow, that is unsaturated and saturated conditions, the model was developed such that it could be applied for both cases. For convenience, Eq. 3. 10 is rewritten with the source/sink term put on the right hand side (RHS).

$$\frac{\partial}{\partial x}\left[K(h)\frac{\partial h}{\partial z}+\right]+\frac{\partial}{\partial z}\left[K(h)\frac{\partial h}{\partial z}+1\right]=\left[\beta S_s+SC(h)\right]\frac{\partial h}{\partial t}-S \qquad 4.1$$

WHISLER and KLUTE (1965) used a modified Crank-Nicholson scheme to solve a one-dimensional groundwater flow. Using similar approach adopted in their study to solve Eq. 4.1, the space derivatives on the left hand side (LHS) are approximated by the finite differences as follows. (refer to Fig. 4.1).

$$\begin{aligned}\frac{\partial}{\partial x}\left[K_x\frac{\partial h}{\partial x}\right]=&\frac{1}{2\Delta x_t}\left[\frac{K_{x_{i+1/2.j}}{}^{n+1/2}}{\Delta x_{t+1/2}}\left(h_{t+1.j}{}^{n+1}+h_{t+1.j}{}^{n}-h_{t.j}{}^{n+1}-h_{t.j}{}^{n}\right)\right]\\&-\frac{1}{2\Delta x_t}\left[\frac{K_{x_{i-1/2.j}}{}^{n+1/2}}{\Delta x_{t-1/2}}\left(h_{t.j}{}^{n+1}+h_{t.j}{}^{n}-h_{t-1.j}{}^{n+1}-h_{t-1.j}{}^{n}\right)\right]\end{aligned} \qquad 4.2$$

$$\begin{aligned}\frac{\partial}{\partial z}\left[K_z\frac{\partial h}{\partial z}\right]=&\frac{1}{2\Delta z_j}\left[\frac{K_{z_{i.j+1/2}}{}^{n+1/2}}{\Delta z_{j+1/2}}\left(h_{t.j+1}{}^{n+1}+h_{t.j+1}{}^{n}-h_{t.j}{}^{n+1}-h_{t.j}{}^{n}\right)\right]\\&-\frac{1}{2\Delta z_j}\left[\frac{K_{z_{i.j-1/2}}{}^{n+1/2}}{\Delta z_{j-1/2}}\left(h_{t.j}{}^{n+1}+h_{t.j}{}^{n}-h_{t.j-1}{}^{n+1}-h_{t.j-1}{}^{n}\right)\right]\end{aligned} \qquad 4.3$$

$$\frac{\partial K_z}{\partial z}=\frac{1}{2\Delta z_j}\left[K_{z_{i.j+1/2}}{}^{n+1}+K_{z_{i.j+1/2}}{}^{n}-K_{z_{i.j-1/2}}{}^{n+1}-K_{z_{i.j-1/2}}{}^{n}\right] \qquad 4.4$$

Where,

$$K_{x_{i+1/2.j}}=\frac{\left(\Delta x_t+\Delta x_{t+1}\right)K_{x_{i.j}}K_{x_{i+1.j}}}{\Delta x_t K_{x_{i+1.j}}+\Delta x_{t+1}K_{x_{i.j}}}$$

$$K_{z_{i.j+1/2}}=\frac{\left(\Delta z_j+\Delta z_{j+1}\right)K_{z_{i.j}}K_{z_{i.j+1}}}{\Delta z_j K_{z_{i.j+1}}+\Delta z_{j+1}K_{z_{i.j}}}$$

All coefficient forming the FF coefficient on the RHS of Eq 4.6 are known either from previous time step or iteration. The set of Eq 4.6 forms a banded matrix having five coefficient in each row representing the cell being considered and its four surrounding cells. A standard matrix solver routine could then be utilized.

$$K_{x_{+1/2.j}}{}^{n+1/2} = \frac{1}{2}\left(K_{x_{i+1/2.j}}{}^{n} + K_{x_{i+1/2.j}}{}^{n+1}\right)$$

$$K_{z_{i.j+1/2}}{}^{n+1/2} = \frac{1}{2}\left(K_{z_{i.j+1/2}}{}^{n} + K_{z_{i.j+1/2}}{}^{n+1}\right)$$

$$\Delta x_{i+1/2} = \frac{1}{2}\left(\Delta x_i + \Delta x_{i+1}\right)$$

$$\Delta z_{j+1/2} = \frac{1}{2}\left(\Delta z_j + \Delta z_{j+1}\right)$$

Superscripts $n, n+1$ and $n+1/2$ indicate time levels at time $t, t+\Delta t$ and $t+1/2\Delta t$, respectively, where Δt is the time interval.

The time derivative on the RHS is expressed in the finite difference form at cell (i, j) as follows.

$$\left[\beta S_s + SC\right]\frac{\partial h}{\partial t} - S = \frac{1}{2}\left[2\beta S_{s_{t.j}} + SC_{t.j}{}^{n+1}\right]\left(\frac{h_{t.j}{}^{n+1} - h_{t.j}{}^{n}}{\Delta t}\right) - 2S_{t.j} \qquad 4.5$$

Summing up Eqs. IV.2, IV.3, and IV.4 and equating them to Eq. IV.5 for every cells form a set of algebraic equations of the form.

$$F1_{t.j}{}^{n+1} h_{t.j-1}{}^{n+1} + F2_{t-1.j}{}^{n+1} - \left[F3_{t.j}{}^{n+1} + \left(\beta S_{s_{i.j}}{}^{n+1} + SC_{t.j}{}^{n+1}\right)\right] h_{t.j}{}^{n+1} + F4_{t.j}{}^{n+1} h_{t+1.j}{}^{n+1}$$

$$+ F5_{t.j}{}^{n+1} h_{t.j+1}{}^{n+1} = -FF_{t.j} + \left(\frac{K_{z_{i.j+1/2}}{}^{n+1/2} - K_{z_{i.j-1/2}}{}^{n+1/2}}{\Delta z_j}\right) - 2S_{t.j}{}^{n+1} \qquad 4.6$$

Where,

$$F1_{t.j} = \frac{K_{z_{i.j-1/2}}}{\Delta z_j \Delta z_{j-1/2}} \qquad F2_{t.j} = \frac{K_{x_{i-1/2.j}}}{\Delta x \Delta x_{t-1/2}}$$

$$F4_{t.j} = \frac{K_{x_{i+1/2.j}}}{\Delta x \Delta x_{t+1/2}} \qquad F5_{t.j} = \frac{K_{z_{i.j+1/2}}}{\Delta z_j \Delta z_{j+1/2}}$$

$$F3_{t.j} = F1_{t.j} + F2_{t.j} + F4_{t.j} + F5_{t.j}$$

$$FF_{t.j} = \frac{\beta S_{s_{i.j}}{}^{n} + SC_{t.j}{}^{n}}{\Delta t} h_{t.j}{}^{n} + F3_{t.j}{}^{n}$$

All coefficients forming the FF coefficient on the RHS of Eq. IV.6 are known either from previous time step or iteration. The set of Eq. IV.6 form a banded matrix having five coeffients in each row representing the cell being considered and its four surrounding cells. A standard matrix solver routine could than be utilized.

