NUMERICAL MODELLING OF TRANSPORT OF POLLUTANT THROUGH SOILS

by

Faheem Ahmad

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APPROVED:

Dr. T. Kuppusamy

Dr. Thomas L. Brandon

Dr. James R. Martin

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(ABSTRACT)

Prediction of subsurface migration of contaminant through soils involves analyses of unsaturated and saturated flow of water and advective dispersive transport of contaminant species. A finite element model is developed here for such an analysis. It is based on the transient nonlinear Richard's equation for the unsaturated flow and the mass transport equation using advective dispersive transport phenomenon. The model makes it possible to make advance predictions of the spread of the contaminant with respect to time and space, into the ground water system. The hydraulic properties of the unsaturated soils and the dispersion characteristics need to be obtained for such an analysis. The unsaturated flow parameters are obtained from a functional relationship between capillary pressure head and moisture saturation, and can be determined from laboratory tests on simple column samples of soils. A general expression is assumed to account for the effect of velocity dependence of the hydrodynamic dispersion coefficient in the mass transport problem. A computer program POLUT2D is developed based on the above assumptions. Pre and post processors for the computer program POLUT2D are also developed for interactive input of data and graphics displays of results. The computer program is first evaluated by comparing the results of a problem given in the literature with the results obtained by POLUT2D. The factors affecting the contaminant movement and distribution such as dispersivities, hydraulic conductivities and the effect of cutoff walls in controlling the spread of contaminant plume are studied. Also in this regard, the movement and spread of a contaminant at a landfill site in New Castle County, Delaware, is studied by comparing the simulated pattern of plume with the observed pattern.

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CHAPTER 1

Introduction

With the increasing concern for the preservation of natural resources, there has been pronounced awareness of the potential for groundwater contamination by leachate from dumps and landfills. Freeze R. and J. Cherry 1979, have defined contaminant as *all solutes introduced into the hydrologic environment as a result of man's activities regardless of whether or not the concentrations reach levels that cause significant degradation of water quality*. Ground water contamination can be linked back to the following:

(1) Industrial pollution, which is carried to the aquifer by used waters which contain chemical compounds and trace elements (for example metals) or waters which are at a rather high temperature. (for example radioactive pollution from atomic plants can be brought in this way.). The major causes are rain infiltrating through waste disposals or by accidents like the breaking of a pipeline.

(2) Domestic pollution, which is carried to the aquifer by causes such as rain infiltrating through sanitary landfills or accidents like the breaking of the septic tanks.

(3) Agricultural pollution, which is mainly due to irrigation water or rain carrying fertilizers, minerals, salts herbicides and pesticides into the aquifer.

(4) Environmental pollution is mainly due to the seawater intrusion in the coastal aquifers.

Predicting the transport of hazardous wastes in soils is a complex problem that requires an understanding and quantification of the physical, chemical and biological mechanisms contributing to the dispersion, retardation and degradation of the wastes. Ground water models have been developed to simulate one or more of the following phenomenon:

- Ground Water Flow
- Solute or Pollutant Transport
- Phased Transport

Ground water flow addresses the physical processes that govern ground water movement.

Solute or pollutant transport couples the hydraulics of ground water flow with the physical, chemical and biological processes that control the migration and degradation of chemical constituent dissolved in ground water. Phased transport includes the physical, chemical and biological processes that control the migration and disposition of chemical constituents that exist in a separate phase within the ground water regime. Ground water models that couple two or more of these models are able to abstract a variety of complex hazardous waste problems.

Pollutant Transport Models

There are three different types of ground water models, as illustrated in figure 1.1, which have been or are in use:

Physical Models

Physical models are the reduced scale versions of the real situation. They are often known as sand boxes and are common in petroleum reservoir engineering (Van Meurs 1957, Muskat 1937). Although physical models can be useful in evaluating certain processes because they duplicate the real world situations including geometric, kinematic and dynamic similarities (Bear 1972), the amount of time required to construct such models is a major disadvantage to their use. They have been largely replaced by other types of models.

Analog Models

Analog models are made of completely different materials from the physical problem. However, there is a one-to-one correspondence between each dependent variable in the analog and the physical systems. The analog models basically mimic hydraulic processes with electrical or thermal systems (Scheidegger 1957). One important advantage of the physical and analog models is that the solution is continuous in the time domain. But now a days they have been generally replaced by mathematical models because of the costs and time involved.

Mathematical Models

Mathematical models rely on the solution of an equation or sets of equations to describe the processes of ground water hydraulics and contaminant migration. Mathematical models have largely replaced physical and analog models due to the recent availability and advancement in the computer technology. The majority of ground water and pollutant transport models are mathematical models. The mathematical models, as shown figure 1.1 can be divided into three categories:

- Analytical or closed form
- Statistical Model
- Numerical Models

In the analytical or closed form, due to the complexity and nonlinear nature of the governing equations, the problem is idealized and over simplified and the analytic solution obtained is expressed in the form of an infinite series or a complex integral. An over simplified problem has less practical value as it is applicable to a specific and simple case. An analytical solution involving any

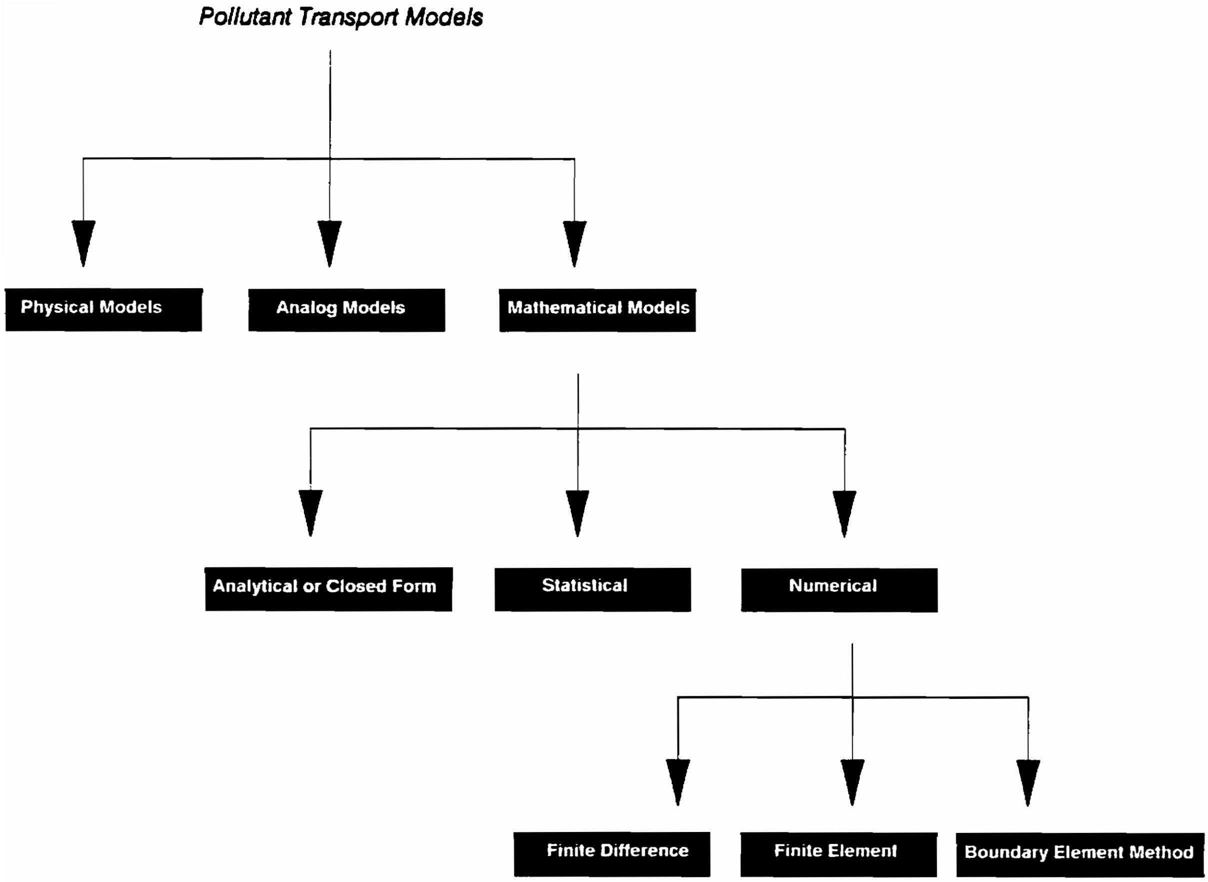


Figure 1.1 Overview of Pollutant Transport Models

form of infinite series or a complex integral may still need a digital computer for evaluation. Bear 1972 and Javendal et al. 1984 have given extensive review of the analytical methods.

because of the limitation of data availability, statistical models rely on probability and statistics to address the complexity of hydrogeological problems. Statistical models are hybrids, composed of an analytical or numerical model and statistical framework.

There are basically two procedures for solving governing differential equations numerically, the finite difference method (Smith 1965, Peaceman 1977), the finite element method (Bathe 1976, Desai 1979, Zienkiewicz 1977) and also there is a relatively new method known as Boundary Element Method (Brebbia and Walker 1980).

Finite Difference Method

In the finite difference method, spatial derivative terms of the dependent variable are approximated by the *finite differences* of the variables and distances between adjacent grid points. Similarly for a time dependent problem, finite difference approximation is made for time derivative terms. The solution proceeds for each discrete time step Δt. The difference equation turns out to be a series of algebraic equations and can be solved for unknowns by substituting the given boundary conditions. The finite difference method has been widely used in solving the flow problems. Tanji et al. 1967 were among the first who employed finite difference models for the simulation of mass transport in saturated-unsaturated porous media. A relatively recent contribution in the area of mass-transport problems is by Wierenga (1977).

Finite Element Method

The finite element method discretizes the whole domain by using smaller elements. By the variational or the residual method, a series of algebraic equations for each finite element is developed. Then the local element level algebraic equations are assembled into global level algebraic equations and unknowns are solved by applying the boundary conditions. A number of books on this subject are available (Zienkiewicz 1977, Bathe 1982, Desai 1979, Reddy 1984). The finite element method has a greater flexibility and capability for handling complex geometric conditions, than does the finite difference method. Thus more and more researchers have applied the finite element method to flow problems since 1970's. A one dimensional finite element model for mass transport problems assuming steady state flow, was developed by Guymon et al. (1970). As an example of two dimensional pollutant transport model, van Genuchten (1983) used Hermitian finite element formulation to solve for two-dimensional saturated-unsaturated flow and mass transport equations.

Boundary Element Method

The boundary element method (BEM) is a relatively newcomer in numerical analysis. This method also creates an integral form of the governing flow or transport equation relying on boundary rather than areal integrals. This method holds promise for reduction in computational effort through reduction in problem dimensionality. The other aspect of the boundary element method is that the resulting matrix is full, whereas in finite element or finite difference methods matrix is sparse and banded, which helps in computer storage and speed. The Boundary element technique can be used to solve the advection dispersion equation (e.g Brebbia and Skerget 1984) but to date, it has not found significant applications in the solution of contaminant transport problems.

Scope of Study

In this thesis, the aim is to study a finite element procedure based on the two dimensional unsaturated-saturated flow and advective dispersive transport of a contaminant. The computer program POLUT2D along with the pre and post processors, which have been developed to allow interactive input of data and graphics displays of results, are used in this study. In order to evaluate the computer program, the solutions of a problem given in the literature are compared to the results obtained using POLUT2D. The effect of various parameters such as dispersivities, hydraulic conductivities are studied including the effect of cutoff walls in controlling the spread of contaminant plume. The program is then used to model spread and movement of contaminant at a landfill site located in Delaware, by comparing simulated values with the limited observed data.

Summaries of Various Chapters

Chapter 2 of this thesis describes the model used for unsaturated flow. It includes a discussion on the unsaturated hydraulic conductivity. Chapter 3 describes the transport phenomenon in a porous medium, and the derivation of the mass transport equation with advection and dispersion with a general discussion of dispersion coefficient. Chapter 4 describes the finite element formulation. The formulation is based on the Galerkin's method for mass transport equation and uses iterative technique for non-linearity and a general time integration scheme. In Chapter 5, an example problem given in the literature is solved and compared with the known solution. In Chapter 6, an attempt is made to model the spread of contaminant at a landfill site in New Castle County, Delaware based, on the observed values of contaminant at well points. Conclusions derived from this study are presented in Chapter 7. A user's guide for the computer program POLUT2D is given in the appendix.

CHAPTER 2

Unsaturated Flow Through Porous Medium

General

The unsaturated subsurface flow is subjected to two conditions: (1) flow through unsaturated medium above the water table and (2) flow through fractured zones or conduits of solid rocks above the water table.

In the case of unsaturated flow through porous medium above the water table, where the surface of solid grains is relatively large as compared to the volume of moving water, the air within the media is in direct contact with the atmosphere, which determines its pressure. Under the second condition, i.e. unsaturated flow through fractured zones or conduits of solid rocks above water table, contact is made to the atmosphere but it is less affected by intermolecular forces.

Darcy's Law

The constitutive law for the flow problem in porous medium is Darcy's Law and it is extended to unsaturated flow in z-direction in an isotropic soil as;

$$V_z = -K(h)\frac{\partial h}{\partial Z} \qquad [2.1]$$

Where :

V_z = specific discharge in z-direction

K(h) = Unsaturated Hydraulic Conductivity

h = Hydraulic Head

Z = Depth

Darcy's Law as expressed in equation [2.1] is an experimental conclusion as concluded by Henry Darcy in 1856. It is generally agreed that Darcy's Law holds for saturated and unsaturated flow with transient and steady state conditions (Freeze R. and J. Cherry 1979). But over the years, many investigators (e.g Rose, H. 1945) have found that Darcy's Law is no longer valid as the specific discharge crosses certain limits. The dimensionless number, Reynold's Number R_e is used as criterion to indicate the flow pattern, i.e laminar or turbulent. For flow through porous medium, R_e is defined as $R_e = q\frac{d}{v}$ where q is the discharge, v is the kinematic viscosity of the fluid and d is the some length dimension of porous medium grain.

It is accepted at low Reynold's numbers, flow in a porous material is laminar, viscous forces are predominant and therefore Darcy's Law is valid. As the Reynold's number increases, inertial forces govern the flow and experimental results deviate from Darcy's Law. This is the upper limit for the validity of Darcy's Law (Bear 1979).

Many investigators (Kutilek 1969, Bolt and Groenevelt 1969, Low 1961) found that if the hydraulic gradient of a fluid in a porous material is lower than a critical value, then there is a very little flow and Darcy's law does not hold true. This is the lower limit for the validity of Darcy's law.

Bear (1979) suggests that for practical purposes, Darcy's Law is valid as long as the maximum value of R_e based on average grain diameter does not exceed some value between 1 and 10.

Unsaturated Flow Equation

Consider a unit volume of porous medium such as that shown in figure 2.1. The control volume considered in figure 2.1 is assumed as partially saturated and by applying the equation of continuity, equation [2.2] is obtained. It reveals the time rate change of storage due to water expansion and aquifer compaction (Freeze, R. and J. Cherry 1979).

$$\rho V_x - \frac{\partial}{\partial X}(\rho V_x) - \rho V_x + \rho V_z - \frac{\partial}{\partial Z}(\rho V_z) - \rho V_z = \frac{\partial}{\partial t}(\rho \eta S) \qquad [2.2]$$

Where:

ρ = Density of Fluid

S = Degree of Saturation

η = Porosity

V_x, V_z = Specific Discharges in X and Z directions

The above equation can be simplified as:

$$-\frac{\partial}{\partial X}(\rho V_x) - \frac{\partial}{\partial Z}(\rho V_z) = \eta S \frac{\partial \rho}{\partial t} + \rho S \frac{\partial \eta}{\partial t} + \rho \eta \frac{\partial S}{\partial t} \qquad [2.3]$$

The above equation can be further simplified by ignoring the first two terms on the right hand side of equation [2.3], because first two terms are much smaller compared to the third term

$$-\frac{\partial}{\partial X}(V_x) - \frac{\partial}{\partial Z}(V_z) = \eta \frac{\partial S}{\partial t} \qquad [2.4]$$

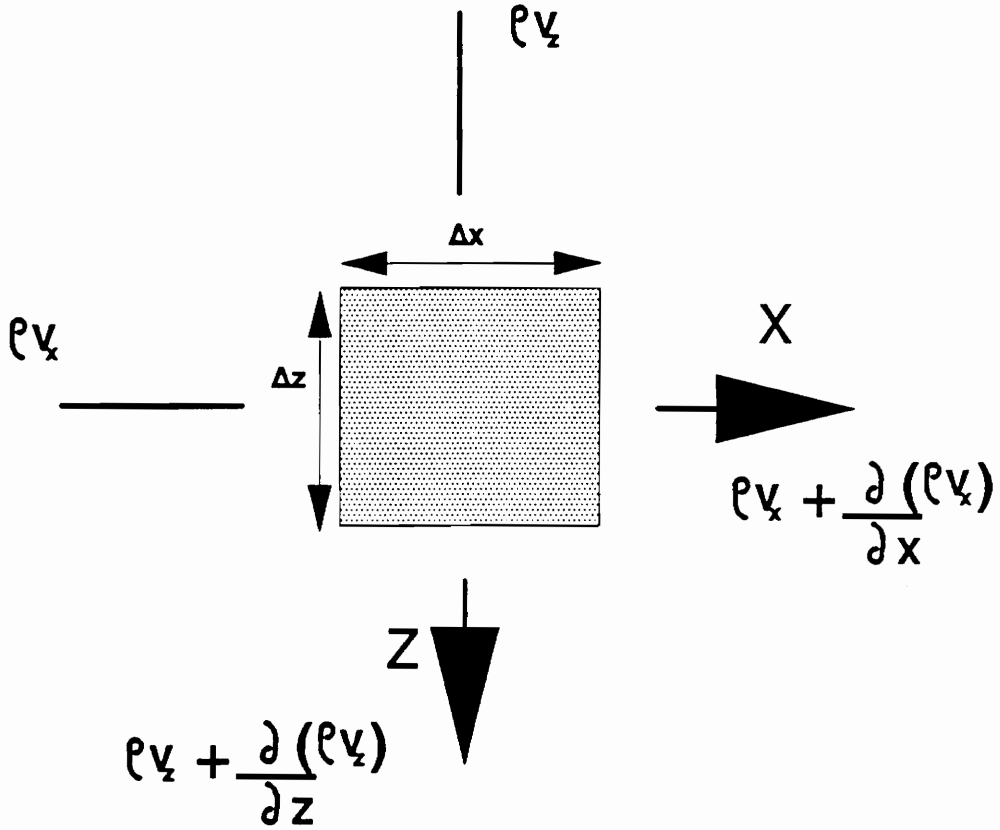


Figure 2.1 (Elemental Control Volume For Flow Through Porous Medium)

The degree of saturation S, is related to the volumetric water content θ by the following relation;

$$S = \frac{\theta}{\eta} \qquad [2.5]$$

The equation [2.4] can be written by using $\eta \partial S = \partial \theta$ and by using Darcy's Law;

$$\frac{\partial}{\partial X}(K(h)\frac{\partial h}{\partial X}) + \frac{\partial}{\partial Z}(K(h)\frac{\partial h}{\partial Z}) = \frac{\partial \theta}{\partial t} \qquad [2.6]$$

The right hand side of equation [2.6] is $\frac{\partial \theta}{\partial h}\frac{\partial h}{\partial t}$ and a coefficient of moisture capacity C_h is defined as $\frac{\partial \theta}{\partial h}$ and hence the following equation is obtained;

$$\frac{\partial}{\partial X}(K(h)\frac{\partial h}{\partial X}) + \frac{\partial}{\partial Z}(K(h)\frac{\partial h}{\partial Z}) = C_h\frac{\partial h}{\partial t} \qquad [2.7]$$

In the above equation [2.7], K(h) and C_h are functions of the type of soil and each is a non linear function of the pressure head. In unsteady or transient flow, the pressure head is varying with time, whereas in the case of a steady state it is no longer time dependent and the right side of the equation [2.7] is equal to zero.

In order to evaluate the parameters, unsaturated hydraulic conductivity K(h) and coefficient of moisture capacity C_h, one has to obtain soil water retention curve for that particular soil.

Water Content Vs Pressure Head Relationship

A typical soil water retention curve (θ - h) or water Content vs. Pressure head relationship is illustrated in figure 2.3. It is obtained by conducting laboratory tests on simple column samples of soils using Tempe Cell.

In the Tempe Cell (figure 2.3), first of all the sample is made saturated. It can be accomplished by exerting a positive head on the sample by filling up the burrett with water. The process of making a sample saturated is a very slow, usually taking about twenty-four hours and also there is a porous stone (with permeability = 1 x 10^{-8} cm/sec) between the sample and the supply of water. This process time can be reduced by pumping air into the burett and thus pushing the water at a much faster rate into the sample.

After the soil sample is made saturated, soil water retention curve is obtained by draining the water from the sample into the burett. It is necessary to determine the time at which soil sample has reached equilibrium, under the pressure of given suction head. This is achieved by taking readings on the burrett every few minutes. After the soil reaches equilibrium, the suction head is increased and the whole process is repeated until no more water can be drained out of the sample. The volumetric water content θ can be obtained for a given suction head by measuring water displaced and a plot similar to figure 2.2 is obtained.

As shown in figure 2.2, soil-water retention curve has hysteresis. If wetting (saturation) and drying (drainage) experiments are conducted on a soil, there will be two different curves showing hysteresis and hence different parameters may be required to define both the curves. For simplicity purposes, it has been decided that drying curve represents in an acceptable way the overall behavior of $\theta - h$ relationship.

In figure 2.2, residual water content θ_r is defined as the water content at which the gradient $\frac{d\theta}{dh}$ in $\theta - h$ curve becomes near zero at very large suction head. The saturated water content θ_s is the point where $\frac{d\theta}{dh}$ becomes zero near the saturation point. The coefficient of moisture capacity C_h is the slope of the soil water retention curve.