4.2 Solute Transport Model

The finite difference form of solute transport equation could be obtained by formal replacement of derivatives by difference approximations on the grid or by taking solute mass balance over each cell of the grid (KINZELBACH, 1986). In the present study the latter was chosen together with the method proposed by LAUMBACH (1975) known as truncation cancellation procedure (TCP) method. The facilitate the use of these method, the Crank-Nicholson finite difference scheme was adopted tos olve the solute transport equation. The same block-centered grid system used in the groundwater flow model was adopted.

The two-dimensional form of Eq. III.36 might be written as follows.

$$-R\frac{\partial c}{\partial t}-\lambda Rc-\frac{\partial}{\partial x}(\upsilon_x c)-\frac{\partial}{\partial z}(\upsilon_z c)+\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial z}\left(D_{zz}\frac{\partial c}{\partial z}\right)+\frac{\partial}{\partial x}\left(D_{xz}\frac{\partial c}{\partial z}\right)+\frac{\partial}{\partial z}\left(D_{zx}\frac{\partial c}{\partial x}\right)-\frac{c^* S}{\theta}=0 \qquad 4.7$$

A typical grid system is shown in Fig.

$$-R\frac{\partial c}{\partial t}-\lambda Rc-\frac{\partial}{\partial x}(\upsilon_x c)-\frac{\partial}{\partial z}(\upsilon_z c)+\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial z}\left(D_{zz}\frac{\partial c}{\partial z}\right)+\frac{\partial}{\partial x}\left(D_{xz}\frac{\partial c}{\partial z}\right)+\frac{\partial}{\partial z}\left(D_{zx}\frac{\partial c}{\partial x}\right)-\frac{c^* S}{\theta}=0 \qquad 4.7$$

at cell (i,j) is explained in the following sections.

$$-R\frac{\partial c}{\partial t}-\lambda Rc-\frac{\partial}{\partial x}(\upsilon_x c)-\frac{\partial}{\partial z}(\upsilon_z c)+\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial z}\left(D_{zz}\frac{\partial c}{\partial z}\right)+\frac{\partial}{\partial x}\left(D_{xz}\frac{\partial c}{\partial z}\right)+\frac{\partial}{\partial z}\left(D_{zx}\frac{\partial c}{\partial x}\right)-\frac{c^* S}{\theta}=0 \qquad 4.7$$

a) The advection terms

Applying upwind difference method to the advection terms results in the following forms.

$$+\frac{\upsilon_{z_{i-1.j}}}{\Delta x_{t-1/2}}\left[\Gamma_1 c_{t-1.j}{}^{n+1}+(1-\Gamma_1)c_{t.j}{}^{n+1}\right]-\frac{\upsilon_{x_{i.j}}}{\Delta x_{t+1/2}}\left[\Gamma_2 c_{t.j}{}^{n+1}+(1-\Gamma_2)c_{t+1.j}{}^{n+1}\right]$$
$$+\frac{\upsilon_{z_{i.j-1}}}{\Delta z_{j-1/2}}\left[\Gamma_3 c_{t.j-1}{}^{n+1}+(1-\Gamma_3)c_{t.j}{}^{n+1}\right]-\frac{\upsilon_{z_{i.j}}}{\Delta z_{j+1/2}}\left[\Gamma_4 c_{t.j}{}^{n+1}+(1-\Gamma_4)c_{t.j+1}{}^{n+1}\right] \qquad 4.8$$

Where,

$$\Gamma_1=\left[1+1*sign\left(\upsilon_{x_{i-1.j}}\right)\right] \qquad \Gamma_2=\left[1+1*sign\left(\upsilon_{x_{i.j}}\right)\right]$$
$$\Gamma_3=\left[1+1*sign\left(\upsilon_{z_{i.j-1}}\right)\right] \qquad \Gamma_4=\left[1+1*sign\left(\upsilon_{z_{i.j}}\right)\right]$$

b) The hydrodynamic dispersion terms

$$+\frac{1}{\Delta x_t}\left[D_{xx_{i+1/2.j}}\left(\frac{c_{t+1.j}-c_{t.j}}{\Delta x_{t+1/2}}\right)\right]-D_{xx_{i-1/2.j}}\left(\frac{c_{t.j}-c_{t-1.j}}{\Delta x_{t-1/2}}\right)$$
$$+\frac{1}{\Delta z_j}\left[D_{zz_{i.j+1/2}}\left(\frac{c_{t.j+1}-c_{t.j}}{\Delta z_{j+1/2}}\right)\right]-D_{zz_{i.j-1/2}}\left(\frac{c_{t.j}-c_{t.j-1}}{\Delta z_{j-1/2}}\right)$$
$$+\frac{1}{\Delta x_t}\frac{1}{2\left(\Delta z_{j-1/2}+\Delta z_{j+1/2}\right)}\left[D_{xz_{i+1/2.j}}\left(c_{t.j+1}-c_{t.j-1}+c_{t+1.j+1}-c_{t+1.j-1}\right)\right]$$
$$-\frac{1}{\Delta x_t}\frac{1}{2\left(\Delta z_{j-1/2}+\Delta z_{j+1/2}\right)}\left[D_{xz_{i-1/2.j}}\left(c_{t-1.j+1}-c_{t-1.j-1}+c_{t.j+1}-c_{t.j-1}\right)\right]$$
$$+\frac{1}{\Delta z_j}\frac{1}{2\left(\Delta x_{t-1/2}+\Delta x_{t+1/2}\right)}\left[D_{zx_{i.j+1/2}}\left(c_{t+1.j}-c_{t-1.j}+c_{t+1.j+1}-c_{t+1.j+1}\right)\right]$$
$$-\frac{1}{\Delta z_j}\frac{1}{2\left(\Delta x_{t-1/2}+\Delta x_{t+1/2}\right)}\left[D_{zx_{i.j-1/2}}\left(c_{t+1.j-1}-c_{t-1.j-1}+c_{t+1.j}-c_{t-1.j}\right)\right] \qquad 4.9$$

Where,

$$D_{xx_{i+1/2.j}}=\frac{\left(\Delta x_t+\Delta x_{t+1}\right)D_{xx_{i.j}}D_{xx_{i+1.j}}}{\Delta x_t D_{xx_{i+1.j}}+\Delta x_{t+1}D_{xx_{i.j}}} \qquad D_{zz_{i.j+1/2}}=\frac{\left(\Delta z_j+\Delta z_{j+1}\right)D_{zz_{i.j}}D_{zz_{i.j+1}}}{\Delta z_j D_{zz_{i.j+1}}+\Delta z_{j+1}D_{zz_{i.j}}}$$
$$D_{xz_{i+1/2.j}}=\frac{\left(\Delta x_t+\Delta x_{t+1}\right)D_{xz_{i.j}}D_{xz_{i+1.j}}}{\Delta x_t D_{xz_{i+1.j}}+\Delta x_{t+1}D_{xz_{i.j}}} \qquad D_{zx_{i.j+1/2}}=\frac{\left(\Delta z_j+\Delta z_{j+1}\right)D_{zx_{i.j}}D_{zx_{i.j+1}}}{\Delta z_j D_{zx_{i.j+1}}+\Delta z_{j+1}D_{zx_{i.j}}}$$

c) The degradation, sorption, and source/sink terms.

The degradation and source/sink terms do not contain any derivatives. They are converted directly into discrete values on the cell. Whereas, the sorption term is included in the retardation factor, *R.* Thus, those three terms could be expressed in the following form.

$$\lambda R c_{t.j}+\frac{c_{t.j}S_{t.j}}{\theta_{t.j}} \qquad 4.10$$

d) The time derivative

The upwind difference scheme used in the advection terms could improve the convergence of the solution, especially when these terms predominates. Difficulties, however, might still arise when the Peclet number becomes large. In this case, the TCP technique is used. TCP was introduced by LAUMBACH (1975). The technique aims to cancel a portion of error in the advection terms with that accumulation term (LAUMBACH, 1975). TCP was used in conjuction by Laumbach, the time derivative of Eq. IV.7 might be expressed in the following form.

$$\frac{\partial c}{\partial t} = (1-\xi_1-\xi_2)\left(\frac{c_{t.j}{}^{n+1}-c_{t.j}{}^{n}}{\Delta t}\right)+\frac{\xi_1}{2}\left(\frac{c_{t+1.j}{}^{n+1}-c_{t+1.j}{}^{n}+c_{t-1.j}{}^{n+1}-c_{t-1.j}{}^{n}}{\Delta t}\right)$$

$$+\frac{\xi_2}{2}\left(\frac{c_{t.j+1}{}^{n+1}-c_{t.j+1}{}^{n}+c_{t.j-1}{}^{n+1}-c_{t.j-1}{}^{n}}{\Delta t}\right) \quad 4.11$$

Where,

$$\xi_1 = \omega_1 + \frac{1}{6}\left(\frac{\upsilon_x \Delta t}{\Delta x}\right)^2 \qquad \xi_2 = \omega_2 + \frac{1}{6}\left(\frac{\upsilon_z \Delta t}{\Delta z}\right)^2$$

ξ_1 dan ξ_2 are known as the TCP weighting parameters, ω_1 and ω_2 are arbitary weighting parameters.

The use of Ceank-Nicholson scheme means that the space derivatives, that is the advection (Eq. $+\frac{\upsilon_{z_{i.j-1}}}{\Delta z_{j-1/2}}\left[\Gamma_3 c_{t.j-1}{}^{n+1}+(1-\Gamma_3)c_{t.j}{}^{n+1}\right]-\frac{\upsilon_{z_{i.j}}}{\Delta z_{j+1/2}}\left[\Gamma_4 c_{t.j}{}^{n+1}+(1-\Gamma_4)c_{t.j+1}{}^{n+1}\right]$ 4.8) mand dispersion (Eq. $-\frac{1}{\Delta z_j}\frac{1}{2(\Delta x_{t-1/2}+\Delta x_{t+1/2})}\left[D_{zx_{i.j-1/2}}\left(c_{t+1.j-1}-c_{t-1.j-1}+c_{t+1.j}-c_{t-1.j}\right)\right]$ 4.9) terms, are evaluated at half time between previous and present time steps. It is done by giving time weighting factor ½ to the difference at time n and $n+1$. Summing up Eqs.

$$-R\frac{\partial c}{\partial t}-\lambda Rc-\frac{\partial}{\partial x}(\upsilon_x c)-\frac{\partial}{\partial z}(\upsilon_z c)+\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial z}\left(D_{zz}\frac{\partial c}{\partial z}\right)+\frac{\partial}{\partial x}\left(D_{xz}\frac{\partial c}{\partial z}\right)+\frac{\partial}{\partial z}\left(D_{zx}\frac{\partial c}{\partial x}\right)-\frac{c^* S}{\theta}=0$$

4.7 to

$$\lambda Rc_{t.j}+\frac{c_{t.j}S_{t.j}}{\theta_{t.j}} \quad 4.10$$

and equating them to Eq. $+\frac{\xi_2}{2}\left(\frac{c_{t.j+1}{}^{n+1}-c_{t.j+1}{}^{n}+c_{t.j-1}{}^{n+1}-c_{t.j-1}{}^{n}}{\Delta t}\right)$ 4.11 form the complete finite difference equating of solute transport at cell (i,j).

$$T1_{t.j}{}^{n+1}c_{t-1.j-1}{}^{n+1}+T2_{t.j}{}^{n+1}c_{t.j-1}{}^{n+1}+T3_{t.j}{}^{n+1}c_{t+1.j-1}{}^{n+1}+T4_{t.j}{}^{n+1}c_{t-1.j}{}^{n\_1}$$
$$+T5_{t.j}{}^{n+1}c_{t.j}{}^{n+1}+T6_{t.j}{}^{n+1}c_{t+1.j}{}^{n+1}+T7_{t.j}{}^{n+1}c_{t-1.j+1}{}^{n+1}$$
$$+T8_{t.j}{}^{n+1}c_{t.j+1}{}^{n+1}+T9_{t.j}{}^{n+1}c_{t+1.j+1}{}^{n+1}=-TT_{t.j}{}^{n}c_{t.j}{}^{n}-\frac{c_{t.j}{}^{z}S_{t.j}}{\theta_{t.j}} \quad 4.12$$

Where coefficients $T1$ to $T9$ and TT are obtained from Eqs.

$$-R\frac{\partial c}{\partial t}-\lambda Rc-\frac{\partial}{\partial x}(\upsilon_x c)-\frac{\partial}{\partial z}(\upsilon_z c)+\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial z}\left(D_{zz}\frac{\partial c}{\partial z}\right)+\frac{\partial}{\partial x}\left(D_{xz}\frac{\partial c}{\partial z}\right)+\frac{\partial}{\partial z}\left(D_{zx}\frac{\partial c}{\partial x}\right)-\frac{c^* S}{\theta}=0$$

4.7 to

$$+\frac{\xi_2}{2}\left(\frac{c_{t.j+1}{}^{n+1}-c_{t.j+1}{}^{n}+c_{t.j-1}{}^{n+1}-c_{t.j-1}{}^{n}}{\Delta t}\right)$$

4.11 for the corresponding cells.

The set of Eq. $$+T8_{t.j}{}^{n+1}c_{t.j+1}{}^{n+1}+T9_{t.j}{}^{n+1}c_{t+1.j+1}{}^{n+1}=-TT_{t.j}{}^{n}c_{t.j}{}^{n}-\frac{c_{t.j}{}^{z}S_{t.j}}{\theta_{t.j}}$$

4.12 for all cells forms a banded matrix having nine coefficient representing the cell being considered and its eight surrounding cells.