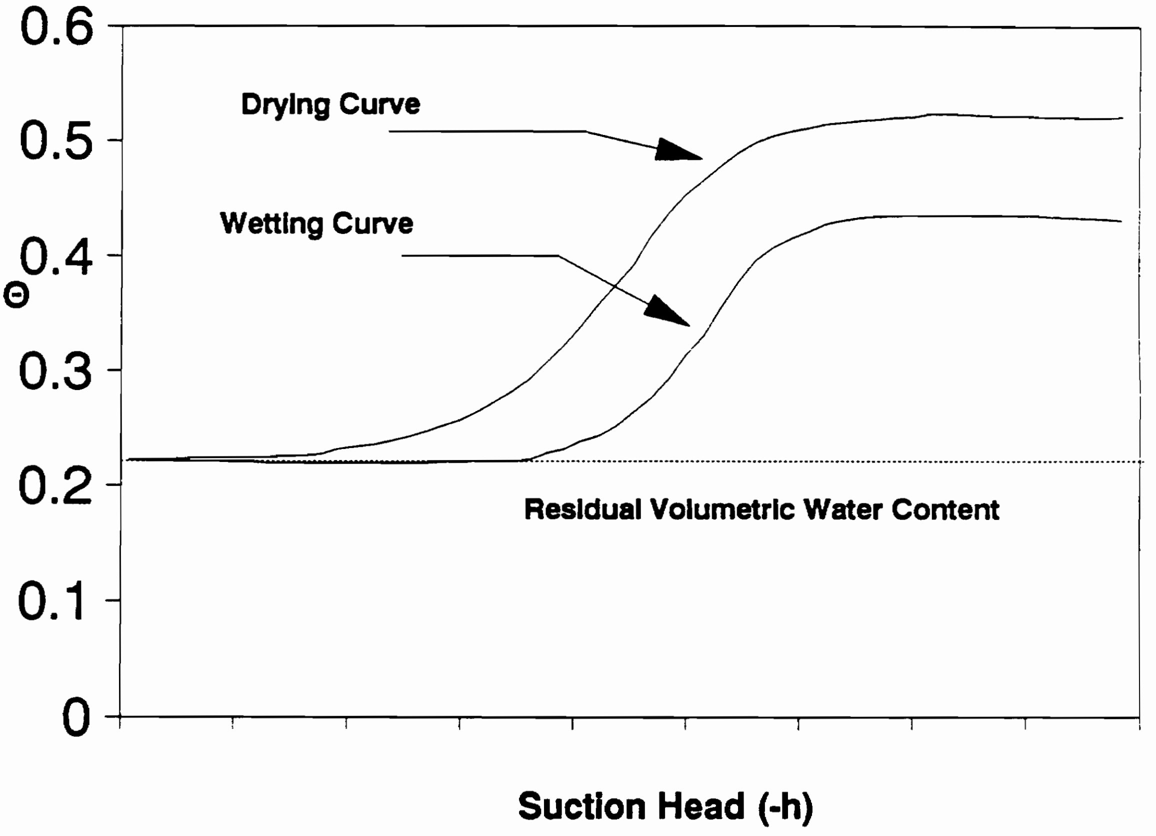


Figure 2.2 (Typical Soil Water Retention Curve Showing Hysteresis)

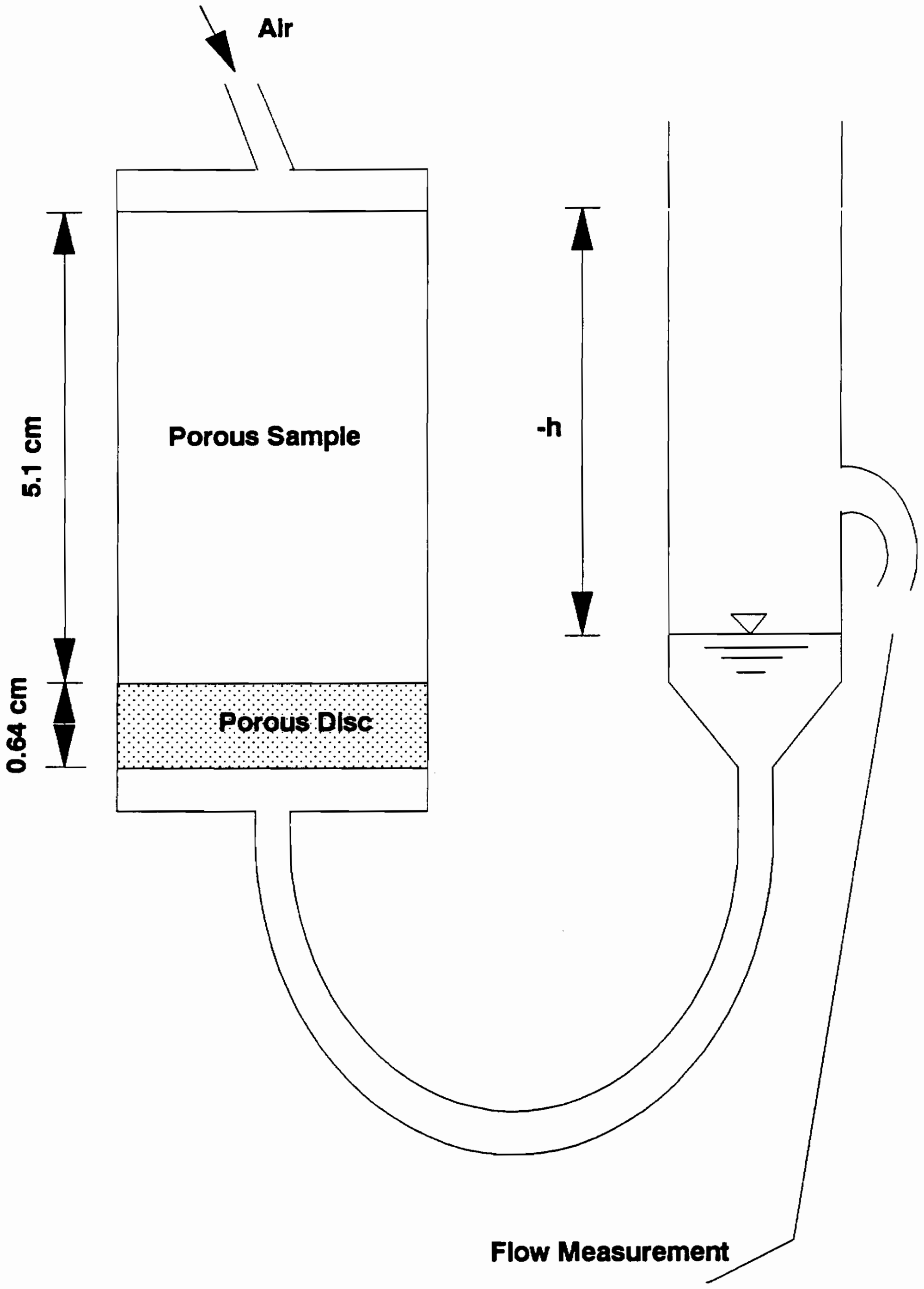


Figure 2.3 (Sketch of Tempe Cell)

Unsaturated Hydraulic Conductivity

The unsaturated hydraulic conductivity is related to the saturated hydraulic conductivity by;

$$K_u = K_r K_s \qquad [2.8]$$

Where:

K_u = Unsaturated hydraulic conductivity

K_r = Relative hydraulic conductivity ratio

K_s = Saturated hydraulic conductivity

According to Mualem, Y. (1976), the methods for obtaining relative hydraulic conductivity in unsaturated soils, can be divided into two categories:

- Relating K_r to Effective Saturation (S_e)
- Relating K_r to Pressure Head and Water Content Relationships

In the first category, expression for relative hydraulic conductivity is based on a generalization of Kozney's approach for saturated and unsaturated porous medium. In this approach, relative hydraulic conductivity is a power function of the effective saturation. (Mualem, Y. 1976)

$$K_r = S_e^{\alpha} \qquad [2.9]$$

and

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \qquad [2.10]$$

Where:

S_e = Effective Saturation

θ_r = Residual Water Content

θ_s = Saturated Water Content

θ = Volumetric Water Content

= 0.0 for $S_e = 0.0$

= 1.0 for $S_e = 1.0$

For this method, Averjanov [1950], suggested that α = 3.5, whereas Irmay (1954) proposed α = 3.0. According to Brooks and Corey [1964] for many types of soils, α = 3.5 leads better agreement with observed values than with α = 3.0.

In the second category, K_r is obtained from $\theta - h$ relationships. The Burdine (1953) equation as used in petroleum engineering, relative hydraulic conductivity to water content vs pressure head relationships;

$$K_r = S_e^{\,2}\,\frac{\displaystyle\int_{\theta=0}^{\theta}\frac{d\theta}{h^2}}{\displaystyle\int_{\theta=0}^{\theta=1}\frac{d\theta}{h^2}} \qquad [2.11]$$

Mualem (1976) developed a equation of the form similar to Burdine's equation;

$$K_r = S_e^{\,0.5}\left[\frac{\displaystyle\int_{0}^{\theta}\frac{d\theta}{h}}{\displaystyle\int_{0}^{\theta=1}\frac{d\theta}{h}}\right]^2 \qquad [2.12]$$

There are other models in this category, i.e Farrel and Larson (1972), Wyllie and Gardner (1958). Mualem (1976) tested his model against those of Wyllie and Gardner, and Averjanov and showed that his model minimized the difference between predicted and measured values.

The Burdine's and Mualem's equations are related to each other by the means of a general equation. (Osmun, D. 1988)

$$K_r = S_e^{\,n} \left[\frac{\int_0^{\theta} \frac{d\theta}{h^a}}{\int_0^{\theta = 1} \frac{d\theta}{h^a}} \right]^b \qquad [2.13]$$

Burdine's Equation: $n = 2, a = 2, b = 1$

Mualem's Equation : $n = 0.5, a = 1, b = 2$

van Genuchten (1980) modelled soil-water retention curve by use of two parameters α and n. He proposed a continuous emperical function for relating effective saturation to pressure head using n and α.

$$S_e = [1 + |\alpha h|^n]^{-m} \qquad \text{for } h < 0 \qquad [2.14]$$

$$= 1.0 \qquad \text{for } h > 0$$

Where:

$$m = 1 - \frac{1}{n}$$

van Genuchten further concluded that the Burdine based equations are less accurate than the Mualem based equations. This is also consistent with the Mualem's comparisons with the Burdine equation.

By substituting equation [2.14] into equation [2.10], the following equation for soil-water retention curve is obtained;

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{[1 + |\alpha h|^n]^m} \qquad \text{for h} < 0 \qquad [2.15]$$

$$= \theta_s \qquad \text{for h} > 0$$

Where:

$$m = 1 - \frac{1}{n}$$

The coefficient of moisture capacity, C_h as it is used in the unsaturated flow equation is;

$$C_h = \frac{\partial\theta}{\partial h} = -\alpha m (\theta_s - \theta_r) S_e^{\frac{1}{m}} (1 - S_e^{\frac{1}{m}})^m \qquad \text{for h} < 0 \qquad [2.16]$$

$$= 0 \qquad \text{for h} > 0$$

Similarly Van-Genuchten derived expression for relative hydraulic conductivity as follows;

$$K_r(S_e) = S_e^{0.5} \left[1 - (1 - S_e^{\frac{1}{m}})^m\right]^2 \qquad [2.17]$$

The above equation can be written by substituting the expression for effective saturation.

$$K_r(h) = \frac{\left[1 - |\alpha h|^{n-1}\{1 + |\alpha h|^n\}^{-m}\right]^2}{\left[1 + |\alpha h|^n\right]^{\frac{m}{2}}} \qquad [2.18]$$

The expression for unsaturated hydraulic conductivity can be written as;

$$K_u(h) = K_s \frac{\left[1 - |\alpha h|^{n-1}\{1 + |\alpha h|^n\}^{-m}\right]^2}{\left[1 + |\alpha h|^n\right]^{\frac{m}{2}}} \qquad [2.19]$$

The equation relating pressure head to relative hydraulic conductivity is displayed as in figure 2.4 for typical values of n and α.

Back Pressure

A typical effective saturation - pressure head relationship for a wetting curve is shown as figure 2.5. However for a wetting curve , the saturation may be less than 1, when the pressure head is positive. The positive value of pressure head, where saturation is reached, is termed as *back pressure.* In order to allow for back pressure in the van Genuchten theory, the following modification is adopted. (Osmun, D. 1988)

let $h = h_{ph} - h_{Bp}$

Where;

h = Pressure value to be used in Van Genuchten′ equation

h_{ph} = Pressure head

h_{Bp} = Back pressure for that particular type of soil

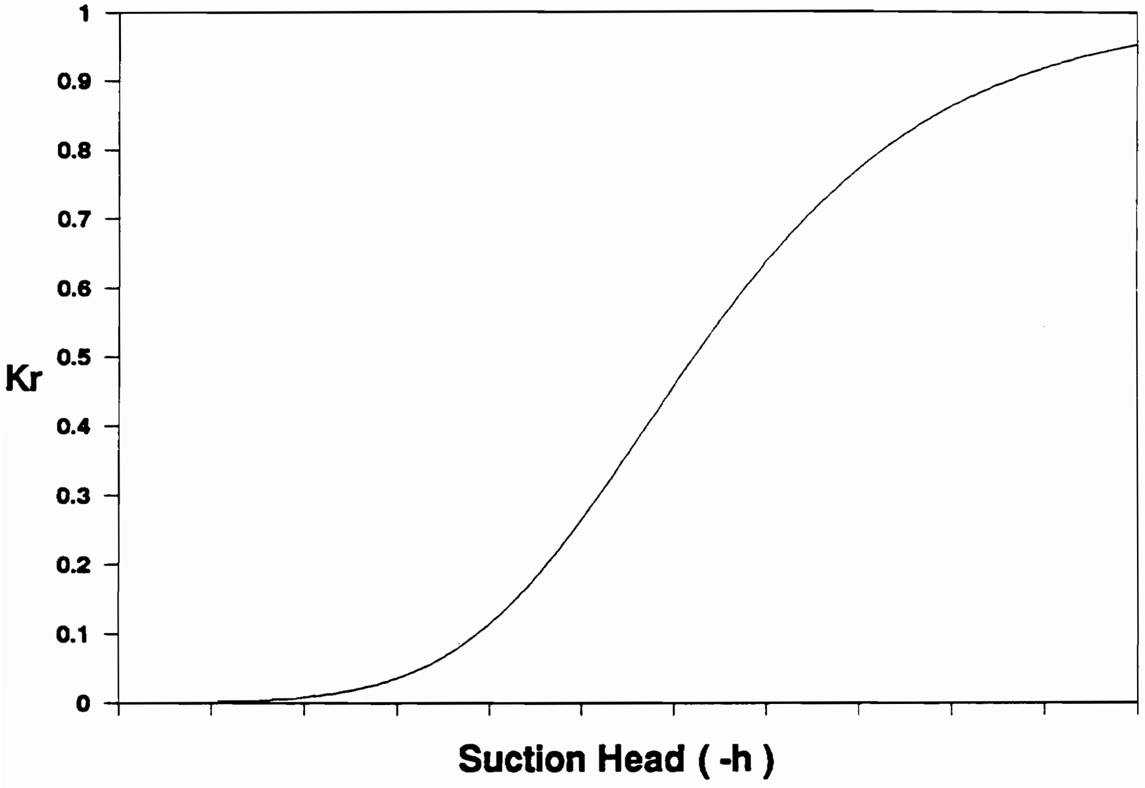


Figure 2.4 (Van Genuchten Relationship For Relative Hydraulic Conductivity)

The Van Genuchten's equations can be rewritten as;

$$S_e = [1 + [\alpha \ |h_{ph} - h_{Bp}|]^n]^{-m} \qquad \text{for h} < h_{Bp} \qquad [2.14a]$$

$$= \quad 1.0 \qquad \text{for h} > h_{Bp}$$

and Volumetric Water Content relationship is written as;

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{[1 + [\alpha\,|h_{ph} - h_{Bp}|]^n]^m} \qquad \text{for h} < h_{Bp} \qquad [2.15a]$$

$$= \quad \theta_s \qquad \text{for h} > h_{Bp}$$

Where:

$$m = 1 - \frac{1}{n}$$

These modifications are implemented in the computer program POLUT2D.

Van Genuchten's Parameters

There are five different parameters K_s (Saturated hydraulic conductivity); θ_s (Saturated water content at h = h_{Bp}); θ_r (Residual water content); α and n, used in the van Genuchten's equations [2.15] through [2.19]. The first two parameters have clear physical significance. The residual water content is strictly a emperical coefficient which yields the best fit to the data over a desired range of θ. Similarly n and α are also curve fitting parameters. The effects of α and n are shown in figure

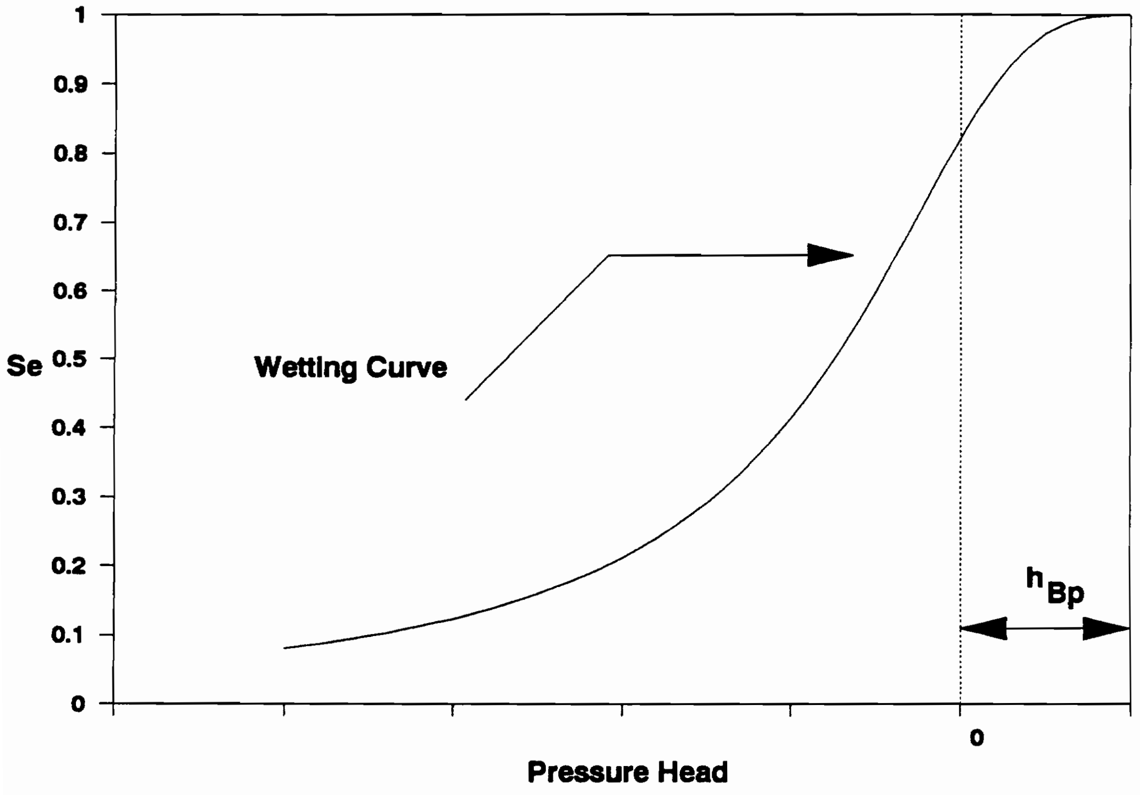


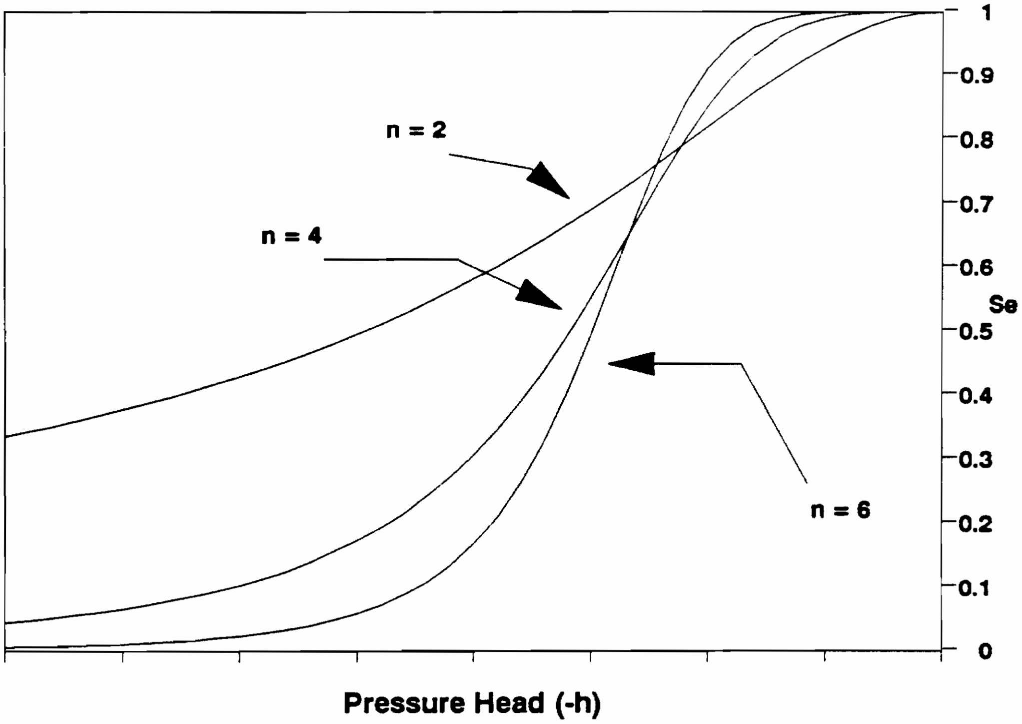
Figure 2.5 (Effect of Back Pressure)

2.6 . In the first part, the value of n is kept constant and α is varied from 1 to 5, the curve shifts towards the vertical axis. In the second part, the value of α is kept constant and n is varied from 2 to 6, here the slope of the curve becomes shallower.

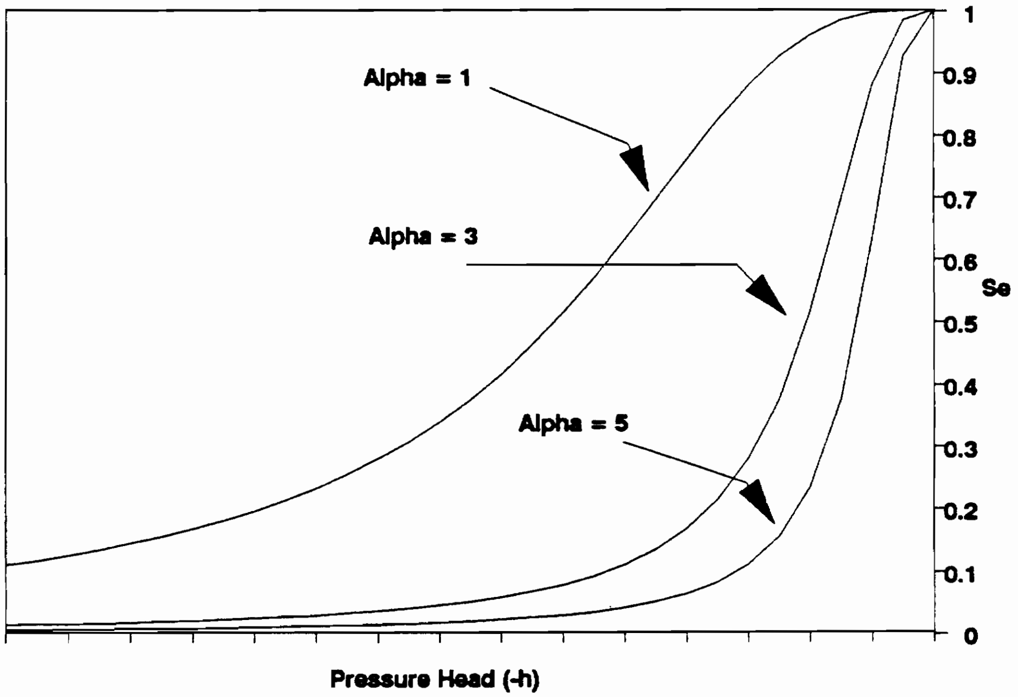
The parameters α and n are inversely related to the air-entry tension and the width of pore size distribution, respectively (van Genuchten 1978a). According to a study by Kool et al. (1985), the value of α generally ranges from 1.6 to 16.0 ft^{-1}, while n ranges from 1.1 to 3.5. The lowest value reported for α is 0.5 ft^{-1} for a heavy clayey soil. The upper value for n is about 10 for materials with extremely narrow pore size distribution. The high values for n and α generally correspond to sandy soils while fine textured soils such as clays have lower values.