4.3 Boundary and Initial Condition

4.3.1 Dirichlet and Neuman type boundary conditions.

Eqs. $$F1_{t.j}{}^{n+1}h_{t.j-1}{}^{n+1}+F2_{t-1.j}{}^{n+1}-\left[F3_{t.j}{}^{n+1}+\left(\beta S_{s_{i.j}}{}^{n+1}+SC_{t.j}{}^{n+1}\right)\right]h_{t.j}{}^{n+1}+F4_{t.j}{}^{n+1}h_{t+1.j}{}^{n+1}$$
$$+F5_{t.j}{}^{n+1}h_{t.j+1}{}^{n+1}=-FF_{t.j}+\left(\frac{K_{z_{i.j+1/2}}{}^{n+1/2}-K_{z_{i.j-1/2}}{}^{n+1/2}}{\Delta z_j}\right)-2S_{t.j}{}^{n+1}$$

4.6and

$$+T8_{t.j}{}^{n+1}c_{t.j+1}{}^{n+1}+T9_{t.j}{}^{n+1}c_{t+1.j+1}{}^{n+1}=-TT_{t.j}{}^{n}c_{t.j}{}^{n}-\frac{c_{t.j}{}^{z}S_{t.j}}{\theta_{t.j}}$$

4.12, a set of boundary conditions was specified. There were two types of boundary conditions, namely Dirichlet- and Neuman- type, used in the present study. Dirichlet-type boundary condition specified prescribed pressure heads or concentrations on the boundary.

$$h(x,z,t)=f(t),\qquad t>0$$
$$c(x,z,t)=g(t),\qquad t>0$$

Where $f(t)$ and $g(t)$ are known functions. In a modeled domain, there must be at lease one point that constitutes a first-kind boundary to guarantee the uniqueness of the solution (KINZELBACH, 1986).

Boundary conditions of the second-kind or Neuman-type specify the boundary flux, which means the pressure head gradient, for groundwater flow, or concentration gradient, for solute transport, normal to the boundary. A special case of this type of boundary is the impervious boundary where the flux is zero. Thus,

$$\frac{\partial h}{\partial t} = 0, \qquad t > 0$$

$$\frac{\partial c}{\partial t} = 0, \qquad t > 0$$

4.3.2 Initial condition

The initial conditions were given by the pressure head and concentration distributions at the starting time of simulation. The initial concentrations at every cell was zero except those at boundary. The initial pressure heads were assigned at every cell with determined values or a result of previous simulation.

4.4 Stability Criteria

The solutions obtained from a finite difference approximation depend on the nodal spacing or grid size and the time increment. A finite difference approximation is said to be convergent if the solution approaches the correct solution as the spacing and the time increment approach zero. A finite difference is stable if, as the solution becomes invalid (WANG and ANDERSON, 1982). The stability criteria apply both for groundwater flow and solute transport models.

The stability criterion of a finite difference approximation for two-dimensional flow ia as follows.

$$\frac{K_x Z_h \Delta t}{S_s(\Delta x)^2} + \frac{K_z Z_h \Delta t}{S_s(\Delta z)^2} < \frac{1}{2} \qquad 4.13$$

In which Z_h is the average flow depth.

There are two criteria for stability of a solute transport finite difference solution. The first one is the Courant criterion which requires that

$$C_{o_x} + C_{o_z} \le \frac{1}{2} \qquad 4.14$$

$$C_{o_x} = \left|\frac{\upsilon_x \Delta t}{\Delta x}\right| \text{ and } C_{o_z} = \left|\frac{\upsilon_z \Delta t}{\Delta z}\right|$$

Where C_o is known as Courant number. In physical terms this creterion says that not modre solute mass can leave the cell via advection during the time interval $\left[t, t+\Delta t\right]$ than is inside at the beginning of the time interval (KINZELBACH, 1986).

The second criterion is the Neuman criterion which implies that concentration gradients cannot be reserved by dispersion fluxes alone. It has the form (REDDERL and SUNADA, 1970).

$$D_{xx} > 0 \qquad D_{zz} > 0$$

$$D_{xx} D_{zz} > \frac{\left(D_{xz} + D_{zx}\right)^2}{4}$$

$$\frac{D_{xx}\Delta t}{\left(\Delta x\right)^2} + \frac{D_{zz}\Delta t}{\left(\Delta z\right)^2} \le \frac{1}{2} \qquad 4.15$$

A common problem encountered in a finite difference solute transport solution is errors due to an artificial numerical dispersion. To avoid such a problem, KINZELBACH (1986) suggested that the above criteria should be satisfied together with a criterion related to the grid-Peclet number, Pe, defined as

$$Pe_x = \frac{\upsilon_x \Delta x}{D_{xx}} < 2 \qquad Pe = \frac{\upsilon_z \Delta z}{D_{zz}} < 2 \qquad 4.16$$

4.5 Mass Balance Computation

The numerical accuracy and precision of the solution can be checked by performing mass balance computations. The principles of conservation of the mass requires that the comulative sums of mass inflows and outflows, that is the net flux, must equal the change in mass stored in the domain. KONILOW and BREDEHOEFT (1984) presented equations to compute the precent error, E, in the mass balance based on the difference between the net flux and the mass accumulation called the mass residual. One of them is chosen in the present study. It takes the following form.

$$E = \frac{100\left(M_t - \Delta M_s\right)}{M_o - M_t} \qquad 4.17$$

Where,

M_t = net mass flux of solute [M]

M_o = initial mass of solute present in the domain [M]

ΔM_s = change in mass of solute stored in the domain [M]

The net mass flux is computed from the advective-disperative inflow and outflow. If there is not any outflow of solute from the domain then this term equals the inflow according to the following equation.

$$M_{\mp} = \sum_t \sum_j \sum_k \left(\frac{\vec{n}\vec{\upsilon}_{t.j}}{R} c_{t.j} - \frac{\vec{n}\overline{D}}{R} \vec{\nabla} c_{t.j} \right) \Delta x_t \Delta t_k , \qquad i, j \text{ on the boundary} \qquad 4.18$$

Where $\vec{n}$ is the direction normal to the boundary.

$$\Delta M_s = \sum_t \sum_j \Delta x_t \Delta z_j \left(\theta_{t.j}{}^{n+1} c_{t.j}{}^{n+1} - \theta_{t.j}{}^{n} c_{t.j}{}^{n} \right) \qquad 4.19$$

4.6 Solution Strategy

4.6.1 Iteration scheme

The model developed consist of two main models, grundwater flow and solute transport models. An iteration scheme, called Picard method (REMSON, 1971), is utilized in the first model to solve the flow equation for pressure mheads due to its non-linearity nature in the unsaturated condition. The iteration starts with an initial guess of pressure heads at every cells which is generally equal to he initial value. The solutions of the groundwater flow equation then give new pressure heads which are then used as improved guesses. The iteration stops when there is not any significant improvement in the solution. In fact, such an iteration scheme is not needed for saturated flow condition. However, since the domain is treated as an integrated unsaturated-saturated one, the iteration scheme is applied for all flow conditions. The second model works upon the completion of the groundwater flow model.

a) The simulation starts with determinded initial pressure head and concentration distributins of the system.
b) Using the iteration scheme explained previously, the groundwater flow equation is solved for pressure heads.
c) Velocities and dispersion coefficient then could be calculated which are used in the solute transport model to give the concentration distribution.
d) Keeping those values calculated in steps b) and c) as initial values for the next time step, the simulation proceeds until the required simulation period is completed.

The convergence of the iteration is archieved when the maximum difference between the computed pressure head values at present and previous iterations is less than a small number. Difficulty in achieving theconvergence might be encountered when a wide range of the water content, and thus of the [ressure head, is expected. This difficulty increases when the wide range of the water content is accompanied by the wide range of the hydraulic conductivity and specific capacity. At early time steps, the pressure head values generally change abruptly and make the iteration difficult to converge. The initial pressure head or water content at the unsaturated zone, therefore, affect the convergence of the iteration. Care should be taken in specifying the initial condition. It is to be noted also that the unsaturated zone is of finite depth with the ground surface and water table at the upper and bottom boundaries, respectively. Hence, specifying a pressure head value that is much greater than the static pressure head should be avoided.

The choice of the time increment is another factor that affects the convergence of the iteration. At early time steps when the pressure gradient is high, small time increments are needed. However, as the simulation proceeds, this gradient decreases, allowing the use of greater time increments. Nevertheless, the time increment is restricted by the stability criteria according to Eqs. $C_{o_x} + C_{o_z} \leq \frac{1}{2}$

4.14and $\frac{D_{xx}\Delta t}{(\Delta x)^2} + \frac{D_{zz}\Delta t}{(\Delta z)^2} \leq \frac{1}{2}$

4.15. in the model developed, the time increment is generated according to the algorithm : $\Delta t_{t+1} = 1.2\Delta t$, while keeping it less than the maximum value according to Eqs. $C_{o_x} + C_{o_z} \leq \frac{1}{2}$

4.14and $\frac{D_{xx}\Delta t}{(\Delta x)^2} + \frac{D_{zz}\Delta t}{(\Delta z)^2} \leq \frac{1}{2}$

4.15.

4.6.2 <u>Computer Program</u>

The computer program of the model was written in Turbo Pascal. It consist of five moduls namely a main program and four units. The main program controls the overall execution of the model. Unit GLOVBVAR list all globals variables used throw out the program and procedure to write the out put. Unit GWFLOW and SOLUTE group routins for solving groundwater flow and solute transport equations, respectively, wereas routns serving the solution of the matrices formed by the groundwater and solute transport equation air grow in unit MATSOLVE.

The special feature of the model lies in the use of the matrix solver routin to solve both the groundwater flow and solute transport equation that needs only once to be set up at the beginning of the simulation. This featuremight be utilized by satisfying to condition, that is the same band with band witch and unknown coefficient for the groundwater flow and solute transport equations. In order to archieve this condition following reqruitments apply.

a) The band witch of the matrix is determined according to the solute transport equation since it is the minimum with required to solve the groundwater flow and solute transport equations.

b) A unified treantment of the boundary conditions is adopted to ensure the same number of unknowns for the groundwater flow and solute transport equations. This methodwas derived based on the similar method explained by KINZELBACH (1986). It is down as follows.

   i. Cells outside the modeled domain are assigned zero hydraulic conductivity and zero dispersion coefficient. It is to ensure a zero grqadient normal to the boundary at the boundary cells. If there is a flux, it is converted to the sourceof sink at those boundary cells of after apropirate division with their grid size.

   ii. Cells that have prescribed pressure head and consentration do not have any unknowns, thus all coefficient related to them are brought to the RHS.

   iii. Cellx that constitute a Dirichlet-type boundary for the flow buta Neuman-type boundary for the solute transport are given an extremely large storage coefficient for instance1E30, and the treated as ordinary internal cells. Acell that can store infinitely much water will not change its pressure head value in reaction to inflows or outflows appreciably (KINZELBACH, 1986).

5 MODEL APPLICATION

5.1 Validation of the Model

The leachate migration model developed in the present study was validated by comparing its results for selected problems with those obtained from exsisting numerical model or analytical solution. Three problems were considered in the validation, namely two problems of solute transport in an unsaturated porous medium, and a longitudinal-lateral dispersion problem in a saturated porous medium.the first two problems were similar ones solved ny HUYAKORN et al. (1985) using their proposed finite element solution,SATURN model. The last validation was carried out by applying the proposed model to a longitudinal-lateral dispersion problem for which an analytical silotion was given by HARLEMAN and RUMER (1963). The validation with an unsaturated-saturated coupled problem was not possible due to unavailability of data.

5.1.1 Solute transport in an unsaturated soil

Figure 5.1 shows a schematic descripton of the problem considered. The soil was orginaly considered as a one-dimensionalproblem solved by finite element solution (HUYAKORN et al., 1984 and 1985), whoever, to suith the proposed model, it was revormulated as a two-dimensional problem in $x-$ and $y-$ direction. The initial condition associated with this problem were a uniform -83.33 cm pressure head and zero consentration distribution. The boundary condition of the flowwere zero constant pressure heads on the left-hand side and -83.33 cm on the right-hand side boundaries. A solute of 1 ppm consentration was injected on the left-hand side boundary and kept constant during the simulation.

The space discratization were $\Delta x = 0.25$ cm for $0 \le x \le 5$ cm, $\Delta x = 1$ cm for $5 \le x \le 20$ cm, and $\Delta z = 1$ cm for $0 \le z \le 4$ cm, whereas the time increment values were $\Delta t = 0.002$ days. The arbitrary weighting parameters ω_1 and ω_2 in the TCP equation were chosen to be 0.10. All physical data pertaining to the problem are presented in Table 5.1. the functional relationships between pressure head and saturation as well as hydraulic conductivity and saturation used in this test were the same ones used in the Huyakorn's study. They are of the form (HUYAKORN et al., 1985).

$$\frac{h - h_\alpha}{h_r - h_\alpha} = \frac{1 - S_w}{1 - S_{wr}}$$

$$K = \frac{S_w - S_{wr}}{1 - S_{wr}} K_s \qquad (5.1)$$

The model was run for 55 time steps and the results of pressure heads and concentrations are plotted against the distance or elevation for times 0.01, 0.06, and 0.11 days, together with those obtained from Saturn model. Figure 5.2 shows the plot of the pressure heads, whereas Fig. 5.3 shows that of the concentrations. It can be seen from the figures, the proposed model gave slower water micement then SATURN model did. On the other hand, the solute tends to move faster,especially at early time steps was steep, especially near the left-hand side boundary. The gradient became less steep as the simulation proceeded, that is when the solute front moved away from the left-hand side boundary.

In order to know the effect of the nodel parameters, a sensitivity analysis was conducted. The model was run with variations in $\omega_1$dan ω_2, Δt and Δx values. Several runs were performed by varying values of ω_1 and ω_2 while keeping the other parameters constant. Similar procedure was adopted for parameters Δt and Δx. Figure 5.4 shows the error percentages of relative concentration $c/c_o = 0.50$ position at time $t = 0.11$ days obtained from the model run as compared to those obtained from SATURN-model's results for different values of ω_1 and ω_2 respectively. These plots show that greater values of ω_1 and ω_2 or Δx slower solute movement. On the other hand greater values of Δt resulted in a faster movement. The use of $\omega_1 = \omega_2 = 0.10, \Delta t = 0.002$ days, and $\Delta x = 0.25$ gave the least errors.