Kool, Parker and van Genuchten (1985) performed numerical studies on hypothetical soils to evaluate factors which effect the determination of soil parameters. They investigated solution uniqueness and sensitivity to error in laboratory experiments. They recommended that initial trial parameters should be reasonably close to their actual values in order to reduce chances of finding an erroneous solution and to enhance the speed of convergence. The "average" initial values, for instance $n = 1.75$, $\theta_r = 0.150$, and $\alpha = 0.762$ ft^{-1} for most medium textured soils should give good results. The initial values can be adjusted for soils with different particle size distribution. Parker, Kool and van Genuchten (1985) then performed *One - Step Outflow Experiments* on four soils. They determined the parameters α and θ_r and n using three different methods of fitting curves to experimental data points. Typical values of these three parameters are given in Table 2.1.

Estimating parameters from any data to some degree of accuracy involves tedious mathematical and statistical procedures. General trends can be interpreted from the existing results until a larger data base is established for soils.



Variation of Se With Pressure Head (Constant α)



Variation of Se With Pressure Head (Constant n)

Figure 2.6 Effect of van Genuchten Parameters

Table 2.1. Parameter Values for van Genucten model (Kool et. al 1985)

Soil	Particle size distribution (%)			Bulk Density lb/ft^3	Θ_s	K_s ft/s
	Sand	Silt	Clay			
Sandy Loam - Granular Structure	61	24	25	97	0.355	2.0×10^{-6}
Silty Loam - Granular Structure	28	56	15	98	0.388	5.0×10^{-5}
Sandy Clay Loam - Granular Structure	56	18	26	96	0.402	3.3×10^{-6}
Clay - Massive Weathered Shale	21	31	48	69	0.589	7.0×10^{-8}

(a) Measured Soil Properties

Soil	Van Genuchten Parameters		
	n	α ft^{1}	Θ_r
Sandy Loam - Granular Structure	1.301	0.375	0.110
Silty Loam - Granular Structure	1.461	1.44	0.173
Sandy Clay Loam - Granular Structure	1.225	0.713	0.199
Clay - Massive Weathered Shale	1.319	0.0244	0.127

(b) Van Genuchten Parameters

CHAPTER 3

Transport Phenomenon In Porous Media

General

There are two main approaches that are commonly used for the prediction of the behavior of most chemically reactive inorganic contaminants in the groundwater (Cherry et al. 1984). The first approach has the objective of predicting the advance rate of the front of contaminant zone emanating from a continuous or a temporary source by incorporating simple chemical mass-tranfer term representing adsorption in the advection-dispersion equation. The second approach has the objective of predicting the contaminant concentrations that will occur in the zone of contamination after chemical mass transport has caused equilibrium concentrations to be achieved by precipitation, dissolution, oxidation or reduction. The first approach has its origins in applied chemical chromatography and the second approach is adapted from the chemistry of electrolyte solutions by geochemists interested primarily in seawater and surface continental waters.

The movement of contaminants in ground water is governed by a complex interaction of four processes;

- Mechanical Dispersion
- Molecular Diffusion
- Hydrochemical Interaction
- Biological Action

Mechanical dispersion is the phenomenon of scattering and is due to the velocity fluctuations resulting from the variability in flow paths of the porous medium. Uniform Sandy soils may yield one particular type of flow velocity as opposed to a fractured rock geological formation.

Molecular diffusion is the phenomenon related to the thermal kinetic energy contained within specific particles. This phenomenon is significant in fine grained soils such as clays, because ground water velocities are normally very small and molecular diffusion can play significant role in the movement of contaminant.

Hydrochemical interaction is the process that occurs between porous medium and fluid and its significance varies to a great extent, based on the type of medium and other natural conditions. For example in clayey soils, the predominant reactions would occur in the form of ion exchange and therefore cation exchange capacity is a major factor. Lime stones tend to dissolve in water producing high hardness of water. These reactions would continue until an equilibrium is achieved. The hydrochemical interaction in contaminant transport models has not been used widely (Cheremisinoff et. al. 1984).

Biological activity in ground water is the most difficult process to quantify. Biological actions are less complex in the saturated zone than in the unsaturated zone because of the filteration of organisms and organic matter by the soil, sometimes in the top few feet of the soil. Data on the biological activity is scarce and it is not normally incorporated into transport models.

The above mentioned four processes usually occur simultaneously in zones of contaminated groundwater; therefore the use of predictive methods that represent certain processes with the exclusion of the effects of processes is usually based on convenience conceptualization rather than a quest for realism.

The movement of contaminants in ground water is an inherently a three dimensional process. According to Domenico and Robbins (1984), that even a low-order transverse dispersion, acting over a long distance, can substantially affect the configuration of contaminant plume. The three dimensional modeling of transport of contaminants can be very expensive, both in terms of human and machine computations, therefore at present time, most of the contaminant modeling is done in two dimensions. Burnett D. and Frind E. (1987a, 1987b) studied the dimensionality effects on the movement of contaminants. They concluded that in a vertical two dimensional plane model, the horizontal transverse mass loss is neglected, and hence the simulated plume advances farther than the real plume. This effect becomes noticeable at a horizontal dispersivity as low as 1 cm. In the case of horizontal two-dimensional plane model, it under estimates the actual concentrations in the aquifer by substantial amount and hence it provides no margin of safety. The vertical two dimensional plane simulation on the other hand can be regarded as conservative in the sense that it predicts concentrations higher than the actually would be expected.

Mass Transport Equation With Advection and Dispersion

In the derivation of mass transport equation, two processes are considered, i.e advection and dispersion. Advection refers to the transport of contaminants at the same speed as the average linear velocity of groundwater. Dispersion in porous material refers to the spreading of a stream or discrete volume of contaminants as it flows through the subsurface. For example, if a spot of dye is injected into porous material through groundwater flowing, the spot will enlarge in size as it moves downgradient. Dispersion causes the contaminant to spread over a greater volume of aquifer than would be predicted solely from an analysis of groundwater velocity vectors. The advection- dispersion equation is derived by combining a mass balance equation with an expression for the gradient of mass flux.

Consider a unit volume of porous medium such as shown in figure 3.1. It is assumed that, porous medium is homogenous and isotropic, and Darcy's Law and Law of Conservation of Mass is applicable. The concentration of the solute, C is defined as the mass of solute per unit volume of solution. The porosity of unit volume is η and therefore the mass of solute per unit volume of porous medium is ηC. The mass of solute transported in Z-direction can be represented as; (Bear 1979, Freeze and Cherry 1979)

$$\text{Mass transport by Advection} \quad = \quad \overline{V}_z \eta \, C \, \mathrm{dA}$$

$$\text{Mass transport by Dispersion} \quad = \quad \eta D_z \frac{\partial C}{\partial Z} \, \mathrm{dA}$$

where $\overline{V}_z$ is the average linear velocity and is obtained by dividing specific discharge by porosity. i.e $V_z = \frac{\overline{V}_z}{\eta}$, V_z is the specific discharge in Z-direcion, D_z is the dispersion coefficient in Z-direction, dA is the elemental cross-section area. Let F_x, F_z represent the total mass of solute per unit cross-sectional area transported in the X and Z direction per unit time, then;

$$F_x = \overline{V}_x \eta C - \eta D_x \frac{\partial C}{\partial X} \qquad [3.1]$$

$$F_z = \overline{V}_z \eta C - \eta D_z \frac{\partial C}{\partial Z} \qquad [3.2]$$

Now applying the law of conservation of mass, i.e total amount of solute entering the unit volume is equal to the amount of solute leaving the unit volume plus the difference in the amount in entering and leaving;

$$\frac{\partial F_x}{\partial X} + \frac{\partial F_z}{\partial Z} = - \eta \frac{\partial C}{\partial t} \qquad [3.3]$$

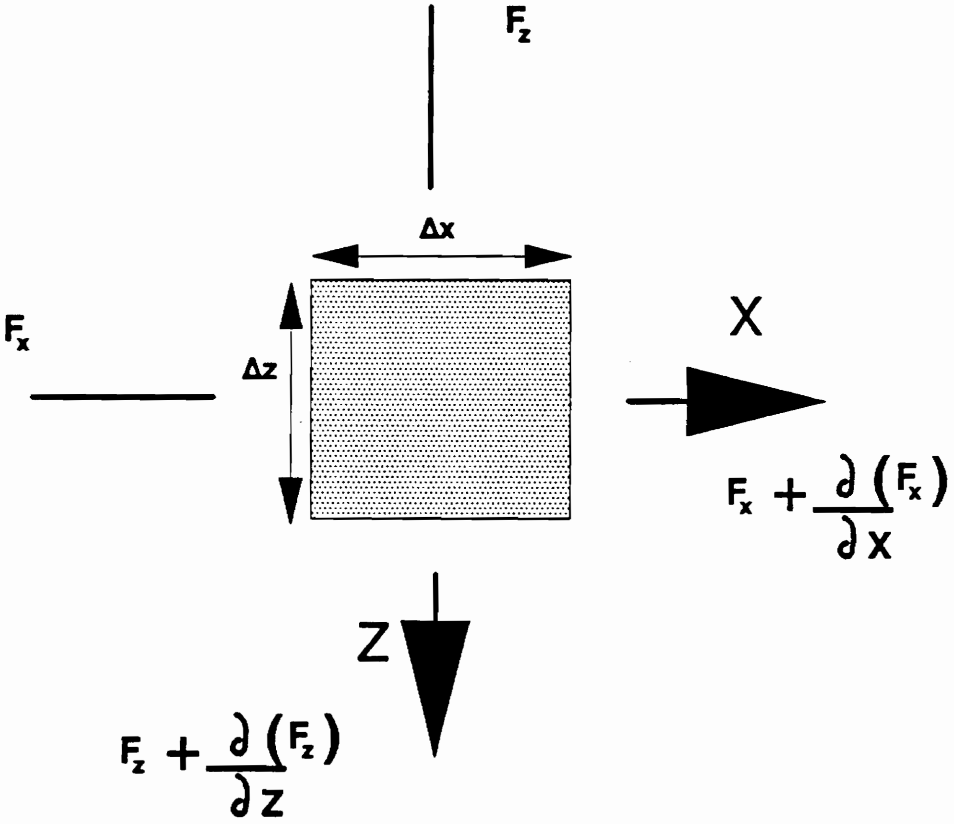


Figure 3.1. Control Volume for Mass Transport Equation

$$\left[\frac{\partial}{\partial X}(D_x\frac{\partial C}{\partial X})+\frac{\partial}{\partial Z}(D_z\frac{\partial C}{\partial Z})\right]-\left[\frac{\partial}{\partial X}(\overline{V}_xC)+\frac{\partial}{\partial Z}(\overline{V}_zC)\right]=\frac{\partial C}{\partial t} \qquad [3.4]$$

It is possible to include the effects of retardation of solute through adsorption, chemical reaction, or radioactive decay. In this case, source - sink term is also included. The following equation is obtained; (Huyakorn, P. and G. Pinder 1983)

$$\left[\frac{\partial}{\partial X}(D_x\frac{\partial C}{\partial X})+\frac{\partial}{\partial Z}(D_z\frac{\partial C}{\partial Z})\right]-\left[\frac{\partial}{\partial X}(\overline{V}_xC)+\frac{\partial}{\partial Z}(\overline{V}_zC)\right]+\overline{F}C+\overline{Q}=R\frac{\partial C}{\partial t} \qquad [3.5]$$

Where:

R = Retardation Factor

$\overline{Q}$ = Zero Order source or sink

$\overline{F}$ = First Order decay coefficient

The retardation factor, R is defined as the measure of the ratio of the velocity of water flow to the velocity of the contaminant in the aquifer. For example low molecular weight compounds or volatile organics may travel quite readily through the saturated zone. Freon is one compound which is not readily adsorbed and is thus able to enter the groundwater and be transported to considerable distances. Some common compounds with their respective retardation factors are: Cholorform 3; 1,1,1- trichloroethane 6; chlorobenzene 35 to 40 (Cheremisinoff et. al 1984).

The coefficient $\overline{F}$ is a first order radioactive decay coefficient and it is used in situations where the material undergoes first order decay. It is defined in terms of the half life of the species. For substances, which are not radioactive in nature, $\overline{F}$ is zero.

Dispersion Coefficient

In order to evaluate dispersion coefficient, there are two approaches which are commonly employed. (Bear 1979). In the first approach, the porous medium is replaced by a fictitious, greatly simplified model, in which the spreading of solute that occurs can be analyzed by exact mathematical models. Examples of this approach are a single capillary tube, a bundle of capillaries, an array of mixing cells. The second approach is to assemble a statistical model of the microscopic motion of solute particles and to average these motions in order to obtain a macroscopic evaluation of them. (Saffman 1959, 1960; Wilson and Gelhar 1974).

In the first approach the coefficient of hydrodynamic dispersion D_h is defined as the sum of the coefficients of mechanical dispersion D and of molecular diffusion in a porous medium D_d (Bear 1979).

$$D_h = D + D_d \qquad [3.6]$$

The works of Saffman (1960) and Bear and Bachmat (1967) are the examples of investigations to obtain the expressions for D_h.

In Saffman's model (1960), he obtained two components of hydrodynamic dispersion coefficients, i.e coefficient of longitudinal dispersion D_{hL} and coefficient of transverse dispersion D_{hT} by introducing the effect of molecular diffusion through Peclet number, P_e. The model is expressed as;

$$D_{hL} = D_d(m + \frac{P_e^2}{15}) \qquad \text{for } P_e << 1$$

$$D_{hT} = D_d(m + \frac{P_e^2}{40})$$

and

$$D_{\mathrm{hL}} \simeq \left[(\frac{P_e}{6}) \ln(1.5P_e) - (\frac{17P_e}{72}) - (R/l)^2 \frac{{P_e}^2}{48} + m + \frac{4}{9} \right] D_d \qquad \text{for} \quad 1 \le P_e \le 8(R/l)^2$$

$$D_{\mathrm{hT}} \simeq \left[\frac{3P_e}{10} + (R/l)^2 \frac{{P_e}^2}{40} + m - \frac{1}{3} \right] D_d$$

Where:

P_e = Peclet Number = $\frac{\overline{V}L}{D_d}$

L being some characteristic length of the pores, $\overline{V}$ is average velocity.

$R = (24K/n)^{0.5}$

K and n are the mediums permeability and porosity respectively.

l = Pore length

m = Emperical coefficient = (1/3 < m < 2/3)

Bear (1979), for an isotropic medium, obtained the following relationship for coefficient of dispersion;

$$D_{\mathrm{hij}} = \alpha_{\mathrm{T}} \overline{V} \delta_{\mathrm{ij}} + (\alpha_{\mathrm{L}} - \alpha_{\mathrm{T}}) \overline{V}_i \overline{V}_j / \overline{V} + D_{\mathrm{d}} \qquad [3.7]$$

Where:

α_{L} = Longitudinal dispersivity

α_{T} = Transverse dispersivity

δ_{ij} = Kronecker's delta

$\overline{V}$ = Magnitude of velocity vector

For cartesian co-ordinates and velocity $\overline{V}$ (Components V_x , V_z) , the equation [3.7] can be written as;

$$D_x = \alpha_L \frac{\overline{V}_x^2}{\overline{V}} + \alpha_T \frac{\overline{V}_z^2}{\overline{V}} + D_d$$

$$D_z = \alpha_L \frac{\overline{V}_z^2}{\overline{V}} + \alpha_T \frac{\overline{V}_x^2}{\overline{V}} + D_d$$

$$\overline{V} = \sqrt{\overline{V}_x^2 + \overline{V}_z^2}$$

$$\overline{V}_i = \frac{V_i}{\eta}$$

η = Porosity

In contaminant movement in aquifers the contribution of molecular diffusion to the hydrodynamic dispersion equation [3.6] is usually negligible in comparison to mechanical dispersion term. In finer grained soils such as unfractured clays, clayey silts, and shales the groundwater velocities are normally low, and molecular diffusion is significant. Diffusion coefficients for various solutes have been given by Rose 1977, and they are given in table 3.1.

The validity of equation [3.7] is a controversial matter. It is generally accepted that equation [3.7] is useful as a emperical relation for laboratory studies of solute transfer through saturated soil columns. The values of dispersivities are in the range of 0.01-1.0 cm. For field applications, many investigators (e.g Fried 1975; Biggar and Nielson 1976; Gelhar and Axness 1983) have shown that equation [3.7] can be used but with the values of dispersivity many times greater than the observed values in laboratory experiments, values of upto 650 ft have been reported. (Freeze et al. 1979). Reddell and Sunada (1970) suggest that this wide difference in the field and laboratory dispersivity estimates is because of the non-homogenous and anisotropic nature of real ground water flow systems in contrast to laboratory studies, which are usually performed on homogenous materials. Values for field dispersivities are normally obtained by trial and error adjustment of the values of α_L and α_T in a mass transport model of a field situation until the simulated migration pattern closely resembles the pattern observed in the field.

For unsaturated porous media, the validity of equation [3.7] is also under discussion. Kirda et al. (1973), Hildebrand and Himmelbau (1977), and Yule and Gardner (1978) report measurements of dispersion coefficients in unsaturated media, which seem to indicate a relationship of equation [3.7] but with a much higher values of dispersivity than for saturated laboratory experiments. De smedt and Wierenga (1984) report for a porous medium of glass beads with a diameter of 0.01 cm, a dispersivity value equal to 0.021 cm under saturated conditions, increasing by a factor of 20 in the case of unsaturated flow. Also for sands of different grain sizes, Klotz (1980) found a significant increase in the dispersivity values under unsaturated conditions as compared to saturated flow.

In the computer program POLUT2D, equation [3.7] is used and the values of the dispersivity can be used in accordance with the conditions.

Table 3.1. Diffusion Coefficients of some solutes (Rose 1977)

Solute	Coefficient of Molecular Diffusion ft^2/day
Gases	10
Inorganic solute ions	10^{-3}
Organic Molecules	10^{-5}

CHAPTER 4

Finite Element Formulation

General

The governing equations for saturated-unsaturated flow using van-Genuchten model and mass transport phenomenon are described in chapters 2 and 3 respectively. Since the equations are nonlinear, numerical analysis becomes the only practical way to solve them. The finite element technique is one of the versatile and favored simulation methods available for the pollutant transport in a porous medium because it involves solving for arbitrary domains and heterogeneous and non linear materials.

Many researchers have modelled the movement of contaminants in the ground water systems. Freeze, R. (1972), developed a finite difference model for predicting the convective transport of contaminants in a cross-sectional subsurface flow system, neglecting dispersion and retardation processes. Pinder (1973), formulated an aerial mass transport model with the Galerkin technique utilizing isoparametric quadrilateral elements and simulated contaminant movement on Long Island, New York. Pickens and Lennox (1976) developed a finite element program based on Galerkin technique to formulate the problem of simulating the cross-sectional subsurface transport of contaminants in a steady state two dimensional ground water flow system. Rowe and Booker (1985a, 1985b) used closed form solution for one and two dimensional contaminant transport models with constant dispersion coefficient. A one dimensional finite element model using unsaturated flow velocities is presented by Senthilkumar (1986).

A one dimensional analysis may be adequate provided the width of landfill is large enough compared with the depth of the layer and transport is predominantly vertical. If however, the plan dimensions of the landfill are comparable with the depth of layer, both horizontal and vertical transport may occur.

In this chapter, finite element formulation of two dimensional mass transport model with advection and dispersion using velocity fields, is presented. The unsaturated flow equation is used to obtain velocities using van Genuchten model. The velocities obtained are then coupled with the mass transport equation to get the concentration spread.

Finite element formulation of flow equation

The flow equation as given as equation [2.7] is;

$$\frac{\partial}{\partial X}(K(h)\frac{\partial h}{\partial X}) + \frac{\partial}{\partial Z}(K(h)\frac{\partial h}{\partial Z}) = C_h \frac{\partial h}{\partial t} \qquad [2.7]$$

Consider a four noded quadrilateral, two dimensional element as shown in figure 4.1 and shape functions are assumed as bilinear. The variable nodal head h within a quadrilateral element is approximated as;

$$h = N_i h_i = [N]\{q_h\}^T = [N_1 \quad N_2 \quad N_3 \quad N_4]\{h_1 \quad h_2 \quad h_3 \quad h_4\}^T \qquad [4.1]$$

Where N_i are the bilinear shape functions and are given as;

$$N_i = \frac{1}{4}(1 + uu_i)(1 + vv_i) \qquad i = 1,2,3,4$$

Where u and v are the local co-ordinates. (figure 4.1).

Differentiating equation [4.1] with respect to spatial co-ordinates as;

$$\begin{Bmatrix} \frac{\partial h}{\partial X} \\ \frac{\partial h}{\partial Z} \end{Bmatrix} = [B]\{q_h\} \qquad [4.2]$$

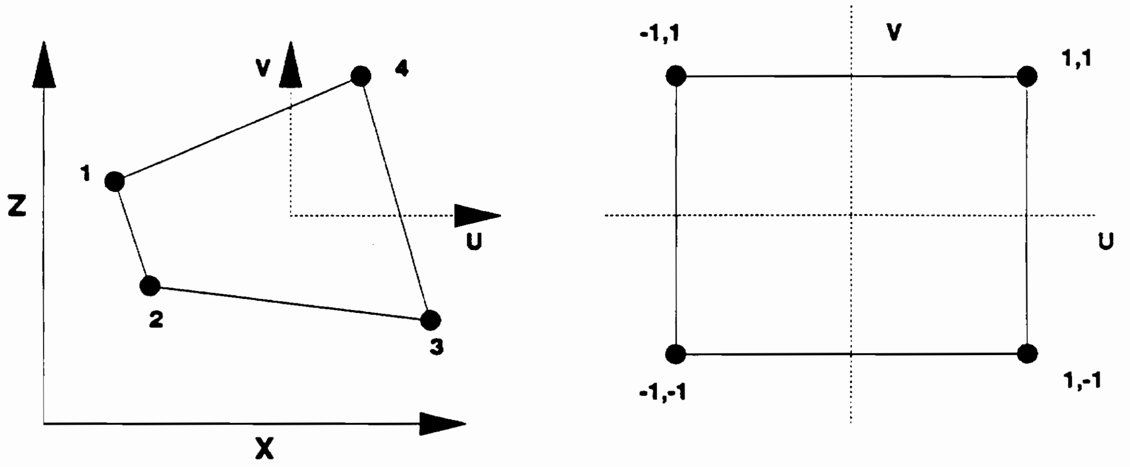
The derivatives of the shape functions with respect to spatial co-ordinates are;

$$[B] = \begin{bmatrix} \frac{\partial N_i}{\partial X} & \frac{\partial N_i}{\partial Z} \end{bmatrix}^T \qquad [4.3]$$

Differentiating equation [4.2] with respect to time co-ordinates as;

$$\frac{\partial h}{\partial t} = [N]\ \{\dot{q}_h\} = [N]\begin{Bmatrix} \frac{\partial h_1}{\partial t} & \frac{\partial h_2}{\partial t} & \frac{\partial h_3}{\partial t} & \frac{\partial h_4}{\partial t} \end{Bmatrix}^T \qquad [4.4]$$

The element equation in matrix from can be derived by applying variational procedure to equation [2.7] as;



Global Co-ordinates

Local Co-ordinates

Figure 4.1 4 - Node Isoparametric Element

$$[K]\{q_h\} + [K_T]\{\dot{q}_h\} = \{Q\} \qquad [4.5]$$

Where:

$$[K] = \int_x \int_z [B]^T [C][B] dxdz$$

$$[K]_T = \int_x \int_z C_h [N]^T [N] dxdz$$

The applied nodal seepage vectors are given by;

$$\{Q\} = \{\bar{q}_1 \ \ \bar{q}_2 \ \ \bar{q}_3 \ \ \bar{q}_4\}^T$$

and

$$\{\dot{q}_h\} = \left\{ \frac{\partial h_1}{\partial t} \quad \frac{\partial h_2}{\partial t} \quad \frac{\partial h_3}{\partial t} \quad \frac{\partial h_4}{\partial t} \right\}^T$$

Also [C] = constitutive matrix

$$[C] = \begin{bmatrix} K_x & K_{xz} \\ K_{zx} & K_z \end{bmatrix}$$

Where K_x, K_z, K_{zx} and K_{xz} are the unsaturated hydraulic conductivities and for the value of angle of anisotropy equal to zero, the values for K_{zx} K_{xz} are zero.

The element equations are assembled to obtain the global equations and are solved for the nodal values of h (head). After substituting the values of nodal heads into equation [4.2], the fluid velocities in x and z direction can be obtained for each element.

Finite element formulation of mass transport equation

The mass transport equation with advection and dispersion is given as equation [3.5];

$$\left[\frac{\partial}{\partial X}(D_x\frac{\partial C}{\partial X})+\frac{\partial}{\partial Z}(D_z\frac{\partial C}{\partial Z})\right]-\left[\frac{\partial}{\partial X}(\overline{V}_xC)+\frac{\partial}{\partial Z}(\overline{V}_zC)\right]+\overline{F}C+\overline{Q}=R\frac{\partial C}{\partial t} \qquad [3.5]$$

Where:

R = Retardation Factor = 1

$\overline{Q}$ = Zero Order source or sink

$\overline{F}$ = First Order decay coefficient

Consider a four noded quadrilateral, two-dimensional element as shown in figure 4.1 and shape functions are assumed as bilinear. The variable concentration within a quadrilateral element is approximated as;

$$C \; = \; N_i C_i = [N]\{q_c\}^T = [N_1 \;\; N_2 \;\; N_3 \;\; N_4]\{C_1 \;\; C_2 \;\; C_3 \;\; C_4\}^T \qquad [4.6]$$

The element equation in matrix form, is derived applying Galerkin's method of weighted residuals on equation [3.5] and the following is obtained.

$$[K]\{q_c\} \; + \; [K_T]\{\dot{q}_c\} \; = \; \{Q_c\} \qquad [4.7]$$

Where:

$\{q_c\} =$ Nodal concentrations $= \{C_1 \ \ C_2 \ \ C_3 \ \ C_4\}^T$

$$[K] = \int_x \int_z \{[B]^T[D][B] \ + \ [N]^T[\overline{V}][B] \ + \ [N]^T\overline{F}[N]\} \, dxdz$$

$$[\overline{V}] = \begin{bmatrix} \overline{V}_x & 0 \\ 0 & \overline{V}_z \end{bmatrix}$$

$$[K]_T = \int_x \int_z R[N]^T[N] dxdz$$

$$\{Q_c\} = \int_x \int_z \overline{Q}[N]^T dxdz \ + \ DN_l \frac{\partial C}{\partial n} \ |_x \, |_z$$

and

$$\{\dot{q}_c\}^T = \left\{ \frac{\partial C_1}{\partial t} \quad \frac{\partial C_2}{\partial t} \quad \frac{\partial C_3}{\partial t} \quad \frac{\partial C_4}{\partial t} \right\}$$

Also [D] = constitutive matrix for mass transport equation

$$[D] = \begin{bmatrix} D_x & 0 \\ 0 & D_z \end{bmatrix}$$

Where D_x and D_z are the dispersion coefficients in x and z directions. [K] is a unsymmetric stiffness matrix and utilizes a matrix solver that uses a full band width and $[K_T]$ is called a *damping matrix* . Assembly of the element equation leads the following global equation and it is written as;

$$[K]\{r\} + [K_T]\{\dot{r}\} = \{R\} \qquad [4.8]$$

Where [K] and $[K_T]$ are assembled stiffness matrices, {R} is a assembled force matrix and {r} is the matrix for nodal concentrations.

Time Integration Method

The time derivative terms in a transient problem are analyzed by the finite difference techniques. There are various time integration schemes available to solve the global equation. The selection of time integrator depends on factors, such as accuracy, stability and ease of computer implementation. A general θ or β (Belytschko and Liu, 1983) is the most common technique used for this purpose, at time t, the equation is written as;

$$[K]_t\{r\}_t \ + \ [K_T]_t\{\dot{r}\}_t \ = \ \{R\}_t \qquad [4.9]$$

and at time t + Δt

$$[K]_{t+\Delta t}\{r\}_{t+\Delta t} \ + \ [K_T]_{t+\Delta t}\{\dot{r}\}_{t+\Delta t} \ = \ \{R\}_{t+\Delta t} \qquad [4.10]$$

from equation [4.9], $\{\dot{r}\}_t$ is derived as;

$$[K_T]_t\{\dot{r}\}_t \ = \ \{R\}_t - \ [K]_t\{r\}_t \qquad [4.11]$$

$$\{\dot{r}\}_t \ = [K_T]_t^{-1}\{ \ \{R\}_t - \ [K]_t\{r\}_t\} \qquad [4.12]$$

Using β method;

$$\{r\}_{t+\Delta t} = \{r\}_t \ + \ \beta\,\Delta t\,\{\dot{r}\}_{t+\Delta t} \ + \ (1-\beta)\,\Delta t\,\{\dot{r}\}_t \qquad [4.13]$$

Where: $0 \leq \beta \leq 1$

and $\{\dot{r}\}_{t+\Delta t}$ can be written as;

$$\{\dot{r}\}_{t+\Delta t} \ = \ \frac{\{r\}_{t+\Delta t} - \{r\}_t - (1-\beta)\Delta t\,\{\dot{r}\}_t}{\beta\,\Delta t} \qquad [4.14]$$

substituting equation [4.14] into [4.10] and multiplying both sides by β.

$$\left(\frac{[K_T]_{t+\Delta t}}{\Delta t} + \beta [K]_{t+\Delta t} \right) \{r\}_{t+\Delta t}$$
$$= \frac{[K_T]_{t+\Delta t}}{\Delta t} \{r\}_t \; + \; [K_T]_{t+\Delta t} (1-\beta) \{\dot{r}\}_t \; + \; \beta \{R\}_{t+\Delta t} \qquad [4.15]$$

substituting the value of $\{\dot{r}\}_{t+\Delta t}$ into the above equation and after rearranging terms;

$$\left(\frac{[K_T]_{t+\Delta t}}{\Delta t} + \beta [K]_{t+\Delta t} \right) \{r\}_{t+\Delta t}$$
$$= \left(\frac{[K_T]_{t+\Delta t}}{\Delta t} - (1-\beta)[K_T]_{t+\Delta t}[K_T]_t^{-1}[K]_t \right) \{r\}_t + (1-\beta)[K_T]_{t+\Delta t}[K_t]_t^{-1}\{R\}_t + \beta \{R\}_{t+\Delta t} \qquad [4.16]$$

Equation [4.16] is the most general expression for the β method on equation [4.9]. In a transient flow problem, $[K_T]_t \neq [K_T]_{t+\Delta t}$ and $\{R\}_t$ is not necessarily equal to $\{R\}_{t+\Delta t}$. The value of β ranges from 0 to 1. The accuracy and stability depends on the eigen values of the matrix [K] and $[K_T]$ and these matrices are dependent on time step Δt.

The forward difference method uses, $\beta = 0$, it simplifies greatly the explicit numerical procedure. It yields either divergent or oscillatory solutions depending upon the value of time step.

In Crank-Nicholson and Galerkin's procedures (i.e $\beta = \frac{1}{2}$ and $\beta = \frac{2}{3}$), when the value of time step becomes large, they yield to oscillatory solutions. But they give more accurate results than any other method.

The backward method uses $\beta = 1$, and the following equation is used;

$$\left(\frac{[K_T]_{t+\Delta t}}{\Delta t} + [K]_{t+\Delta t} \right) \{r\}_{t+\Delta t} \;\; = \;\; \frac{[K_T]_{t+\Delta t}}{\Delta t} \{r\}_t \overset{+}{\downarrow} \{R\}_{t+\Delta t} \qquad [4.17]$$

It is less accurate for large values of time step. However, this method is unconditionally stable and the calculated values do not oscillate about the correct values.

Iteration methods for nonlinearity

In equation [4.16] $[K_T]_{t+\Delta t}$ and $[K]_{t+\Delta t}$ are functions of $\{r\}_{t+\Delta t}$. Thus it is non-linear and requires an iteration technique to handle non-linearity numerically. There are two types of methods which are commonly used;

- Direct Iteration Method
- Tangent Method

The direct iteration method is simple in numerical implementation but is not as efficient as compared to the tangent method. (Huyakorn et al. 1983) In direct iteration technique (such as Picard's method) non-linear problems are usually solved by taking a series of linear steps. An equilibrium equation can be written in this form $[K]\{r\} = \{R\}$, it is non-linear when the stiffness matrix [K] is a function of {r}. In this method, first step is to assume a value for {r} and calculate [K]. The current value of [K] is used to compute the next value of {r} and the process is repeated until the convergence to the solution, r_o as shown in figure [4.2]. Usually the criterion for convergence is selected as $| r_{i+1} - r_i | \leq \varepsilon r_i$, where i is the number of iterations and ε is the desired accuracy. In the case of contaminant transport problem, the non-linearity involved in the governing equation presents an S shaped curve as in figure 4.3. A modification to handle this type of non-linearity is adopted, in which after each iteration, from the new value of r_2 obtained and the previous value r_1, the average is taken to get the r_3 (i.e, $r_3 = \frac{r_1 + r_2}{2}$), which is used to get the updated stiffness matrix. This process is displayed as in figure 4.3.

In Newton-Raphson method, a series of tangents to the curve are taken to obtain the solution. The method is shown as in figure 4.4. The equilibrium equation can be written as a function of r as i.e f(r) = [K]{r}-{R} = 0 and it converges at at $r = r^o$. The equation can be expressed in terms of Taylor Series expansion, ignoring second and higher order order terms, it can be written as;

$$f(r^{i+1}) = f(r^i) + \left(\frac{df}{dr}\right)_i \delta r^i = 0$$

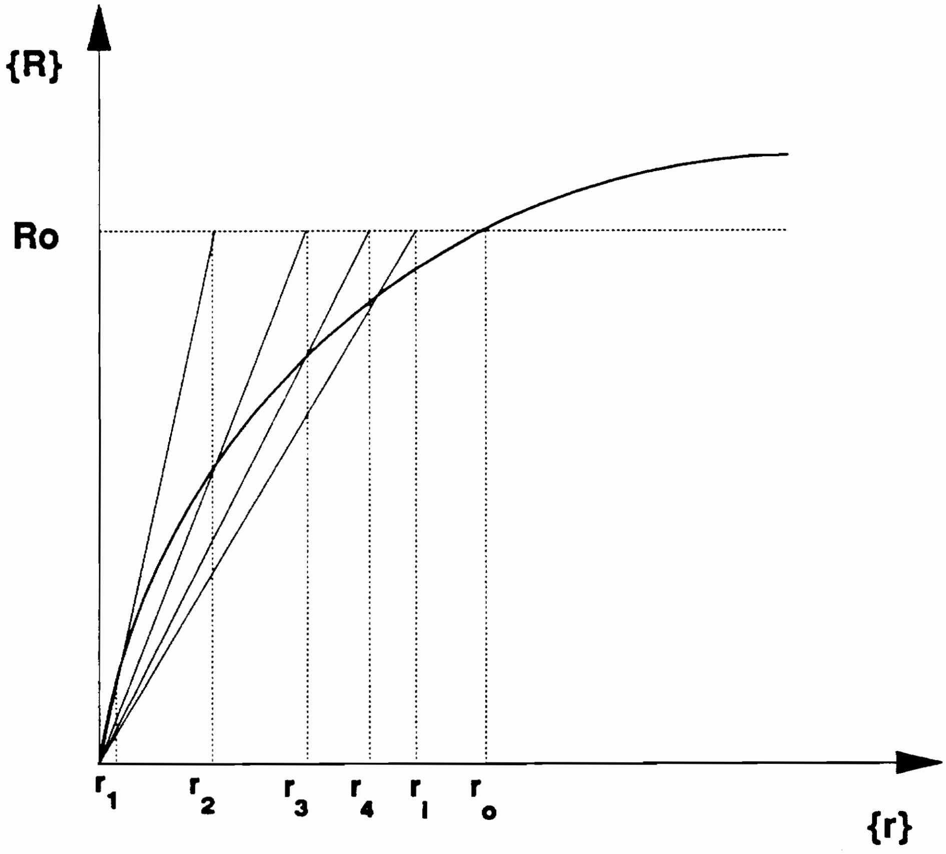


Figure 4.2 (Picard's Method)

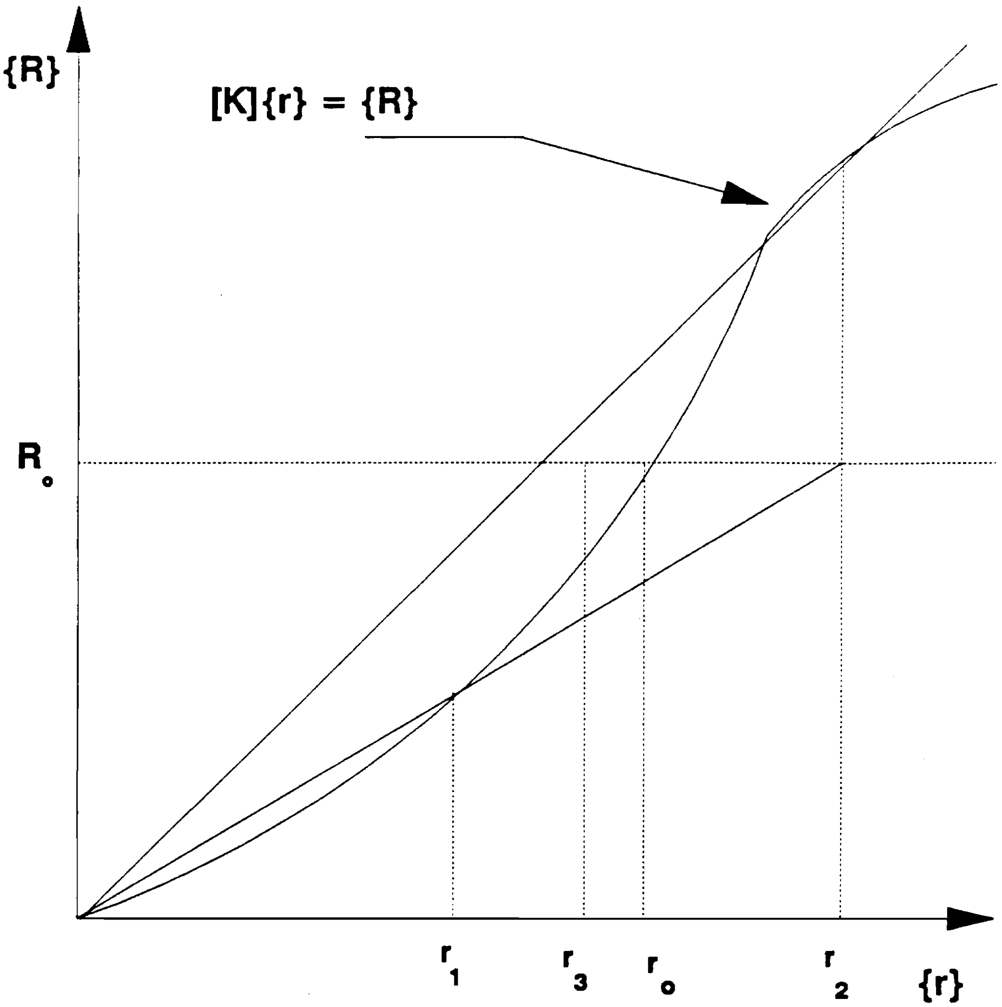


Figure 4.3 (Modified Picard's Method)

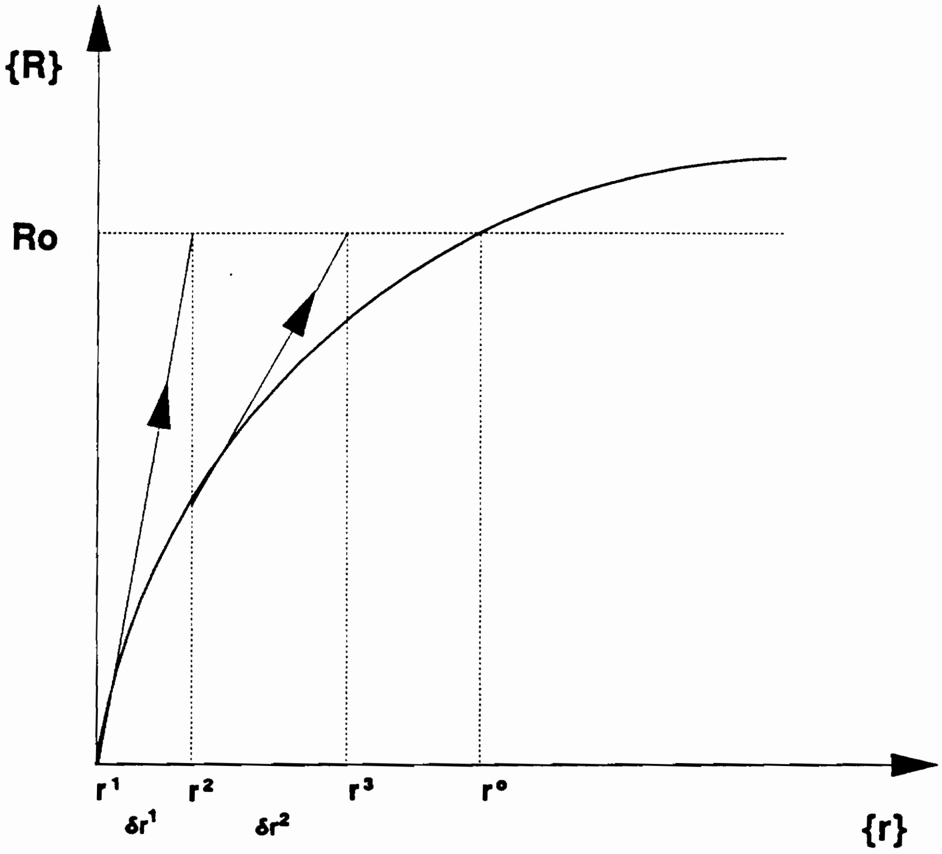


Figure 4.4. Newton - Raphson Method

where $r^{i+1} = r^i + \delta r^i$

The revised value of r^{i+1} is obtained by using

$$\delta r^i = -\left[K^i_{\mathrm{Tangent}}\right]^{-1} f(r^i)$$

The rate of convergence in the case of Newton-Raphson Method is faster as compared to the Picard's method. Newton's method requires the computation of tangent, which requires more computation effort. In POLUT2D, modified Picard's method is adopted.

Computer Program POLUT2D

Computer program POLUT2D has been developed, to perform the finite element modelling as described in this chapter. The pre processor and post processor for this program have been developed to input the data on screen graphics and to display the results. The pre processor program is written in 'C' language. The description of the screens and user's guide are described in Appendix. The post processor includes plot of mesh, concentration front and concentration contour plots.

The analysis program computes the nodal values of head h, and mean pore velocity using the techniques mentioned in chapter 2. The values of velocities are then used in the advection-dispersion mass transport equation and also dispersion coefficient is calculated as suggested by Bear (1979). The values of nodal concentrations at each time step are then obtained.

The program uses four-noded, two-dimensional quadrilateral element and a general β method for the time integration scheme. The solution procedure involves iterations by Picard's method to handle the non-linearities.

CHAPTER 5

Evaluation of Finite Element Program and Parametric Studies

Introduction

The finite element program POLUT2D is a general program, which can be used to solve the problems of contaminant or solute transport in a vertical two dimensional plane. The formulation of POLUT2D is given in the Chapter 4 and the user's guide is described in the appendix, given at the end of this thesis. A contaminant transport problem as presented by Pickens and Lennox (1976) is solved here using POLUT2D. The material properties and other boundary conditions were kept same as used in the above mentioned paper. They studied this problem by using a finite element procedure based on the Galerkin technique to formulate the problem of simulating the two dimensional transient movement of conservative or non conservative contaminants in a steady state saturated ground water flow system. This chapter describes the comparison of the solutions obtained by POLUT2D with those obtained by Pickens and Lennox (1976), including the effects of various parameters involved in the two dimensional pollutant transport problem in a porous medium.

Problem description

The groundwater flow and mass transport model with advection and dispersion is applied to a cross section of a hypothetical groundwater flow system as shown in figure 5.1. The soil domain considered is about 1000 m wide, a variable depth of 50.0 to 37.5 m with an impermeable base. The impervious base is considered as datum for the analysis. The upper boundary of the saturated flow system is the water table, which receives an aerial recharge flux. The source, which is located at the upstream side of the aquifer, provides a constant flux of contaminant to the water table. The contaminant itself is assumed to be non reactive, conservative species with an input concentration value of C_o. The effects of density, sorption, reactions and decay are not considered.

Pickens and Lennox (1976) studied this problem, which is illustrated as figure 5.1, by discretizing the cross section into 720 linear triangular elements with 410 nodes. The procedure involved solution for the steady state head distribution in the cross section, to calculate the average linear groundwater velocity in each element by using the nodal head values, and then to solve for the transient concentration distribution at the nodes, subject to the specified input conditions and porous medium properties.