5.1.2 <u>Two-dimensional transport in an unsaturated soil slab</u>

A schematic representation of the problem domain with defined boundary condition is given in Fig. 5.5 the rectangular soil slab was initially dry and water and solute were allowed to enter the system at the upper portion of the left-hand side boundary, $x = 0$ dan $x \le z \le 4$. The right-hand side boundarywas Dirichlet-type boundary with a constant pressure head, $h = -90$ cm. At the inlet, the pressure head was maintained at $h = z - 4$ and the solute concentration was assumed to be 1 ppm.no flow and zero normal protions of the entire boundary. Physical parameters and used in the test are given in Table 5.2.

The groundwater flow and solute transport equations with the stated initial and boundary conditions were solved usinga uniform grid size of $\Delta x = \Delta z = 1$ cm. The weighting parameters ω_1 and ω_2 were aken to be 0.10 and the time increments were determined according to the following algorithm.

$$\Delta t_1 = 0.01 \qquad days$$

$$\Delta t_t = 1.2 \Delta t_{t-1} \quad days, \quad i > 1$$

The simulation was performed for 15 time steps and the results are presented in Fig. 5.6 and 5.7 for the horizontal distribution at $z = 10$ cm and vertical distribution $x = 3$ cm of the relative concentration, respectively. The use of the block-centerd in the proposed model, in fact, gave those distributions at $z = 9.50$ cm and $x = 2.75$ cm. Similar to the first case, a better agreement between the results by proposed model and those by SATURN model was achieved at latter time steps.

A sensitivity analysis for the weightng parameters ω_1 and ω_2 was conducted, and then results of which were presented in Fig.5.8 through 5.15. These plots indicate that the most appropriate value for these parameters is 0.10.

5.1.3 Longitudinal-lateral dispersion in a saturated soil

The problem of longiytudinal and lateral in an isotropic porous medium is diagrammatically shown in Fig. 5.16. This problem was similar to that considered by REDDEL and SUNADA (1970), and also by KHALEEL and REDDELL (1985) to test their proposed solutions. The solute transport equation describing longitudinal-lateral dispersion problem might be expressed in the following form.

$$\frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} + D_z \frac{\partial^2 c}{\partial z^2} - \upsilon_x \frac{\partial c}{\partial x} \qquad 5.2$$

Subject to the following boundary and initial conditions

$$\begin{aligned}
&c(0,z,t) = c_o, && 0 \le z \le l_1, && t \ge 0 \\
&c(0,z,t) = 0, && l \le z \le l_z, && t \ge 0 \\
&\frac{\partial c}{\partial z}(x,0,t) = 0, && t > 0 && \\
&\frac{\partial c}{\partial z}(x,l_z,t) = 0, && t > 0 && \\
&c(l_x,z,t) = bounded && && \\
&c(x,z,0) = 0, && x > 0, && 0 \le z \le l_z
\end{aligned} \qquad 5.3$$

An analytical solution for the steady-state condition to Eqs. $\frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} + D_z \frac{\partial^2 c}{\partial z^2} - \upsilon_x \frac{\partial c}{\partial x}$

5.2and

$$\begin{aligned}
&c(l_x,z,t) = bounded && && \\
&c(x,z,0) = 0, && x > 0, && 0 \le z \le l_z
\end{aligned}$$

5.3 was given by HARLEMAN and RUMER (!963).

$$\frac{c}{c_o} = \frac{1}{2} erfc\left(\frac{z - l_1}{2\sqrt{\frac{D_z x}{\upsilon_x}}} \right) \qquad 5.4$$

The following data were used in the test.

$\Delta x = \Delta z = 0.40\, cm$

$l_x = 10\ cm, \quad l_z = 4.4\ cm, \quad l_1 = 2.2\, cm$

$D_x = 0.01\, cm^2 / \sec, \quad D_z = 0.001\, cm^2 / \sec$

$\upsilon_x = 0.10\ cm / \sec, \quad \Delta t = 2 \sec$

$$\frac{c}{c_o} = 1, \qquad z < l_1$$

$$\frac{c}{c_o} = 0.5, \qquad z = l_1$$

$$\frac{c}{c_o} = 0, \qquad z > l_1$$

The simulation was conducted for 99 time steps or 198 hr when the steady state transport was reached, that is when the change of the relative concentration was less than a small number. The results are shown in Tables 5.3 and 5.4. and the numerically computed results compared with analytical results (from Eq.5.4) are plotted in Figs. 5.17 and 5.18. A good agreement between the results could be achieved, although some discrepancy could be found in the region near the source boundary, similar to the observation by KHAleel AND reddel (1985). As in the case of unsaturated problems, this phenomembon might be explained as due to the steep gradient in that region. A small grid size should be used to discretize this region near the source boundary in order to get a good accuracy of the solution (REDDEL and SUNADA,1970).

5.2 Application of the model

This simulations performed in the validation stage of the present study so far had not utilized the complete part of the proposed model. The simulation was carried out either for the case of unsaturated or saturated porous medium. An integrated unsaturated-saturated case had not been considered.

In order to demonstrate its ability and applicability, the proposed model was used to simulate a leachate migration from a surface impoundment at the ground surface to the groundwater environment. The problem is depicted in Fig. 6.19. it concerned with a leachate migration in a vertical cross-section of an unconfined aquifer system bounded on the left-hand and right-had sides by drainage ditches where the water levels were known to be 275 cm and 325 cm below at 400 cm from the left-hand side boundary with an infiltrating leachate concentration of 1 ppm. The total depth and length of the modeled domain were 650 cm and 1000 cm,respectively.

The boundary conditions imposed to the domain were constant pressure heads of $z-275$ cm at EG and $z-325$ cm at FH, shilst AE and DF were simukated as zero pressure head gradient boundaries. The botton layer GH wass an impervious boundary. The ground surface was simulated as zero flux boundary or boundary of specified flux depending on wheter there was rainfall coming. The boundary condition associated with the solute transport was specified as constant concentration of 1 ppm at the surface impoundment and zero concentration gradient for the rest of the entire portion of the boundary.

The time increment at each time step was generated within the model according to the stability criteria starting with an initial value of $\Delta t = 0.5$ hr. Values of physical parameters required for the simulation are presented in Table 5.5. The domain consisted of a single layer of fine sand G.E. #13. Experimental data of the soil characteristics of this sand was presented by BROOKS and COREY (1964). Based on these data, RAO et al. (1989) and KASHYAP et al. (1989) derived functional relationships of $\theta - h$ and $K - \theta$ as discussed in Section 3.1.2. Their relationships were used in this simulation.

The initial condition of the simulation should reflect the natural condition of an aquifer, that is they should simulate the equilibrium of the system. However, since it was a hypothetical aquifer without a real field data, such equilibrium was snot known. To get a close approximation to a natural condition, the initial condition of the simulation was sought by initially running the model with a given uniform water content, $\theta = 0.20$, at the unsaturated part and static pressure head values at the saturated part. The boundary conditions were the same as stated earlier, expect that the surface impoundment was not considered yet. The simulation was stopped at this time $t = 5hr$ and the pressure head distribution obtained was used as the initial conditions for the actual simulation. The initial condition for solute concentration was taken as of zero concentration through out the modeled domain.