Assumptions

In order to solve the problem with POLUT2D, the following assumptions are made to simplify the problem:

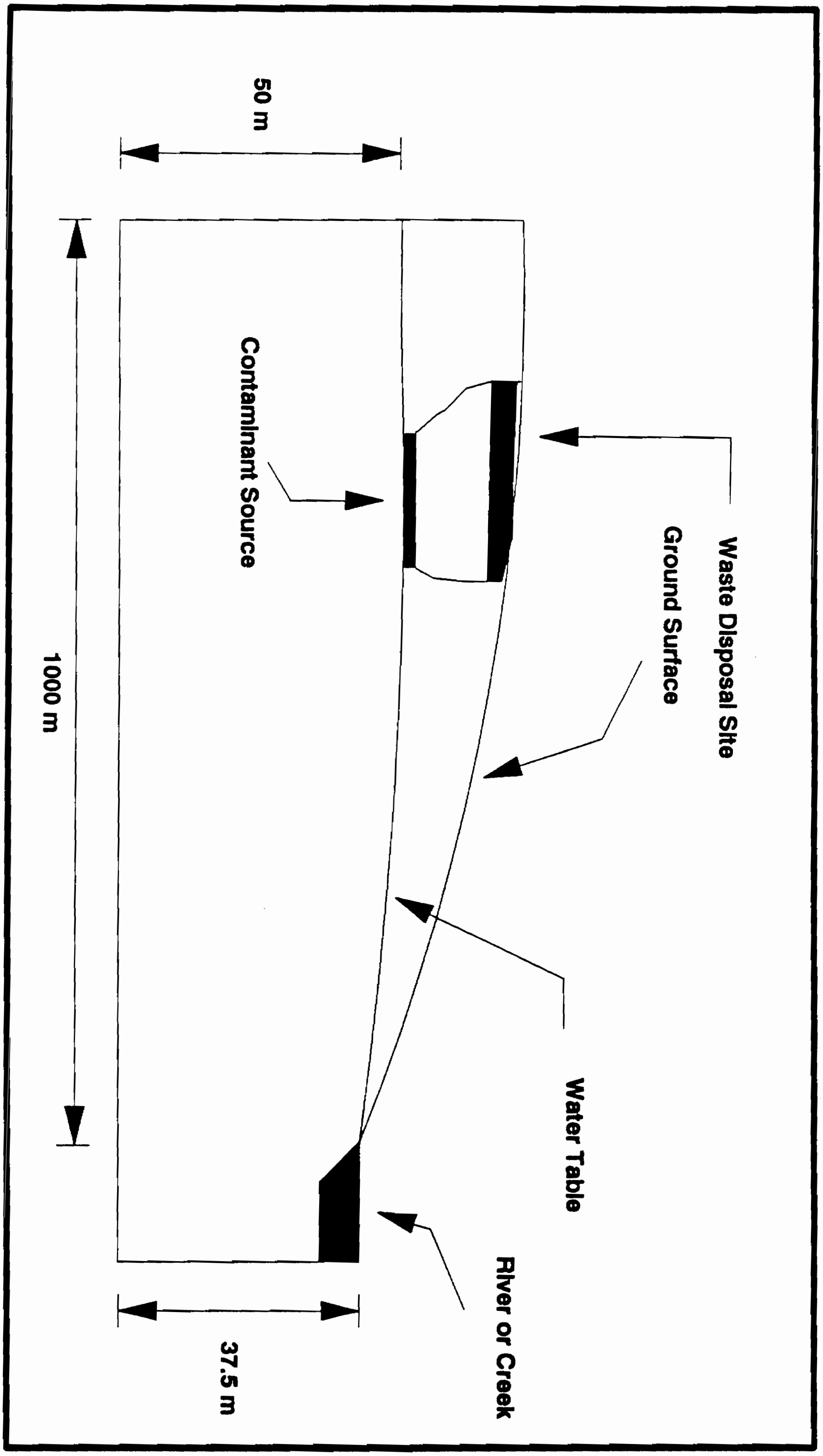


Figure 5.1 Geological Cross-section
(Adapted from Pickens, J. and Lennox, W. (1976))

- The groundwater basin is bounded on the sides and on the bottom by a reflection or impermeable (no-flow) boundary, by a specified flux boundary, or by a specified head boundary. The upper boundary of the saturated flow system is the water table. The contaminant modeled is within the saturated zone of ground water flow system. However the program POLUT2D can also be used in the unsaturated zone, but in order to compare two solutions, conditions are selected similar to the one presented by Pickens and Lennox (1976).

- The flow system chosen is assumed to exhibit steady state water flow.

- All contaminant movement is assumed to be in the plane of the section and thus neglecting the horizontal mass transverse loss. This assumption tends to be satisfied if the lateral extent of the contaminant source is large. Thus the concentration distributions predicted would be in error in a conservative sense because of the movement that occurs in the direction normal to the cross section; the true fronts would be behind the results predicted by the model.

- The porous media can be anisotropic and non-homogenous with respect to hydraulic conductivity (but within each element of this continuum the properties of the medium are constant). The porous medium is assumed isotropic with respect to dispersion.

- The seepage velocities are within the range of validity of Darcy's Law which is generally the case for intergranular porous media flow.

- The density and viscosity of the groundwater flow is essentially constant, which is true for ranges of temperature encountered in most groundwater flow systems.

- The groundwater flow pattern is not altered by the presence of contaminants in either the solution or the sorbed phase. This and the preceding assumptions imply that density variations as a result of the contaminant concentration are negligible. This leads to the decoupled form of the flow and mass transport equations.

Solution Procedure

The nodal arrangement for the finite element discretization, using 4-node quadrilateral elements, of the selected cross section, is illustrated in figure 5.2. In order to keep the mesh generation simple, cross section was divided into 315 quadrilateral elements with 384 nodes. The element shapes were kept close to a rectangular shape.

In the paper by Pickens and Lennox (1976), the contaminant distribution is modelled within the saturated zone of groundwater flow system, using steady state flow equation to get the nodal heads and seepage velocities. In POLUT2D, unsaturated flow equation or the Richard's equation is used to obtain the nodal head and element velocities. In the case of saturated - steady groundwater flow system, the right side of the following equation (Eqn. [2.7]) is zero.

$$\frac{\partial}{\partial X}(K(h)\frac{\partial h}{\partial X}) + \frac{\partial}{\partial Z}(K(h)\frac{\partial h}{\partial Z}) = C_h\frac{\partial h}{\partial t}$$

where

$$C_h = \quad -\alpha\, m\,(\theta_s - \theta_r)S_e^{\frac{1}{m}}\ (1 - S_e^{\frac{1}{m}})^m \qquad \text{for h} < h_{Bp}$$

This can be accomplished by making C_h term equal to zero. i.e setting residual volumetric water content θ_r equal to the saturated volumetric water content θ_s. Table 5.1 summarizes the material properties used for the evaluation of POLUT2D. The saturated hydraulic conductivities used are isotropic, with a values of 0.5 m/day in both x and z directions. The porosity of the soil is taken as 0.35. The coefficient of dispersions, which are used in mass transport equation are calculated as;

Table 5-1. Parameter Values Used in the POLUT2D

Parameter	Value
Sat. Hyd. Conductivity (Kx)	0.5 m /day
Sat. Hyd. Conductivity (Kz)	0.5 m /day
Back Pressure	0.0 ft
Longitudinal Dispersivity (α_L)	0.5 m
Transverse Dispersivity (α_T)	0.5 m
Residual Volumetric Water Content	0.5
Saturated Volumetric Water Content	0.5
Van Genuchten Parameter α	Not Applicable
Van Genuchten Parameter m	Not Applicable
Angle of Anisotropy (Degrees)	0.0

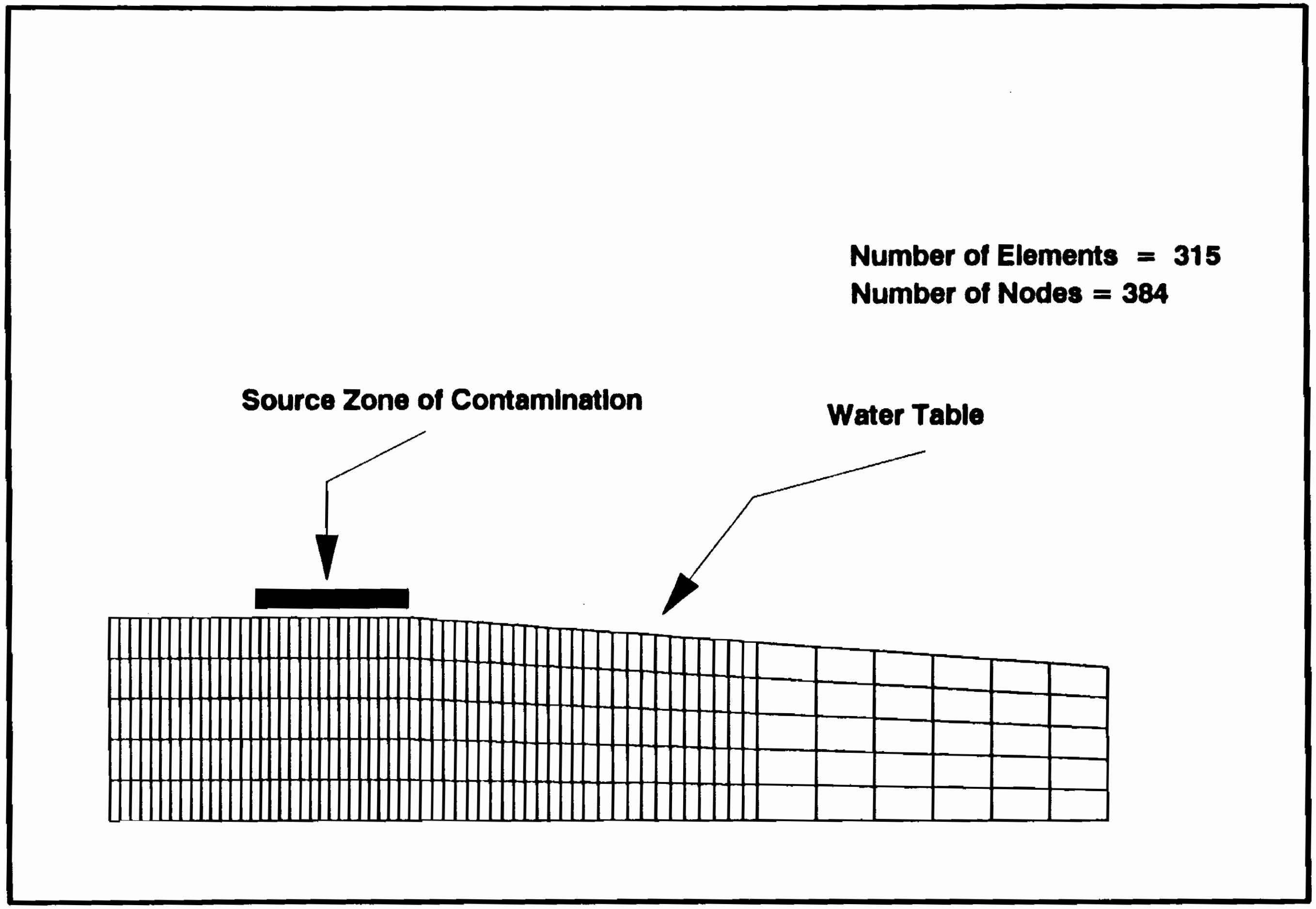


Figure 5.2 Finite Element Discretization for the Figure 5.1

$$D_x = \alpha_L \frac{\overline{V_x^2}}{\overline{V}} + \alpha_T \frac{\overline{V_z^2}}{\overline{V}} + D_d$$

$$D_z = \alpha_L \frac{\overline{V_z^2}}{\overline{V}} + \alpha_T \frac{\overline{V_x^2}}{\overline{V}} + D_d$$

Where

α_L = Longitudinal Dispersivity

α_T = Transverse Dispersivity

D_d = Coefficient of Molecular Diffusion

D_x = Coefficient of Dispersion in x direction

D_z = Coefficient of Dispersion in z direction

V_x , V_z = Velocities in x and z directions respectively

$\overline{V}$ = Magnitude of Velocity Vector

The values for dispersivity are taken as 5 m, and the ratio of transverse to longitudinal dispersivity is kept as 1.0. The coefficient of molecular diffusion term used in the evaluation of dispersion coefficient is kept equal to zero, in order to match the term used by Pickens and Lennox (1976). As a measure of check, a computer program SEEP (Duncan, 1988) which is a finite element program for the groundwater flow in saturated zone, was used to compare the nodal head values computed by POLUT2D. After comparison it was found, the maximum percentage of error was less than 0.2 %.

In the problem, it is assumed that there is no sink or source affecting the groundwater flow, therefore $\overline{Q}$ in the mass transport equation is zero. Similarly the contaminant is assumed as inorganic chemical, which is not biodegradable or radioactive, therefore first order decay coefficient is taken as zero and retardation factor is taken as 1. The water table boundary condition is of the prescribed or known head (Dirichlet type). The values of hydraulic head at the 64 different nodes at the water table boundary are used as input, assuming that the head at these nodes doesn't change with respect to time. The contaminant source is located between 150 m and 300 m from the upstream end of the domain. For the purposes of analysis, it is assumed that concentration input C_o remains con-

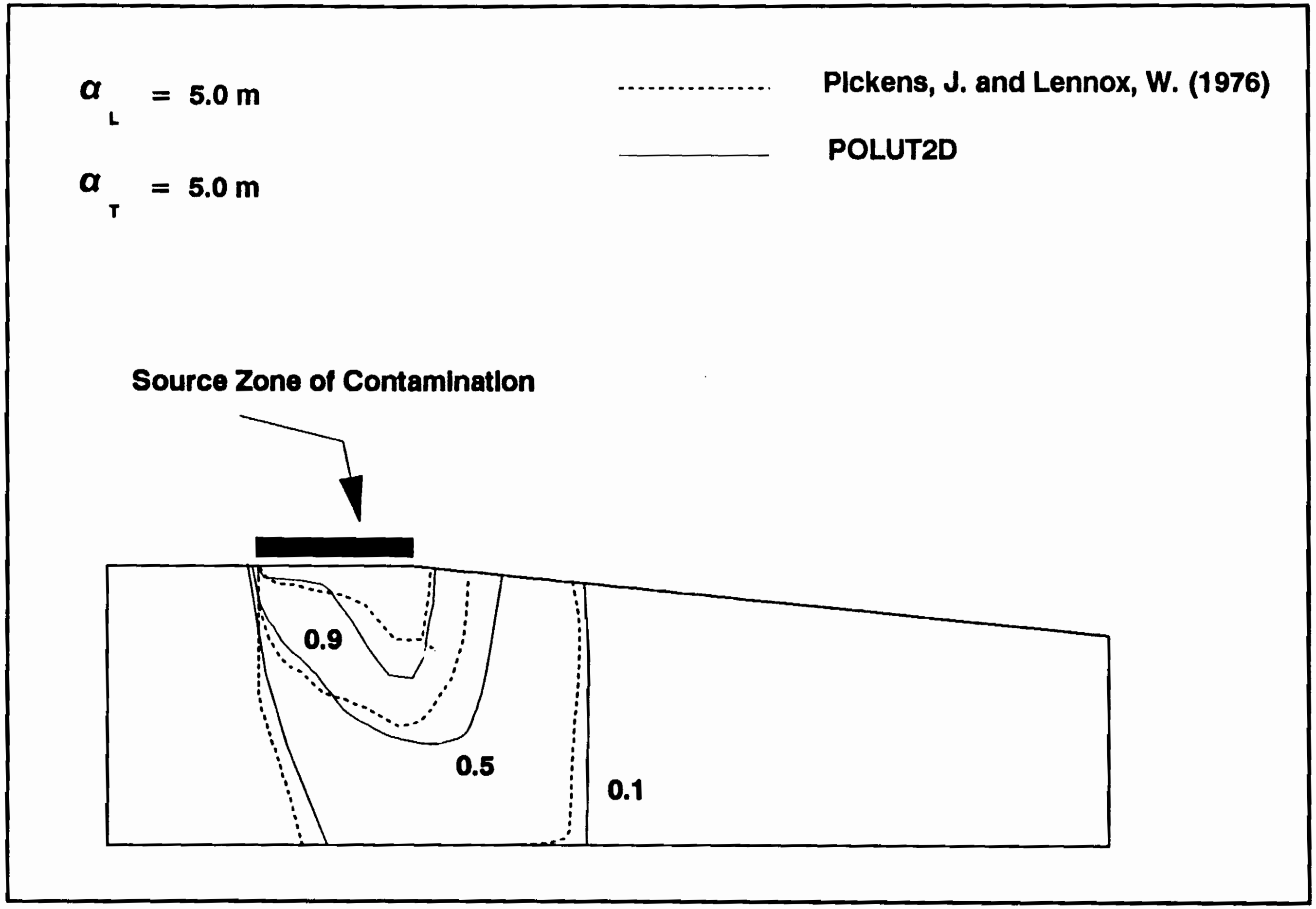


Figure 5.3 Comparison of Contours at C/C_o of 0.9, 0.5, and 0.1 at t = 15 years

stant with respect to time, although which may or may not be the case in a real situation. In many cases in waste disposal problems, the input concentration starts at a low value, increases to a peak value and then it stabilizes to a lower value. Since in this case the problem is being modelled for saturated conditions which indicate long term conditions, therefore it might be appropriate to assume a constant value for the input concentration.

Figure 5.3 shows a comparison of values for the concentration spread obtained by Pickens and Lennox (1976) and the program POLUT2D. In the presentation of results, the concentration C in the porous domain is given as a ratio C/C_0 where C_0 is the concentration introduced at the surface. The figure shows the computed contour levels for C/C_0 of 0.9, 0.5, and 0.1 at time level of 15 years. The saturated hydraulic conductivity in x and z direction is assumed to be 0.5 m/day, where as the longitudinal and transverse dispersivities are used as 5.0 meters. The dotted line contour plots shows values obtained in the paper (Pickens and Lennox, 1976) and solid line contour plots shows values obtained by POLUT2D. The computed contour lines obtained by POLUT2D deviate only slightly from the paper and difference between the two decreases as the contours of C/C_0 approach 0.1. The contours obtained by POLUT2D, exhibit the same shape as obtained in the paper by Pickens, J. and Lennox, W. but the contour levels obtained by POLUT2D spread out a little more towards the downstream of the water table. The conditions for the solution of this problem were kept same as used by Pickens and Lennox (1976)., and this slight deviation could be attributed to the factors such as the discretization, type of the element used, time step and iteration technique.

Pickens and Lennox (1976) discretized the geological cross section into 720 triangular elements with 410 nodes, whereas for POLUT2D, 315 linear quadrilateral elements with 384 nodes were used to discretize the cross section. The use of quadrilateral elements yield better solution than that obtained by using triangular elements, on account of the bilinear shape functions of the quadrilateral element compared to the linear shape functions of the triangular elements and as such the gradients are constant in a triangular element leading to step change of flow from element to element.

The factors such as time integration technique, time step affect the performance of the numerical model. The time integration technique used by POLUT2D is backward difference scheme and the same method is used by Pickens and Lennox (1976) in their numerical model. In backward finite difference scheme, the time step Δt affects only the accuracy but not the stability of the numerical performance. However, the solution may become less accurate if the time step Δt is too large, especially in the early time stages. The number of time steps used by Pickens, J. and Lennox, W. as indicated in their paper were close to 20 where as the number of time steps used in POLUT2D were more than 50, which could be one of the reasons for slight deviation obtained as shown in figure 5.3.

The computer program POLUT2D was run on a 80386 based machine and the program employs double precision for variables used in the program and the average execution time was about 30 minutes. The maximum size of the size of mesh on the PC version of the program was limited to 400 elements with upto 500 nodes. Pickens and Lennox (1976) employed a IBM 360/75 computer using single precision variables.

Parametric Study

In this part of the chapter, the effects of some of the parameters involved in two-dimensional pollutant transport problem in a porous medium are studied. For this purpose the problem as shown in figure 5.1 with the finite element discretization illustrated as figure 5.2, is chosen. The solution of the problem for the parametric study involves the same boundary conditions as used before.

Effect of Dispersivity in the Aquifer

The effects of both horizontal and transverse components of dispersivity are studied here by changing the values of α_L and α_T (See Eqn. 3.7)

Figure 5.4 shows the effect associated with change in dispersivity values from 1.0 m to 100.0 m on the spread of concentration distribution. The values for the parameter dispersivity were varied while all other parameters were held constant. The concentration distribution contours displayed in figure are obtained at time 15 years with C/C_0 values of 0.2. The ratio of longitudinal disperivity to transverse dispersivity α_L/α_T is kept equal to 1. The results illustrated by figure 5.4 show, in general that as the value of dispersivity increases, the contaminants move further in the aquifer and the plume size is larger and thus indicating the role of the dispersion as a transporting agent, in this problem. In this problem (figure 5.4), for a 100 fold increase in the values of dispersivity, the plume size area grew by $2\frac{1}{2}$ times and the plume moved further down 200 m towards the river.

The results also show that the concentration gradient (C/C_0) decreases with the increase in dispersivity value. In figures 5.5 and 5.6 the effects of transverse and longitudinal dispersivity are shown using contours of concentration value of 0.2 at time 15 years. The figure 5.5 was obtained by keeping the longitudinal dispersivity a constant (10 m) while varying transverse dispersivity from 10.0 to 200 m. The figure 5.6 displays concentration spread values obtained by keeping the transverse dispersivity at 10 m and varying longitudinal dispersivity from 10.0 to 200.0 m. The

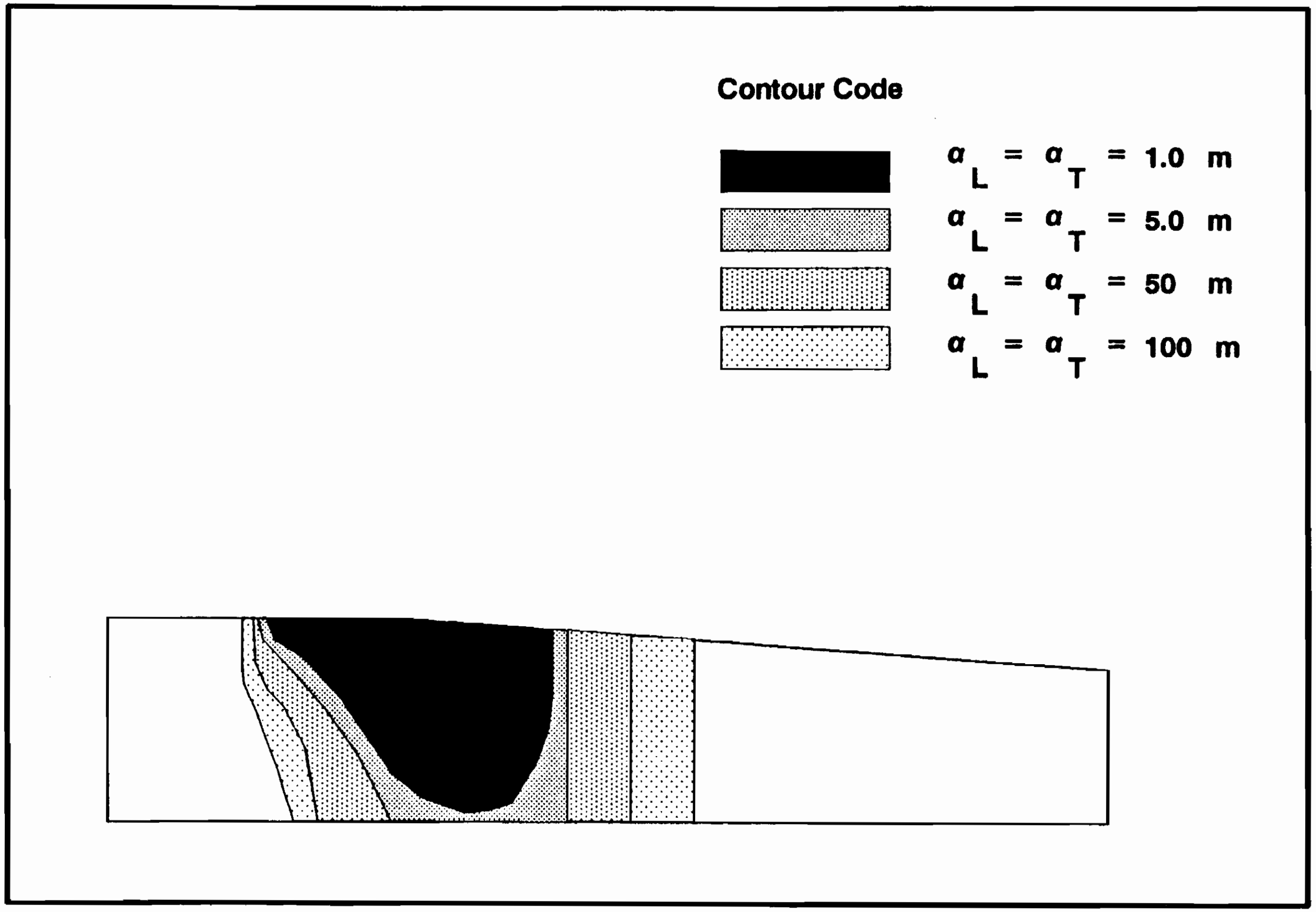


Figure 5.4 Effect of Dispersivity Values on the Spread of Concentration Distribution at t = 15 years. Contours at C/C_o Values of 0.2

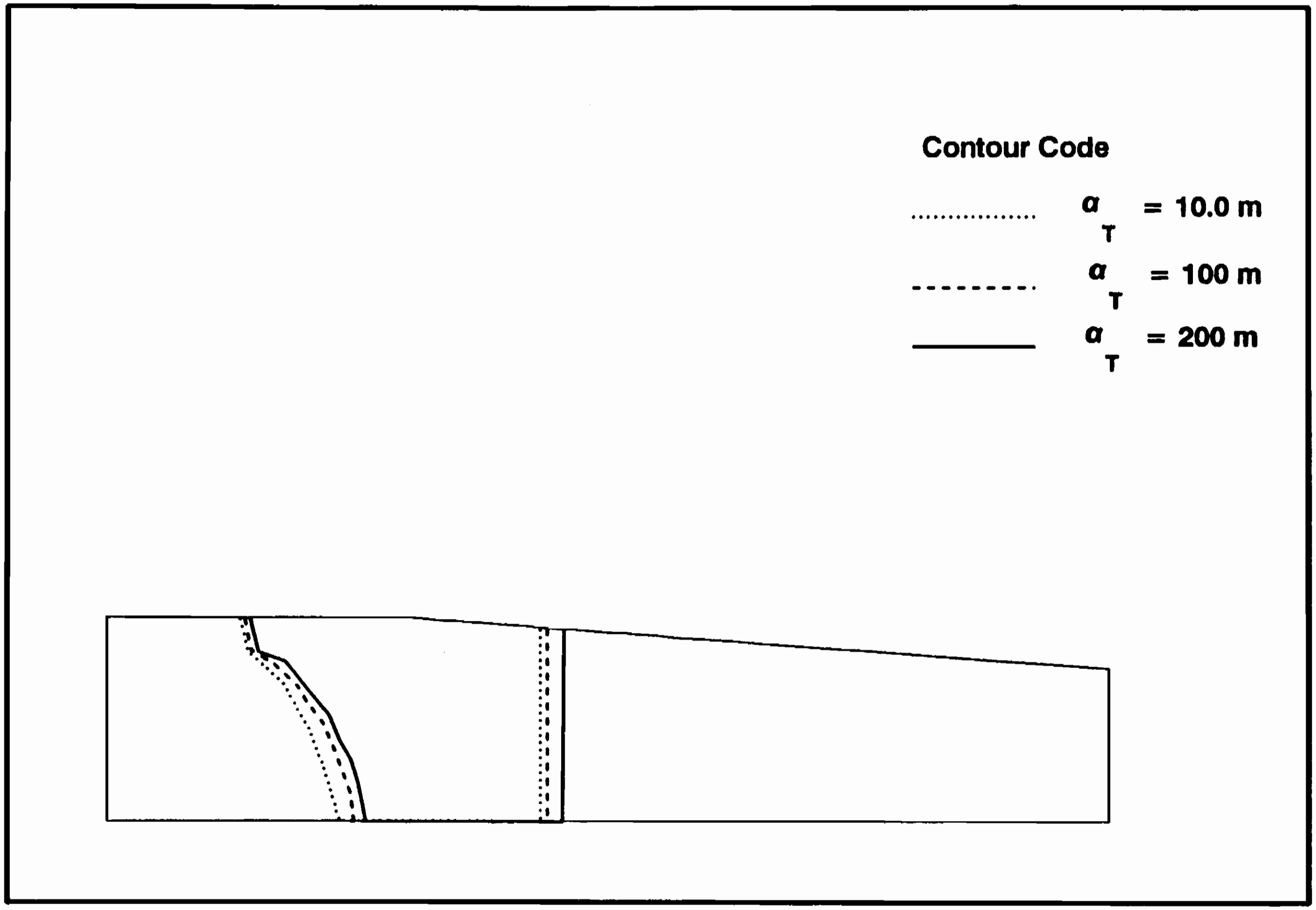


Figure 5.5 The Effect of Transverse Dispersivity on Concentration (α_L = 10 m, time = 15 years, all contours at C/C_o = 0.2)

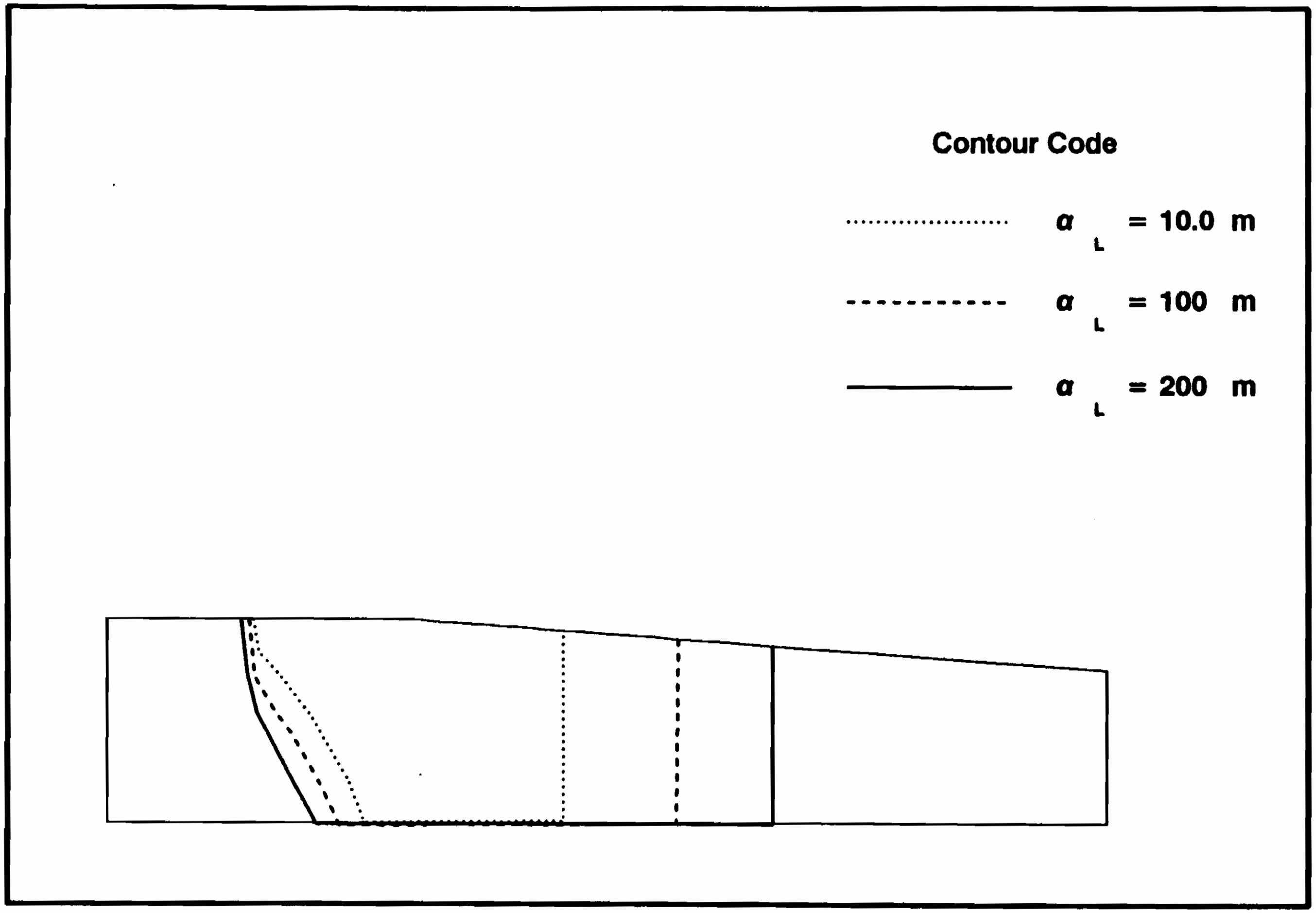


Figure 5.6 The Effect of Longitudinal Dispersivity on Concentration
(α_T = 10.0 m, Time = 15 years, All Contours C/C_o = 0.2)

groundwater flow in this problem is horizontal, therefore by increasing the value for the transverse dispersivity has less effect on the spread of the concentration distribution (figure 5.5) as compared to the varying the longitudinal dispersivity (figure 5.6). However at early time levels the variation in transverse dispersivity effects the downward movement of the concentration contour until it reaches the bottom boundary at late time levels. In figure 5.5, for a 20 fold increase in the transverse dispersivity increased the plume area by 5 % whereas in figure 5.6, with 20 fold increase in the longitudinal dispersivity increased the plume size (area) by 85 %.

Effect of Saturated Hydraulic Conductivity

The groundwater velocity has a significant effect on the dilution of contaminant, since it is used in the mass transport equation as the convective term. Figure 5.7 demonstrates the effect of hydraulic conductivity by keeping the dispersivity constant. In the case(1) of figure 5.7, the value of conductivity in x - direction is kept at 0.01 m/day, while conductivity value in z - direction is varied from 0.01 to 1.0 m/day. As the value of conductivity in z - direction increases the movement of contaminants towards the base increases as expected. flow system. In figure 5.7 (cases 1 thru 3), considering the isotropic cases, i.e where ($K_x = K_z$), by increasing the values of saturated hydraulic conductivity by 100 times, the size of plume grew by 15 fold. The values of 0.01 m/day for Kx and Kz are the representative values for clay, 0.1 m/day for silty clay and 1.0 m/day for loose sand, and thus the increase in the size of plume (figure 5.7) stresses the need for caution in selecting the values of hydraulic conductivity for this problem. The cases (1) thru (3) in this figure also indicate that, since the groundwater flow system is horizontal therefore increasing the saturated hydraulic conductivity in x direction contributes significantly to the spread out (largely towards right) of contaminants in the aquifer.

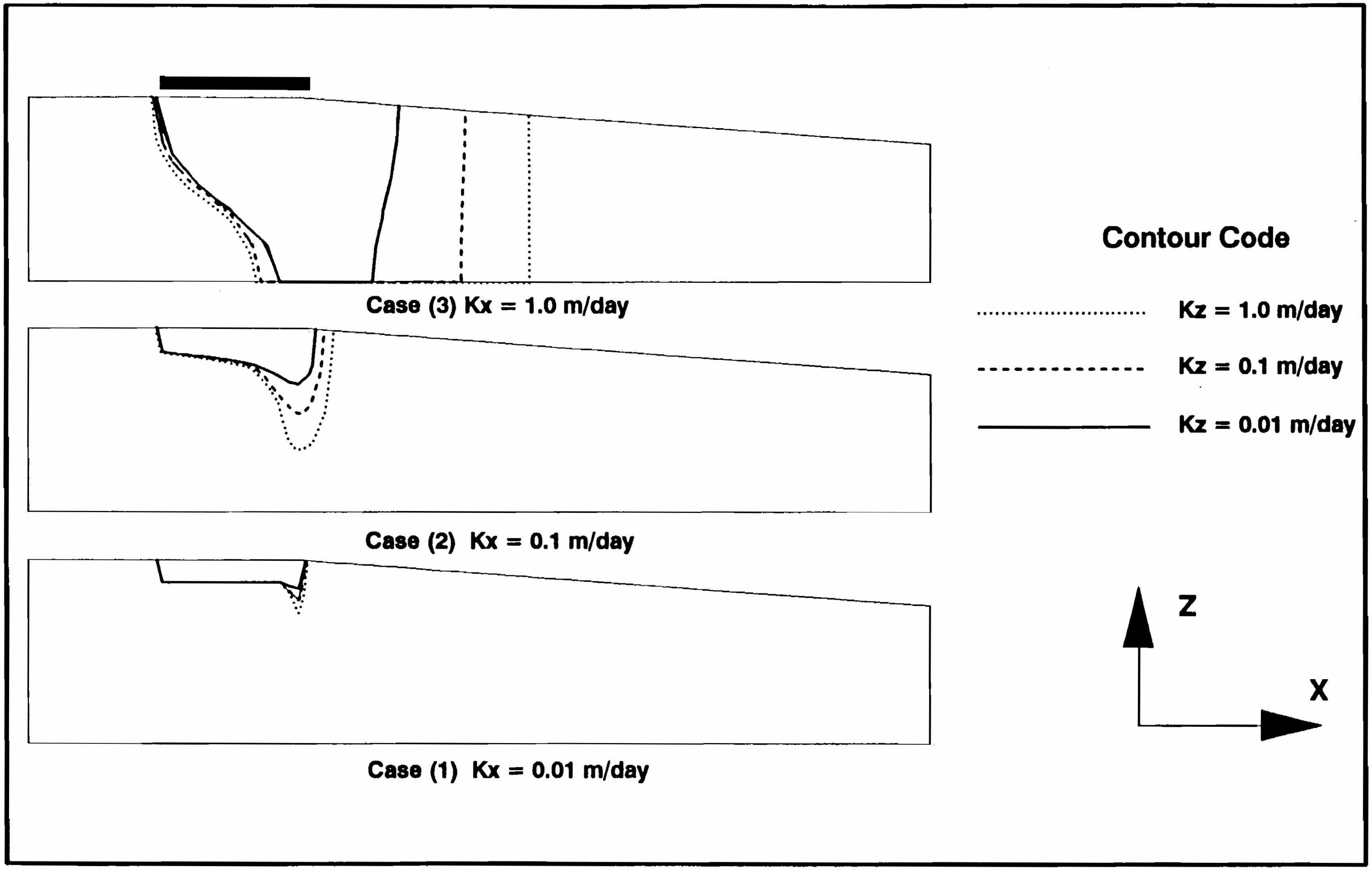


Figure 5.7 Effect of Saturated Hydraulic Conductivity on the Concentration Distribution (Time = 15 years). Contours at C/C_o of 0.4

Effect of Barriers in the Control of Pollution

According to Rowe (1988), for the control of pollution spread in the groundwater system, the preventive measures or barriers usually come under one of the following categories:

- Compacted and Natural Clay Liners
- Synthetic Liners (Including Geomembranes, hydraulic asphalt concrete)
- Hydraulic Controls such as Contaminant recovery wells to isolate the flow system
- Cut-off Walls

Compacted clay liners are frequently used in the design and construction of new waste disposal facilities. The clay layer can be present naturally or can be constructed easily, since clay is one of the most readily available construction materials. The clay liners have adsorption capacity for many wastes and their capacity to withstand cracking is the other advantage.

Synthetic liners are usually relatively thin and they have extremely low hydraulic conductivity and are used in the construction of new waste disposal landfills. However they do not exhibit contaminant adsorption characteristics as in clay liners. Factors such as temperature during installation, bonding and orientation of seams are some of the factors affecting their performance (Mitchell and Brandon 1984).

Hydraulic controls can be used to isolate groundwater from contaminants in existing and new waste disposal sites. The hydraulic barriers can also be coupled with cutoff barriers thus reducing the pumping requirements. The hydraulic controls usually consist of well point systems and deep well systems. The dewatering of the site causes an inward hydraulic gradient toward the leachate and controlling the outward spread of contaminant plume, although care must be exercised to use this method.

Cutoff walls are most commonly (Rowe, 1988) used to control contaminant movement from existing waste disposal sites. There are various types of cutoff walls; including slurry trench cutoff walls, grouted cutoff walls, sheet piles and diaphragm walls (Mitchell and Brandon, 1984).

For the problem shown in figure 5.1 with the finite element mesh shown in figure 5.2, the effect of slurry trench cutoff wall on the movement of contaminant plume is evaluated. The slurry trench

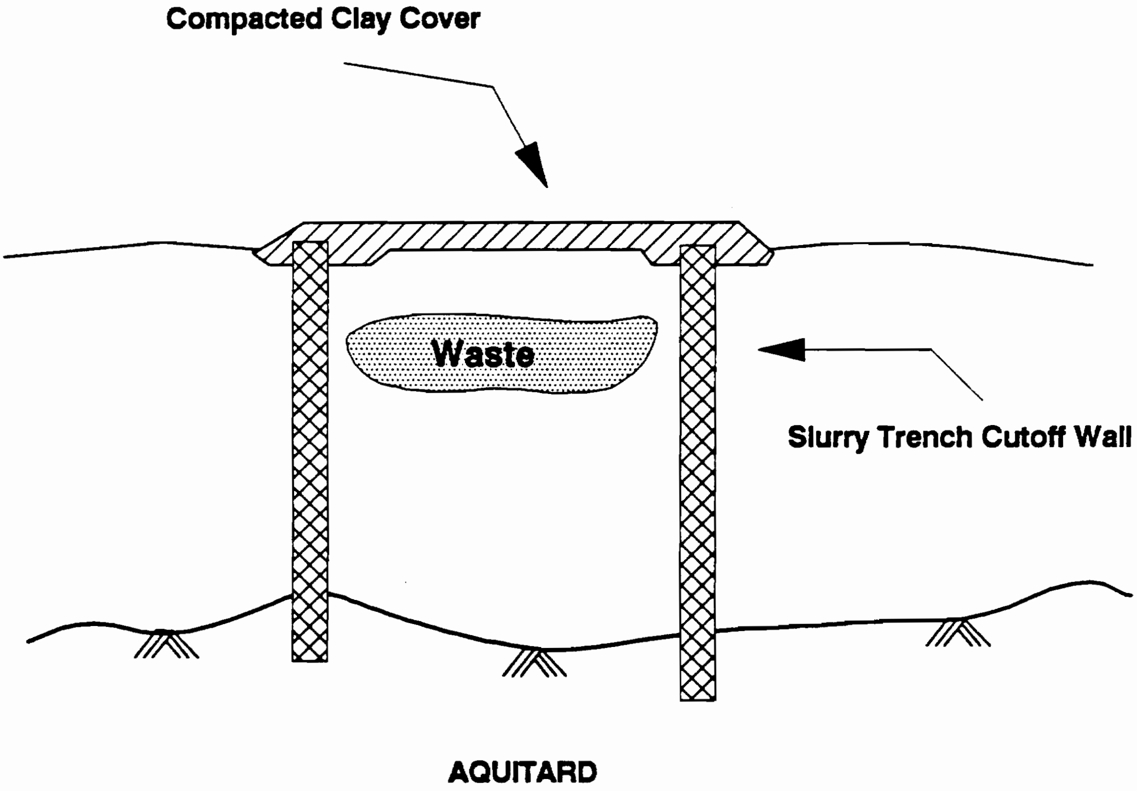


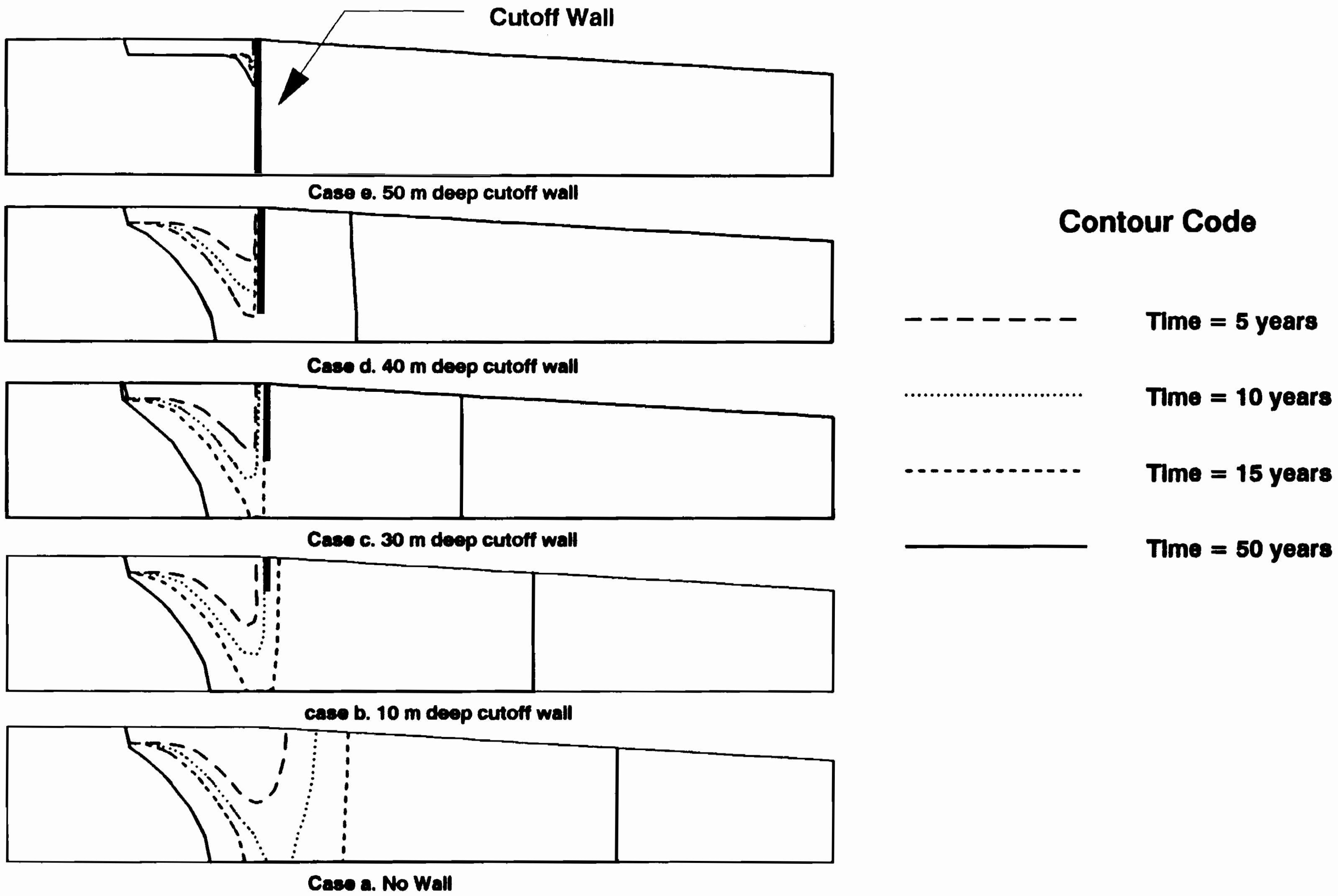
Figure 5.8 Slurry Trench Cutoff Wall with Compacted Clay Cover
(Adapted from D'Appolonia, 1982)

cutoff wall is selected for this problem because they can be constructed for depths upto 100 ft and below the water table. (D'Appolonia, 1982). Slurry trench cutoff walls (Figure 5.8) consist of narrow, clay-filled or cement-bentonite filled trench excavated into an aquitard by a backhoe or clamshell excavator. Hydraulic conductivities as low as 1 x 10^{-8} cm/sec can be achieved (Tallard, 1984).

The slurry trench cutoff wall presented in figure 5.9 is 1.5 m thick. The hydraulic conductivity of the wall is taken as 1 x 10^{-7} cm/sec. The depth of the cutoff is taken as depth from the water table surface. (figure 5.9). In this figure five different cases are studied, in case (a) there is no cutoff wall and in case (e), the depth of the cutoff wall is 50 m, equal to the depth bottom impermeable boundary. The parameter values for the hydraulic conductivity, horizontal and vertical components of dispersivity and the boundary conditions were kept constant. For comparison, the predicted concentration plumes at four different time levels of 5, 10, 15 and 50 years are shown in figure 5.9. It can be seen that, for time level of 5 years, the concentration plume does not go beyond the cutoff wall for cases (b) thru (e). If the time frame under consideration is greater than 50 years, it is worth to note that a depth of 50 m is required to prevent the movement of plume beyond the cutoff wall, however if it is upto 15 years, a depth of 25 to 30 m can be used for the cutoff wall.

Summary

The computer program POLUT2D is evaluated and the results were compared to the solution obtained in the literature. The predicted spreading of the plume is presented at different time levels. The effects of dispersivity, hydraulic conductivities are described and discussed. The effect of depth of a cutoff wall for the control of spread of contaminants is studied.