The scenario of the simulation was performed for three cases : (a) considering the transport process in the unsaturated zone, (b) neglecting the unsaturated zone and introducing the leachate input to the unsaturated domain at the water table, and (c) introducing a uniform rainfall at the ground surface. These scenarios are discussed in the following section.

5.2.1 Case 1 : Leachate migration froma surface impoundment

Leachate from the surface impoundment infiltrates into the unsaturated zone together with infiltring water. To simulate this infiltring water, the boundary at the surface impoundment BC was taken as of zero pressure head and remained constant during the simulation, whereas the remaining boundary conditions were the same as described before. Physical parameter values used in the simulation are presented in Table 5.5 and the calculation was continued for 49 time steps or 102.286 hr.

The simulation was performed by transferring the concentration of 1 ppm from the ground surface to the groundwater table below the surface impoundment. At this place, recharge rate of 4 cm/hr, which was equal to the saturated hydraulic conductivity, was introduced to simulate zero pressure head boundary condition at the surface impoundment in case 1. The remaining initial and boundary conditions were the same with those used in Case 1. Values of physical parameters used were also kept same.

The model run lasted for 53 time steps or 101.752 hr. the equipotential lines at time $t = 50.733$ hr and $t = 101.752$ hr are presented in Figs. 5.25 and 5.26, respectively; whereas the relative concentration distributions at the corresponding times are given in Figs. 5.27 and 5.28. similar to Case 1, the flow reached steady-state at the early time. These figures show that the relative concentration $c/c_o = 0.50$covered an area of $0.691L_x$ at the water table and $0.382L_z$, below the water table at time $t = 50.733$ hr, half time of the simulation. At the end of the simulation, $t = 101.752$ hr, this concentration covered the entire length of the domain at the water table and reached the whole depth of the saturated zone beneath the surface impoundment.

The importany point that could be drawn fro the results of this simulation was the significant difference in the concentration distributions obtained from Case 1 and Case 2. The area covered by leachate of relative concentration $c/c_o = 0.50$in the groundwater environment according to the former was less than that according to the latter. In indicates that a considerable amount of leachate was distributed at the unsaturated zone and thus was retarded from reaching the groundwater environment directly. The difference between the concentration distributions obtained from both cases was illustrated in the plots of their horizontal distributions at $z = 425$ cm and vertical distributions at $x = 425$ cm at the end of simulations as shown in Figs. 5.29 and 5.30, respectively. Here, the over estimation in predicting the leachate concentration in the groundwater environment caused by neglecting the transport processes in the unsaturated part is clearly demonstrated. According to Case 1, leachate of relative concentration $c/c_o = 0.92$reached the water table at the end of the simulation, while according to Case 2, leachate of $c/c_o = 1$was found at the same place at the beginning of the simulation.

5.2.2 Case 3 : Leachate migration subject to a uniform rainfall

In this case, a uniform rainfall of 2 cm/hr was introduced at the ground surface boundary at AB, BC and CD (Fig. 5.19). the remaining boundary conditions, initial condition, and physical parameters used were similar to Case 1. Results of the simulation are shown in Figs. 5.31 and 5.32 fpor the equipotential lines and relative concentration isolines at time $t = 103.765$ hr, respectively.

The water table profile shows the contribution of the rainfall to the water table rise. The maximum rise of the water table was 91.7 cm or $0.141L_z$ less than that in Case 1. A nearly uniform water table rice was observed in this

Case. Relative concentration isolines as shown in Fig. 5.32 indicates small spreading of the leachate. Compared with Case 1 where at the end of the simulation a relative concentration of $c/c_o = 0.92$ was observed at the original water table, the leachate movement in this case was very slow with leachate of relative concentration $c/c_o = 0.26$observed at the original water table at time $t = 103.765$hr.

The relative concentration isolines at time $t = 103.765$ hr as shown in Fig. 5. 32 do not clearly demonstrated the leachate migration along with the groundwater flow.therefore, to have a better illustration of the effect of the groundwater flow to a leachate migration, the simulation was continued until time $t = 722.207$hr or 203 time steps. The relative concentration isolines at this time is given in Fig. 5.33. this figure clearly illustrates the migration of leachate along with the groundwater flow as well as the effect of the rainfall to the leachate distribution at the unsaturated zone. The verticalmovement of leachate in the unsaturated zone was dominant forming a $0.15L_x$wide stramline-shaped area below the surface impoundment covered by leachate of relative concentration $c/c_o = 0.50$ and leaving the remaining part of the unsaturated zone remain clear of leachate. At the groundwater environment, the flow forced the leachate coming from the unsaturated zone tomove toward the right ditch leaving the left-hand side part of the groundwater remain clear.

5.3 Effect of the Boundary Condition

A unified treatment of the boundary conditions as explained in Section 4.5.2 is useful tool to accommodate the use of one coefficient matrix for flow and solute transport equations since it ensures the same number of unknowns in these equations. However, problems arise due to incompatibility of the flow boundary to the solute transport boundary.there are two possibilities of a boundary incompatibility,that is a boundary that constitutes a prescribed flux and concentration, and a boundary that constitutes a prescribed pressure head and zero concentration gradient.the first type of boundary incompatibility gives unknown valuesof pressure head but known concentration at the boundary, hence gives different number of unknowns in the flow and solute transport equations.it disables the use of one coefficient matrix to solve the flow and solute tranposrt equations. Examples of such boundary are BC' in Case 2 (Fig. 5.20) and surface impoundment boundary BC in Case 3 (Fig. 5.19).in the simulations carried out in this study,an approximation was used to overcome this difficulty. In Case 2,boundary B'C' was considered to be a prescribed pressure head boundary with pressure head values were assumed to be the same with those at the nearest cells at the ground surface. In Case 3,similar approachwas adopted except that the pressure head values at boundary BC was assumed to be the same with those at cells one grid distance further inside of the domain and the flux was transferred to these cells.

Examples of the second type of boundary incompatibility are boundaries EG and FH in Fig. 5.19.the specification of zero concentration gradient in these boundaries implies that the outflow through these boundaries was a clear water. As a result, there was an accumulation of solute massin these regions as clearly shown in Fig. 5.31. Such region, in fact should be specified as a dispersive, or convective boundary, or a prescribed concentration flux boundary known as Cauchy-type boundary (KINZELBACH,1986).however,this kind of boundary is not considered in this study.

5.4 Mass Balance Check

The mass balance computations were performed at each time step to help checkthe numerical accuracy and precision of the solution.the computation of the mass inflow needed in determining the net flux according to Eq. 4.18required approximation since the boundary condition specified in the surface impoundment was aconstant concentration. The concentraton gradient across this boundary was not known, thus the dispersive flux could not be determined. Moreover, its velocity was also not known, hence computation of the advective flux was not possible.as an approximation, the advective-diepersive flux was calculated by taking the velocity and concentration gradient at cells one grid-distance further inside the domain.