Case e. 50 m deep cutoff wall

Case d. 40 m deep cutoff wall

Case c. 30 m deep cutoff wall

case b. 10 m deep cutoff wall

Case a. No Wall

Figure 5.9 Effect of Slurry Trench Cutoff Wall on the Concentration Spread Contours at C/C_o of 0.4 at Various Time Levels

CHAPTER 6

Finite Element Modelling of Army Creek Landfill

In this chapter, computer program POLUT2D is used to model the flow of pollutants at well points from a landfill known as Army Creek Landfill, located in New Castle County - Delaware. In the previous chapter of this thesis, the program POLUT2D was evaluated by studying an example problem given in the literature.

The Army Creek Landfill is presently closed, but in 1960's till 1968 it received solid and liquid industrial wastes including municipal wastes. After its closure, it was also listed under CERCLA with the with the Environmental Protection Agency (EPA). According to EPA (1984), the New Castle County has spent over 4 million dollars to control the flow of pollutants to an aquifer that supplies water to over 100,000 people, by implementing a program of contaminant recovery wells.

The study of the contaminant plume migration described in this chapter is strictly a modeling exercise. For purposes of modeling, it is important to be able to specify the time history of conditions of contamination at the source. It is also useful to have reliable water-quality data for comparison of the field situation with the numerical prediction. In the present instance these data bases were not available. Also there were not any data collected to compensate for inadequacies of the available data.

Site History

The Army Creek Landfill (previously known as Llangollen Landfill) is located in New Castle County in Northern Delaware (figure 6.1). It is situated approximately two miles southwest of the city of New Castle in Northern Delaware.

The landfill is about 4,000 ft long, 200 ft to 900 ft wide and covers an area of about 60 acres. The thickness of refuse varies from 6 to 35 ft with an average depth of 25 ft. the estimated volume of refuse is about two-million cubic yards (Figure 6.2).

Between 1960 and 1968, New Castle County, Delaware utilized an abandoned sand and gravel pit as the primary disposal site for the municipal and industrial wastes. From the records and test borings, it was determined that a modified area fill method was used to emplace the above mentioned refuse. The refuse burial started on the eastern end of the site and proceeded towards the pit entrance on the west. All intermittent refuse cover material was obtained within the excavation from residual sand, tailing piles and siltation basin deposits. As the time progressed, cover materials and landfill space became critically depleted; this situation encouraged deeper excavation, especially on the western end of the pit. The excavation removed some, and in few places all of the confining clay on top of the Potomac sands. This situation probably created direct access routes for the leachate from the landfill to enter the Potomac sands. During placement of refuse, compaction and covering operations were conducted by the sand and gravel operator and daily covering was not practiced. This coupled less than adequate compaction within the areas, caused differential settling and uneven finished surface when the final lift was emplaced in 1968. In 1970 the landfill was cov-

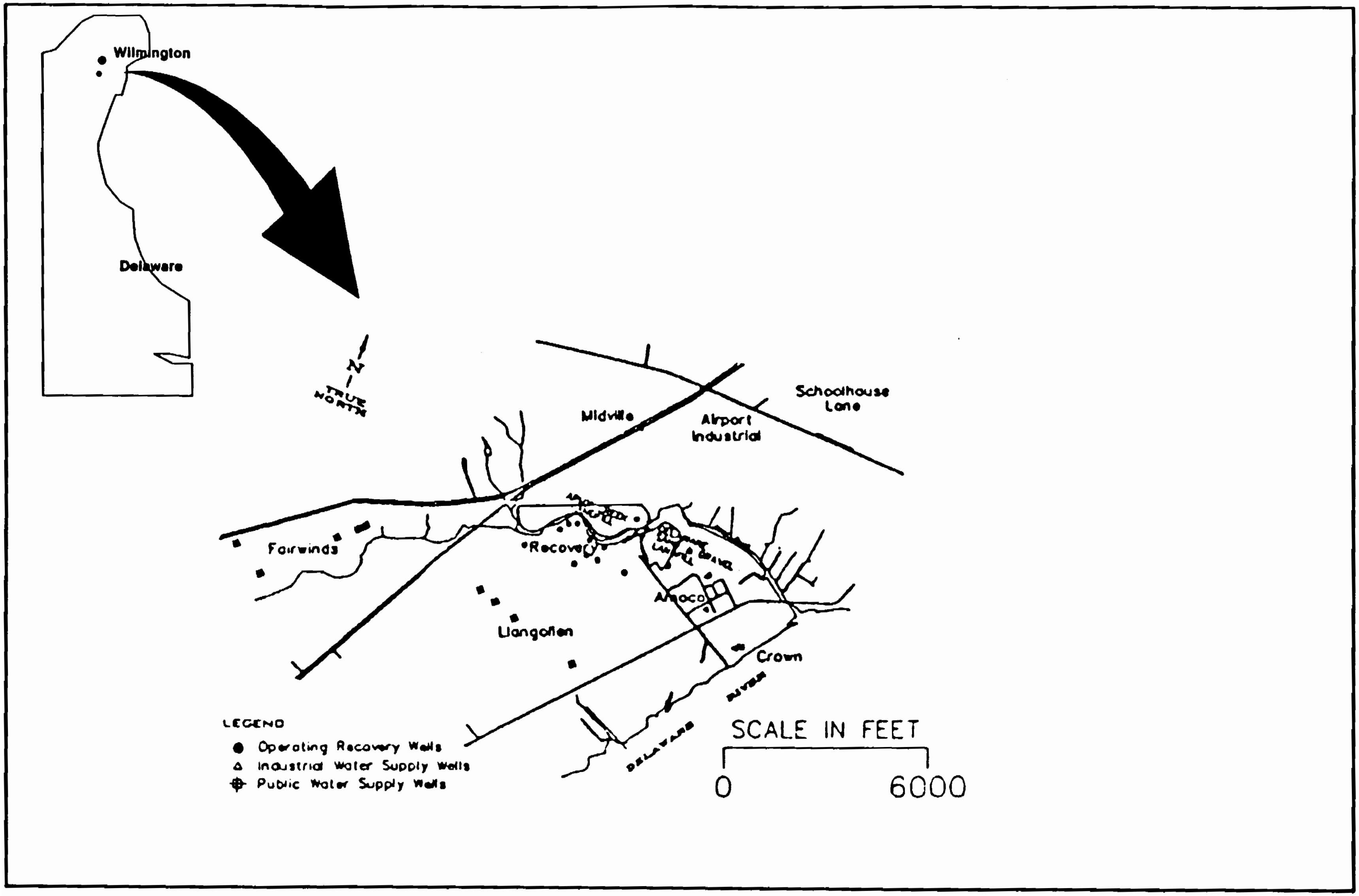
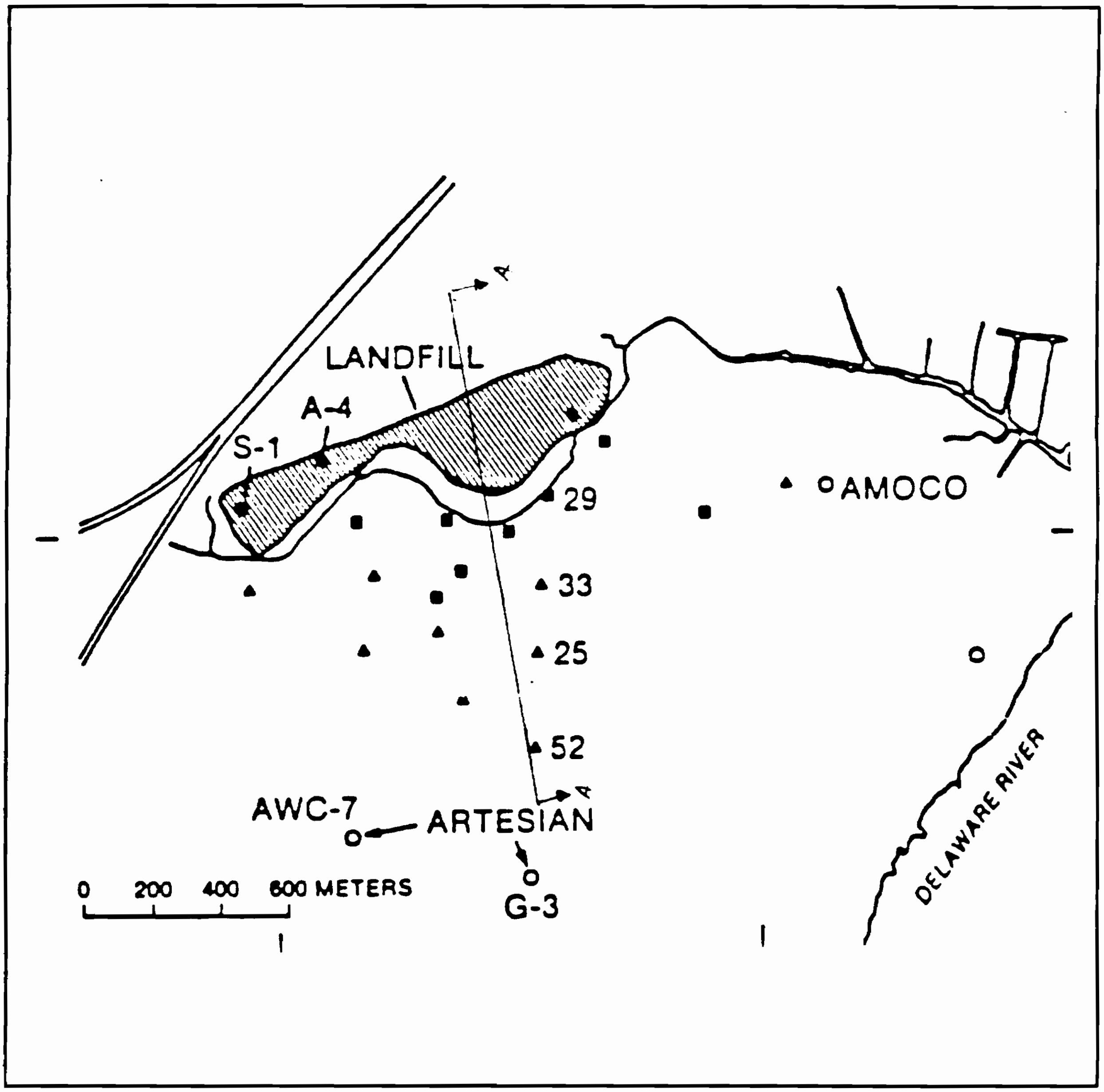


Figure 6.1 Location of Army Creek Landfill and Delaware Sand and Gravel Landfill (Adapted From Clark, D. C. 1979)



Key ● Landfill Wells ■ Recovery Wells ▲ Landfill Wells ○ Suplily Wells

Figure 6.2 Plan View of Army Creek Landfill Site with Location of Wells (Adapted from Baedecker, M. and Apgar, M. 1984)

ered with about 2 ft of soil - mostly sand. It was then purchased by New Castle County and turned over to their Department of Parks and Recreation with the intention that it became a county park. Many types of wastes were buried, including solid and liquid industrial wastes and municipal wastes. It is estimated that about 30 percent (or 600,000 cubic yards) of refuse was beneath the seasonal high water table (Clark, 1979 and Baedecker and Apgar, 1984).

Late in 1971, water in a residential well, located about 900 feet southwest of the landfill, developed quality problems such as a distinctly disagreeable odor and permanent staining of fixtures. Gradually, this situation became more pronounced and the water supply well was abandoned. Analyses conducted by the Delaware Geological Survey and New Castle County Public Works Department indicated the presence of leachate in the ground water. In early 1972 intensive field study was started by New Castle County through its consultant, Roy F. Weston, Inc., and the Delaware Geological Survey to determine the hydrogeologic circumstances responsible for this problem. Later to limit the spread of contaminants, a co-ordinated effort was undertaken to reduce pumping from supply wells and to initiate a program of recovery-well pumping between the landfill and the supply wells. Pumping of the contaminant recovery wells caused a local cone of depression, which reduced contaminant movement towards the supply wells. The recovery well program was started in 1973 and expanded in 1974 to the 10 wells and some of them still operate today. The recovery wells discharge into Army Creek, which flows into Delaware River (Niessen, 1974).

Geological Setting of the landfill

The vicinity of Army Creek Landfill lies in the Atlantic Coastal physiographic province Plain and includes both the saturated and unsaturated zones. The sand excavated from the present landfill site was a part of the Columbia Group, a Pleistocene stream deposit which consists of medium to coarse sand with interbedded gravel. (Jordan, 1976) The Columbia Group forms continuous surficial cover ranging from 10 to 60 feet in thickness. The base of Columbia Group ranges from 10 to 20 feet below mean sea level in the vicinity of the landfill (Clark, 1979).

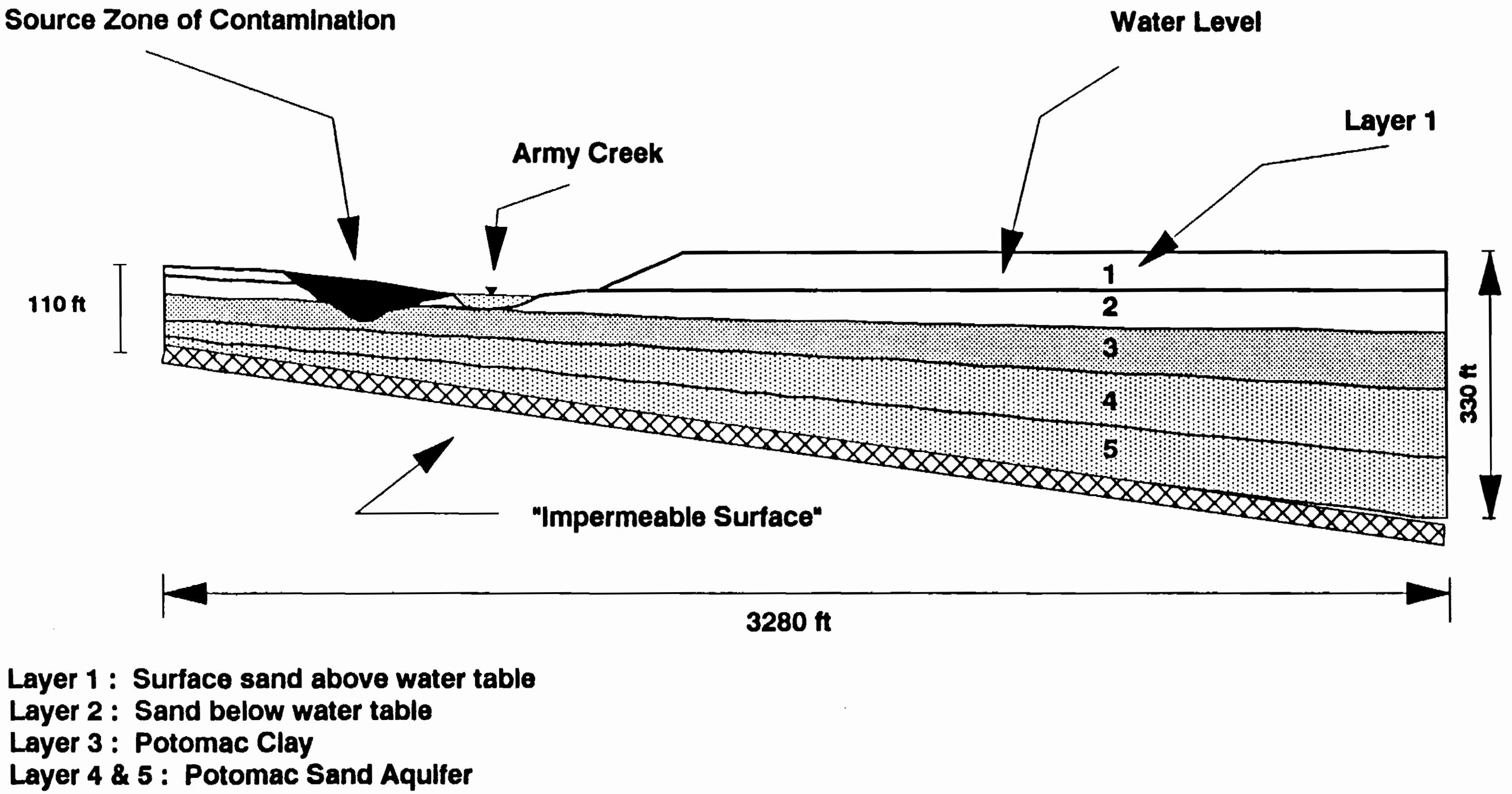


Figure 6.3 Geological Cross section of Army Creek Landfill
(Adapted From Baedecker, M. and Apgar, M. 1984)

A geological section A-A obtained from Figure 6.2, is described in the figure 6.3. The layer 1 and layer 2 in figure 6.3, belong to the Columbia Group and underlying the Columbia Group sand is the Cretacious Potomac Formation. The layer underlying Potomac Formation (below layer 5 in figure 6.3) is Precambrian rocks and is assumed as "impermeable" for the purpose of pollutant transport modelling.

The Potomac Formation consists of silt and clay interbedded quartz sand and some gravel (Pickett, 1970). The Potomac Formation sand units are generally channel shaped, though often laterally extensive lenticular clay and silt deposits are interbedded with thin lenses and thick blankets of clay and silt which accumulated on ancient flood plains with estuaries. A fairly consistent Potomac layer also consist of a clay layer of variable thickness. Due to the lensatic depositional nature of the Potomac Formation, this clay layer varies in thickness and textural character throughout a cross section of the landfill in north-south direction. This is also shown in Figure 6.3, which is also a north-south section (Baedecker, and Apgar, 1984).

The layer underlying Potomac Sand is a layer consisting of Precambrian rocks and stream deposited unconsolidated sands, silts, and clays of Early Cretacious Age. The formation is approximately 600 feet thick in the vicinity of landfill and rests on a seaward-dipping bed rock surface (Clark, 1979).

Hydrologically the generally coarse Columbia Group deposits serve as an infiltration and recharge gallery for Potomac sands. Ground water in the Potomac sands becomes confined (artesian) beneath the relatively impermeable beds of clay and silts as it travels seaward down dip in the formation. Immediately beneath the landfill these clay and silt deposits appear shallow or thin. In the area off the southeast corner of the landfill they are absent (Niessen, W. 1974).

The relatively thin clay layer in the area of landfill probably created direct connections between the base of the refuse and the Potomac Sand aquifer (Apgar, M. 1975).

Previous Studies

In late 1971, water in a residential well, located about 900 feet southwest of the landfill, developed water quality problems such as a distinctly disagreeable odor and permanent staining of the fixtures. Gradually this situation became more pronounced and that water supply well was abandoned. The New Castle County Public Works Department and Delaware Geological Survey conducted analyses and came to the conclusion of presence of leachate in the groundwater.

In early 1972, intensive field study was launched to investigate the magnitude and extent of this problem by New Castle County through its consultant Roy F. Weston. Hydrogeologic analysis revealed a large plume of leachate migrating towards the well field of a major water supply company. Roy F. Weston, Inc. (Niessen, 1974) came up with several options to control the flow of leachate, including: (1) Hydrogeological Control, (2) Incineration control, (3) Haul - Dump Control. Hydrogeological control involved the use of pumping and treatment for an indefinite period, whereas Incineration control involved excavation and incineration of the landfill, although it was the most desirable from the standpoint of permanent solutions but it was abandoned because of the prohibitive capital cost. The haul - dump control required the relocation of the landfill to a new location which would be constructed using liner and leachate collection system but it was also abandoned because it lacked political appeal. Roy F. Weston recommended the use of hydrogeological control program to minimize leaching in the near-term but to date it has been the only control program in operation.

In 1982, William Miller, studied the geology and water resources of the Army Creek vicinity, as a part of his MS thesis. He used a USGS (U.S Geological Survey) two- dimensional, finite difference flow code for the evaluation of the regional groundwater flow system incorporating natural aquifer boundaries. This study provided a insight into the material properties such as the hydraulic conductivity of the area. In 1984, Mary Baedecker and Michael Apgar published a paper (Baedecker, M. and Apgar, M. 1984) titled "Hydrogeochemical Studies at a Landfill in Delaware" in which they analyzed the leachate characteristics and also provided actual Cl^- concentrations at different well points at different time levels. In 1990, William Miller (Miller, W. 1990) used a computer program SWIFT (Sandia Waste Isolation, Flow, and Transport - developed under contract to the Nuclear Regulatory Agency) to model contaminant transport in the vicinity of Army Creek Landfill from an other landfill known as Delaware Sand and Gravel landfill. SWIFT is a fully three-dimensional code which uses finite difference techniques to solve problems involving fluid flow, heat transport, and transport of trace or dominant (density dependent) species. This 3-D modelling also provided another look at the material properties and geological setting and various boundary conditions involved.

Two Dimensional Finite Element Modelling

The finite element program POLUT2D is used here to model Cl^- levels at well points 25 and 52 (see figure 6.2 for their location) at various time levels by considering advection and dispersion processes. The 2-D finite element procedure included several steps: assumptions to simplify the problem, discretization of the geological section, selection of the material properties such as hydraulic conductivities, establishment of initial and boundary conditions (both Neumann and Dirichlet types) and finally the solution for the unknowns. After the input of data, the model was "calibrated" for the present site conditions. This procedure included a series of adjustments of unknown transport parameters in such a way that the numerical solution corresponding to these parameters should coincide with the concentrations values observed at the monitoring wells as closely as possible.

Assumptions

The following are the general assumptions, which were made to simplify the analysis:

The seepage velocities are within the range of validity of Darcy's Law which is generally the case for intergranular porous media flow.

The density and viscosity of the groundwater flow is essentially constant, which is true for ranges of temperature encountered in most groundwater flow systems.

The groundwater flow pattern is not altered by the presence of contaminants in either the solution or sorbed phase. This and the preceding assumptions imply that density variations as a result of contaminant concentrations are negligible. This leads to the decoupled form of the flow and mass transport equations.

For this problem, as shown in figure 6.2, there are various types of wells such as Recovery wells, Landfill wells and supply wells. It is assumed that the flow of contaminants is not altered by their operation. Although this assumption is not true because the flow of contaminant has been controlled by their operation since 1970's, it may be noted that at the time of analysis there were no pumpage rates available and the location of well points 25 and 52 is far as compared to other wells and the pumpage rates are usually low at these distances from the source. The predicted values of concentrations at these well points could be higher than the actual values because of this assumption.

Selection & Discretization of Study Region & Boundary Conditions.

The geological cross section as shown in figure 6.3 was used to model the flow of contaminants. This geological cross section is taken as south-east section A-A (Figure 6.2) in the vicinity of the landfill because the contaminant movement had been primarily in this direction (Apgar, 1975).

The nodal arrangement for the finite element discretization, using 4-node quadrilateral elements, of the selected cross section, is illustrated in figure 6.4. In order to keep the mesh generation simple, cross section was divided into 299 elements with 375 nodes. The element shapes were kept close to rectangular shape but at some points due to geometric conditions triangular elements were used. For finite difference modeling of solute transport, grid blocks must be sized according to the Peclet critirion which, simply stated, relates grid block size to dispersivity values. The values for dispersivities used, are higher because the size of a element is bigger and the use of finer mesh (more elements and nodes) would have permitted smaller dispersivity values but in turn would have made computational costs prohibitive.

For the purposes of 2-D modeling, the geologic cross section A-A (figure 6.3) was divided into five layers; the layer 1 represents surface sand above the water table, layer 2 is part of surface sand situated below the water table and is assumed as saturated. The layers 1 and 2 are part of Columbia Group. The layer 3 represents clay and is known as Potomac Clay. The layers 4 and 5 belong to Potomac sand aquifer and underlying layer 5 is Precambrian rocks and is assumed as "impermeable". Thus bottom of layer 5 provides an no-flow boundary condition to be used in the model. At the lateral boundaries no-flow conditions were used.