Results of the massbalance calculations are plotted at each time step togetherwiththe time increment generated within the model, as shown in Figs. 5.34 and 5.35. The plots show that the mass balance errors are high at early time of the simulation with values as high as 23% and 32% in Case 1 and Case 2.respectively. The important pointthat cen be drawn fromthese plots is that the mass balance error is very sensitive to the time increment. Constant time increments result in a less mass balance error compared to variable time increments do. In Case 1 the time increment reached its maximum value according to the stability criteria at time $t = 22$ hr and kept constant was 23 at the first simulation. The corresponding error in the mass balance was 23% at the first time and steadily decreased to3% at the last. The variable time increment for the whole period of the simulation in Case 2 resulted in the fluctuation of the mass balance error within a range from 32% to 2% as shown in Fig. 5.35.

6 CONCLUSIONS

6.1 Model Development

The main difficulty encountered in the present study is the modeling of the unsaturated flow. The problem is due to the non-linearity of the unsaturated flow equation. The dependence of the hydraulic conductivity, K, to the pressure head, h, as well as that of the specific capacity, SC, to h whilst the functional relationships between these parameters are generally specific or particular cases, cause the convergence of the iteration hard to be achieved. Many relationships were tried to suit the problems being considered, but unfortunalety none of them gave satisfactory results. It was found that the iteration hardly converged when the water content was closed to its residual value at which the negative pressure head became very high. In fact, value of the pressure head is limited since the unsaturated zone is of finite depth and it is unsaturated depth.

The modeling of the saturated zone, unlike that of the unsaturated zone, did not give any major problem. The validation of the solute transport in this zone gave quite satisfactory results. The coupling of the unsaturated and saturated zone which was expected to be a difficult problem to be solved could be tackled rather successfully. Results of the simulations proved that the conyinuity of the flow line between these zones was achieved as shown in the plot of the equipotentiallines.

6.2 Leachate Migration in an Unconfined Aquifers

It has been demonstrated that the migration of leachate from ground surface starts immidately at the base of surface impoundment upon the introduction of infiltrating water. Leachate spreads out over the entire portion of the aquifer, at the unsaturated surface soil part as well as at the groundwater environment as indicated by the concentration distribution observed in both regions.

The role of the unsaturated zone of an aquifer in a eachate migration was studied. It was found that this zone plays an important role in the spreading of leachate concentration. Unsaturated zone acts not only as a conduit to pass leachate from ground surface to groundwater environment but also as an environment where the transport processes of leachate take place. In the simulations of leachate migration from a surface impoundment conducted in the present study, a considerabe amount of leachate concentration was observed in the unsaturated zone. It was shown that a much greater leachate concentration was found in the groundwater environment when the unsaturated zone was not considered in the computation. Therefore, neglecting the unsaturated zone in modeling leachate migration leads to an over prediction of leachate concentration in the groundwater environment.

6.3 Features of the Program Developedand Limitations of the Model

The computer program of the model was written in Turbo Pascal and was developed for use in personal computers. The model uses one matrik solver that needs only once to be set up at the beginning of the computation to solve the banded matrices formed by groundwater flow equation.Eq. 4.6, and solute transport equation, Eq. 4.12, provided these equations have the same number of unknowns to be solved. In order to satisfy this requirement, that is the same number of cells to be solved for pressure heads and concentrations, the boundary conditions must be handled by a unified treatment explained in Section 4.5.2. The use of such matrix solver reduces the execution time of the program. Moreover, since only the elements within the band of the matrices are stored, the effective use of memory space is ensured.

The size of the domain that can be considered in the simulation is restriced to its maximum value depending on thememory space available in the computer. In fact, the size of the band width of the matrices determines the maximum size of the domain. The numbering of the grid system gives the size of this band widtt. To have the minimum size of the band width, the grids are numbered either column wise or row wise to give the least difference in consecutive columns or rows.

The modeled domain under consideration do not need to be discretized into a uniform grid size. The proposedmodel can be applied for non-uniform grid size system. The use of a non-uniform grid size might be necessary to seek a better accuracy in the solutions. Regions near the boundaries,for instance, might sometime need smaller grid sizes. This might be needed aso for regions near the water table, especially when small fluctuation is expected. Even though varying grid size is permitted, provision should be made to have the ratio of the greatest and smallest grid size not so high. It is recommended to have this ratio less than 100. The maximum grid size is governed by the grid-Peclet number. In order to get an accuracy of the solutions, this number should be less than 2. However, it was found that this requirement was hardly satisfied. The use of TCF metjod is expected to compensate the errors caused by this problem.

The most promising feature of the proposed model is its suitability for application to a non-uniform geometric domain. This feature is very important since the real field problems do not constitute uniform geometric domain. However, this feature has not been verified in this study.

6.4 Recommendations for Further Work

The present study has not given satisfactory results for unsaturated flow case, even though much effort has been made to overcome the difficulties encountered in the modeling of this part. Therefore, it is recommended that further studies on leachate migration should emphasize to the unsaturated zone. Different approaches, or even different numerical methods, might be used to solve the finite difference equations governing flow and solute transport.

The types of boundary conditions considered in the present study need to be extended to include the convective and dispersive boundary conditions. It was observed that inaccurate results might occur due to the limitation of the types of boundary conditionsconsidered.

The proposed model, as far as possible, was developed such that it could be applied to general leachate migration problems. The model, however, was verified for its unsaturated or saturated part seoarately. Its validity for an integrated unsaturated-saturated condition was not verified. Moreover, the model was pplied to a typical specific problem. Thus, a verification with a real field data and subsequently the application to a real unsaturated-saturated problem might be conducted to test its validity as well as applicability.

The sink term was not considered in the present study. It might be in the form of water uptake by plant, evaporation, or pumping. The model needs a small modification co facilitate the consideration of this term. The inclusion of this term in the simulation could give a better approximation to the real problem.

The convergence of the iteration is achieved when the maximum difference between the computed pressure head values at present and previous iterations is less than e small number. Difficulty in achieving the convergence might be encountered when a wide range of the water content, and thus of the pressure head, is expected. This difficulty increases when the wide range of the water content is accompanied by the wide range of the hydraulic conductivity and specific capacity. At early time steps, the pressure head values generally change abruptly and make the iteration difficult to converge. The initial pressure head or water content at the unsaturated zone, therefore, affect the convergence of the iteration. Care should be taken in specifying the initial condition. It is to be noted also that the unsaturated zone is of finite depth with the ground surface and water table at the upper and bottom boundaries, respectively. Hence, specifying a pressure head value that is much greater than the static pressure head should be avoided.

The choice of the time increment is another factor that affects the convergence of the iteration. At early time steps when the pressure gradient is high, small time increments are needed. However, as the simulation proceeds, the gradient decreases, allowing the use of greater time increments. Nevertheless, the time increment is restriced by the stabily criteria according to Eqs. 4.14 and 4.15. in the model developed, the time increment is generated according to the algorithm : $\Lambda t_{t+1} = 1.2 \Lambda t$, while keeping it less than the maximum value according to Eqs. 4.14 and 4.15.