Pumping records are important to a contaminant transport modeling because pumping can accelerate (or decelerate) the spread of a contaminant plume, and also alters the head profile. In this case of contaminant transport modeling sources of discharge and recharge are not included. Although as shown in figure 6.2, there are various types of wells such as Recovery wells, Landfill wells and supply wells, but the rates of pumpage from these wells were not available at the time of analysis. The location of well points 25 and 52 is far as compared to other wells and pumpage rates are usually low at these distances from the source zone of contamination. The predicted values of concentrations (by not considering pumpage.) at these well points could be higher than the actual values.

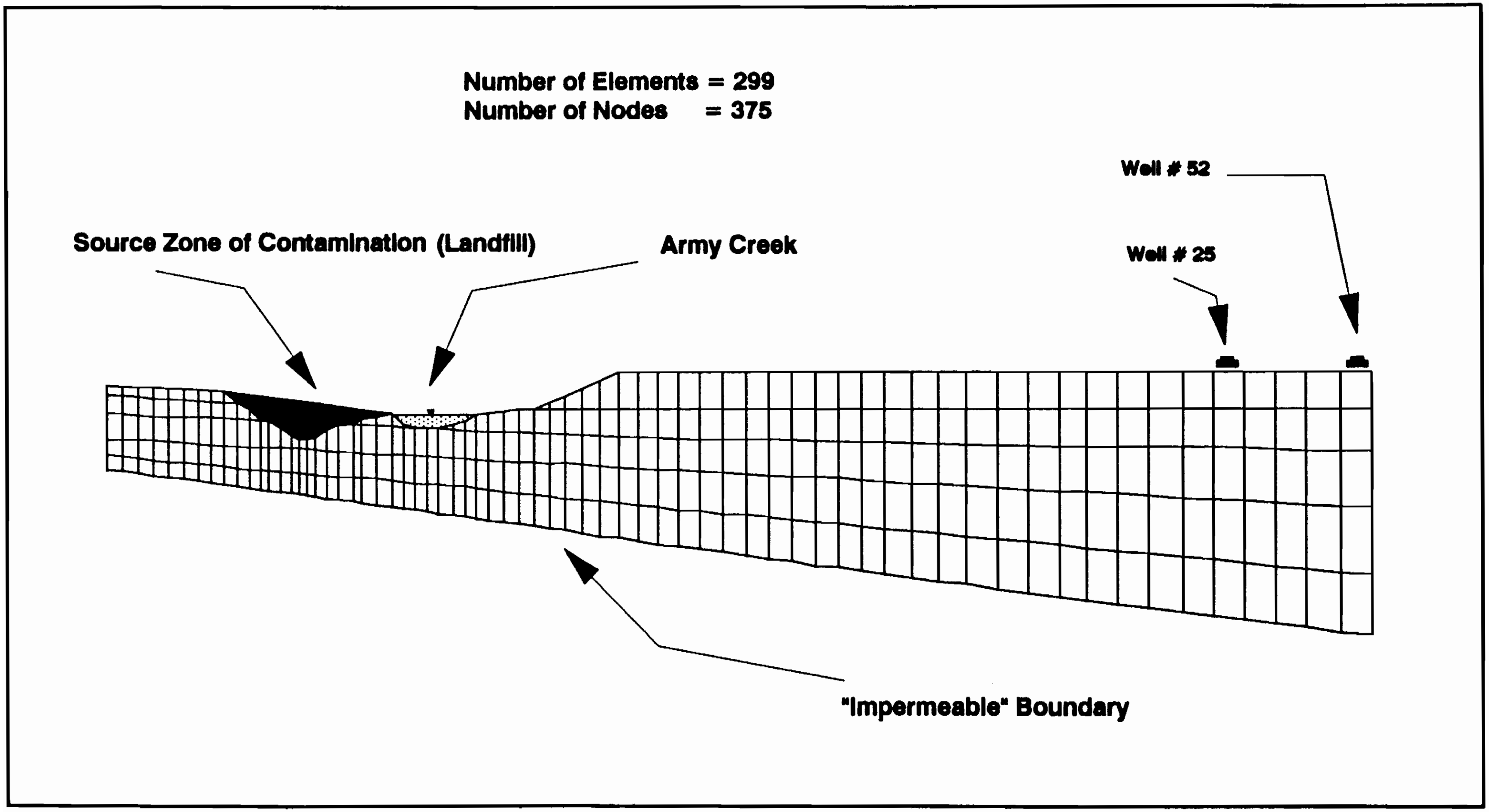


Figure 6.4 Finite Element discretization for the geological section shown in figure 6.3

The Army Creek (See figure 6.2) is a small tributary and it imposes a Dirichlet type condition of prescribed head on the nodes in the finite element mesh (see figure 6.4) under Army Creek.

Source Zone of Contamination

The Army Creek Landfill was used as a primary disposal site from 1960 to 1968, for the industrial and municipal wastes. Many types of wastes were buried, including solid and liquid industrial and municipal wastes. For the purposes of modeling, it is important to be able to specify the time history of conditions of contamination at the source. In the present instance, this information is not available.

According to Miller, W. (1990), the source Army Creek Landfill was initiated in November 1965. For the purposes of analysis, it is assumed that Concentration input $\mathbf{C_0}$ remains constant with respect to time. This assumption has limitations in that no possible decrease of contamination due to flushing is accounted for; on the other hand, no increase of contamination due to the possible rupure of waste drums is explicitly accounted for. The $\mathbf{C_0}$ values used are listed in Table 6.1, the $\mathbf{C_0}$ value was assigned to all the nodes (Figure 6.4) under Army Creek Landfill.

In this instance, available data is the Cl^- concentration levels on well 25 and 52. Chlorides are considered as conservative contaminants, which means that they are not sorbed by the soil or rock matrix, do not undergo radioactive or significant biological decay and do not precipitate. $\mathbf{Cl^-}$ concentration levels are often considered as being the primary indicator of a contaminant plume when monitoring contaminant transport from existing facilities. By considering modeling of conservative contaminants, there is no retardation and decay which leads to Retardation Factor of 1 and Decay coefficient of zero.

Table 6.1 Parameter Values used in 2-D Model

PARAMETERS	SOIL LAYERS				
	Surface Sand Above Water Layer 1	Surface Sand Below Water Layer 2	Potomac Clay Layer 3	Potomac Sand Aquifer Layer 4	Potomac Sand Aquifer Layer 5
Sat Hyd. Conductivity (Kx) ft/year	18250	18250	1.0	10000	10000
Sat Hyd. Conductivity (Kz) ft/year	18250	18250	1.0	10000	10000
Back Pressure	0.0	0.0	0.0	0.0	0.0
Angle of Anisotropy (Degrees)	0.0	0.0	0.0	0.0	0.0
Longitudinal Dispersivity (α_L) *ft*	1000.0	1000.0	1000.0	1000.0	1000.0
Transverse Dispersivity (α_T) *ft*	100.0	100.0	100.0	100.0	100.0
Coeff. of Molecular Diffusion	0.0	0.0	0.0	0.0	0.0
Residual Vol. Water Content	0.15	0.25	0.5	0.4	0.4
Saturated Vol. Water Content	0.4	0.4	0.5	0.4	0.4
van Genuchten Parameter α ft^{-1}	0.8	0.8	0.4	0.6	0.6
van Genuchten Parameter m	0.2	0.3	0.3	0.3	0.3
Input Concentration Value C_o	5 lb/ft^3/day				
Time of Initiation for Source (T = 0)	End of 1965				
Time Step	0.10 Year				

Soil Properties and Other Parameters

The groundwater velocities used in this 2-D pollutant transport model are obtained by using transient unsaturated flow equation as described in Chapter 2 of this thesis. For obtaining groundwater velocities following parameters are needed; Saturated hydraulic conductivities $\mathbf{K_x}$ and $\mathbf{K_z}$, back pressure, angle of anisotropy, saturated volumetric water content θ_s , residual volumetric water content θ_r and van Genuchten parameters α and m. The parameters $\mathbf{K_x}$, $\mathbf{K_z}$, θ_s , angle of anisotropy and back pressure have clear physical significance and are considered as "true soil properties", whereas residual volumetric content θ_r and van Genuchten parameters α and m are simply curve fitting parameters. The values of various parameters used in this study are summarized in Table 6.1.

The hydraulic conductivities control the velocities of groundwater by virtue of Darcy's Law and the velocities in turn control the subsurface movement of contaminant. For this 2-D model, both the field data and laboratory data on the hydraulic conductivities of soil was not available but "best match" data from a recent study was available (Miller, W. 1990). In the study by Miller (1990), 3-D modelling of flow of contaminants from a nearby landfill was studied by taking into account pumping rates at various recovery wells and by "matching" values of computed head with the observed head values at various time levels ranging from pre-pumping in 1961 to 1984. The values of saturated hydraulic conductivities range from 18250 ft/year (1.8x10E-2 cm/sec) for surface sand to 1.0 ft/year (9.67x10E-7 cm/sec) for clayey soil and the value of porosity or saturated volumetric water content ranges from 0.4 to 0.5. The values for residual volumetric water content and van Genuchten parameters α and m are taken as average values as described for these materials in Table 2.1.

The parameters necessary for the simulation of solute concentration include dispersivities in longitudinal and transverse directions α_L and α_T , coefficient of molecular diffusion and the velocities from the solution of flow equation. The coefficient of molecular diffusion was neglected by setting it to 0 (Miller 1990). In a contaminant transport model of a field situation, the values of field dispersivity are usually obtained by trial and error adjustment of the values of longitudinal and transverse components of dispersivity until the simulated transport pattern closely resembles the pattern or values of solute concentration obtained in the field. In this 2-D modelling, the values of dispersivity were assumed so as to obtain the match with the known values of solute concentration at wells 25 and 52.

Solution Procedure and Results

POLUT2D is used to solve the problem, the velocity field is obtained by solving transient unsaturated flow equation for nodal head values. The velocity field is then coupled with the mass transport equation to get the concentration spread at each time level by using backward difference scheme. For the time integration scheme, the value of time step was taken as 0.1 year. The geological cross-section is taken as south-east section A-A (Figure 6.2) in the vicinity of the landfill. The location of wells 25 and 52 is also shown in Figure 6.4. For this geological cross section only wells 25 and 52 were along the cross section. Figure 6.5 consists of two parts i.e first part displays comparison of concentration values with observed values for well 25 and the second part illustrates comparison for well 52. As it can be seen from figure 6.5, the observed values vary or fluctuate over the time whereas computed values don't show much variation. For example in the first part of figure 6.5, observed values show variation in the initial time period but later on values are not varying much, this could be the effect of pumping in the initial time period and later on pumpage on some wells was either reduced or stopped (Miller 1990). The fluctuation may be due to some events which are not recorded clearly or available. The events could have been heavy rains, heavy pumpage which could have effected the rate of flow. These events are not modelled in this FEM. However, the average concentration values (35 mg/l in Well 25 and 25 mg/l in Well 52) were matched between the FEM predictions and the field observations. This study is strictly a modeling excercise because lack of certain databases, however the solution can be

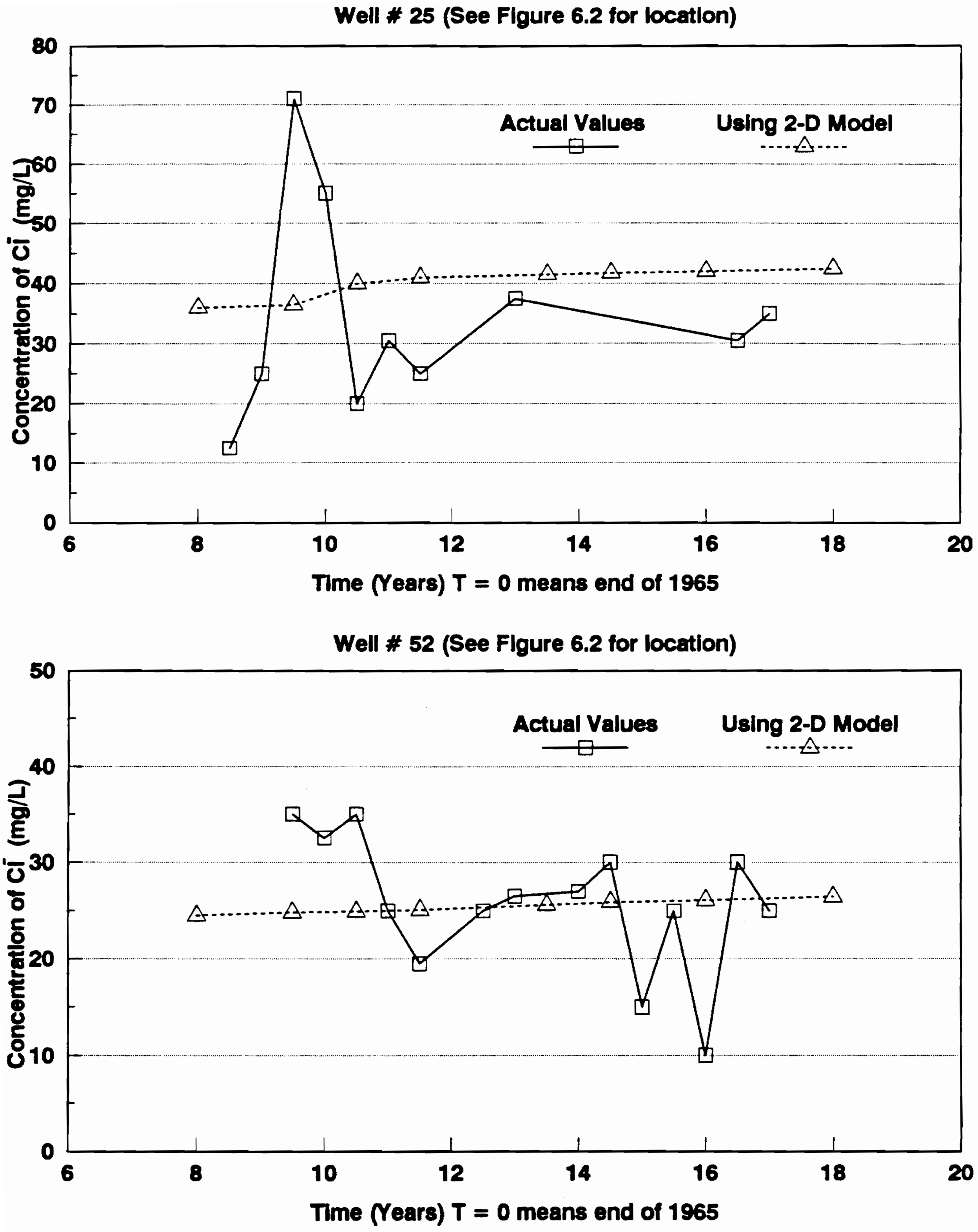


Figure 6.5 Comparison of Cl⁻ Concentration Values at Wells 25 and 52

improved by including pumpage rates, historical hydraulic head data, concentration values at various other locations and time levels.

Summary

In this chapter, vertical 2-D spread of contaminant from a site known as Army Creek Landfill located in Delaware, was studied using a finite element formulation for advective dispersive transport of pollutant through soils. The contaminant modelled was assumed as non-reactive inorganic species. The data regarding the hydraulic conductivities and porosity of soils concerned were taken from a contaminant modelling study conducted on another nearby landfill. (Miller 1990). The results, comparison of observed and computed concentration values at wells 25 and 52, are illustrated as figure 6.5. The fluctuations in observed concentration levels at both wells as compared to the computed values, may be due to some events which are not included in the F.E. model. These events could have been heavy rains or heavy pumpage which could have effected the flow rate and pattern. However, the average concentration values (35 mg/l in well # 25 and 25 mg/l in well # 52) match between the Finite Element model predictions and the field observations.

CHAPTER 7

Summary and Conclusions

Summary

The study has been concerned with the modeling of advective dispersive transport of dissolved contaminant through soils. The model is based on the flow and mass transport equations, and a finite element formulation was used to study the problems.

The flow equation used in this model was Richard's equation, which is applicable to both transient unsaturated and saturated flow. The equation uses the values of coefficient of moisture capacity C_h and hydraulic conductivity K from a soil water retention curve of a soil. The van Genuchten model employs two curve fitting parameters α and m to relate to soil water retention curve. The dispersion coefficient for the use in mass transport equation, is computed as suggested by Bear (1979). The finite element formulation based on the variational formulation for flow equation and Galerkin's method for mass transport equation was used. In order to obtain solution in time domain, backward finite difference scheme was used. The non-linearities imposed in the finite element formulation were handled by employing Picard's method.

An example problem given in the literature (Pickens and Lennox, 1976) was analyzed. Also for this problem, the effects of dispersivity, hydraulic conductivities, and the use of cutoff wall as an example of barriers to control spread of contaminant was studied. Another landfill problem known as Army Creek Landfill, located in Delaware was modelled and the results were compared with the field observed data.

Conclusions

The finite element formulation code POLUT2D, was evaluated by studying an example problem presented by Pickens and Lennox (1976). The study of this problem by Pickens and Lennox, (1976) used 720 triangular elements whereas POLUT2D used 315 quadrilateral elements. The results obtained by POLUT2D were reasonably close to those obtained by Pickens and Lennox (1976).

For the same problem, the effects of dispersivity (α_L and α_T) were studied. For a 100 fold increase in the values of the dispersivity (by keeping ratio of longitudinal to transverse dispersivity equal to 1), the plume size grew by 2 1/2 times and plume moved further down 200 m towards the river. For a 20 fold increase in the transverse dispersivity, by keeping longitudinal dispersivity constant, the plume area increased by 5 % whereas with a 20 fold increase in the longitudinal dispersivity increased the plume size (area) by 85 %.

As an example of barriers to control the movement of contaminant, a slurry trench cutoff wall of varying depth ranging from 50 m deep to 10 m deep was used to study the effects on the plume movement on this example problem. It was concluded that a cutoff wall of 50 m deep was required to block the plume movement for more than 50 years, whereas a cutoff wall of 25 to 30 m may be used to block plume movement for time period of 15 years.

The problem of Army Creek Landfill was studied and the computed concentration levels in the observation wells 25 and 52 were reasonably close to the average observed values. (35 mg/L in well # 25 and 25 mg/L in well # 52). However, there are fluctutations of observed concentration levels in these wells which may be due to some events which were not modelled in this study.

Appendix A. Computer Program POLUT2D

POLUT2D

POLUT2D is a finite element program, that can be applied to problems of contaminant or solute transport involving single chemical species in a vertical two dimensional plane. The program enables one to make advance predictions of the spread of pollutants with respect to time and space, into the ground water system in saturated as well as unsaturated porous medium.

In order to model the ground water flow in unsaturated zone, it uses Van Genuchten model and obtains average velocities. The velocities obtained are then coupled with the mass transport equation with advection and dispersion to get the concentration spread. The model also allows to consider isotropic and anisotropic hydraulic conductivity, hydrodynamic dispersion (Bear, J. 1979) and source or sink terms.

The type of the element used in POLUT2D is a four noded quadrilateral, isoparametric element and it uses bilinear shape functions.

The program POLUT2D, can be run on DOS and UNIX based Intergraph systems. The program was run on the UNIX based Intergraph's Interpro 120 and DOS based PC with hard disk and EGA or VGA graphics screen with math co-processor. The instructions for installation and operation of the program on either system are provided as README file on the disk.

The computer program POLUT2D consists of three parts and the structure of the overall processes is shown as figure A.1:

- Pre Processor
- Processor or Analysis Program
- Post Processor

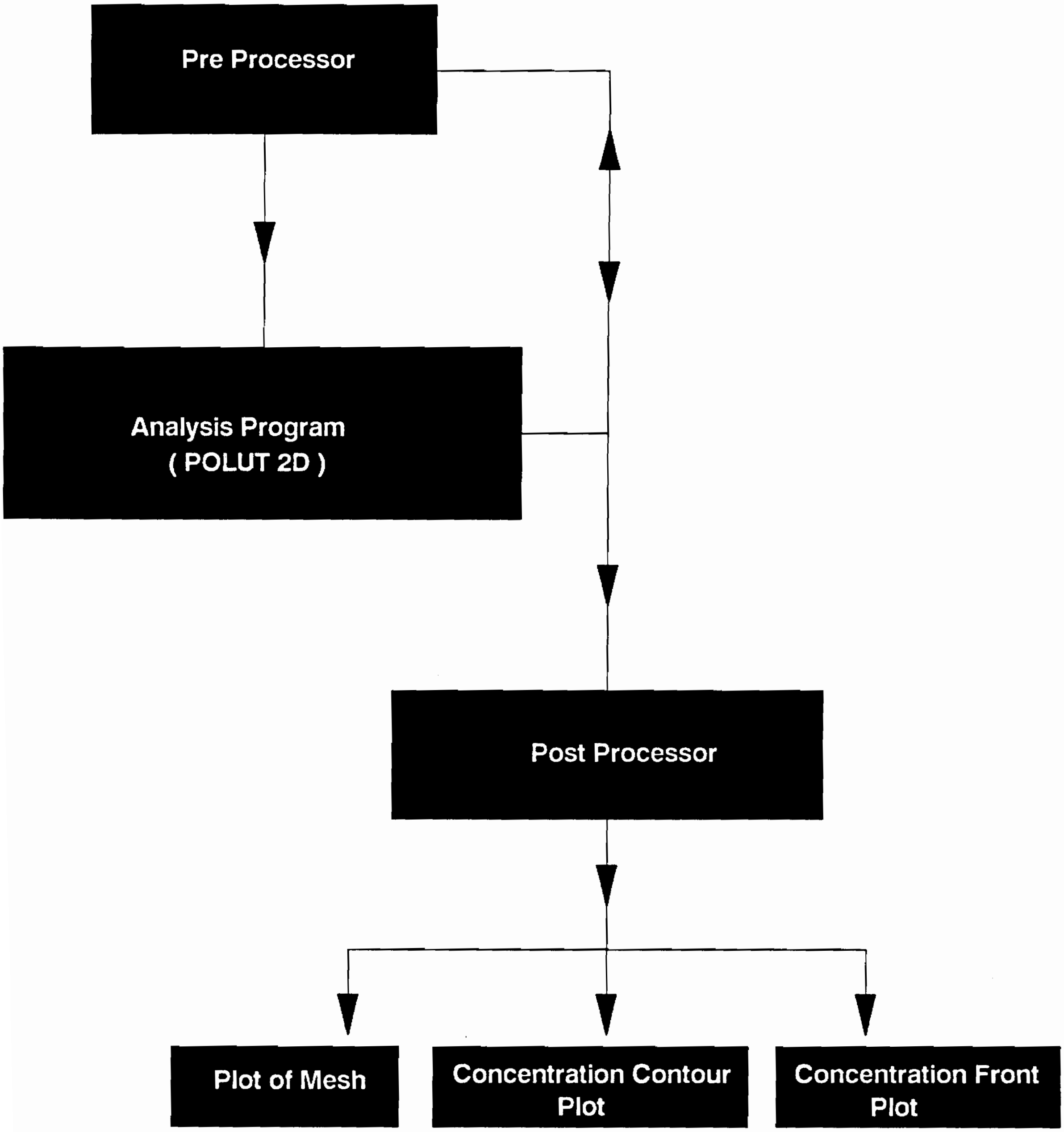


Figure A-1. Scheme of Overall Processes

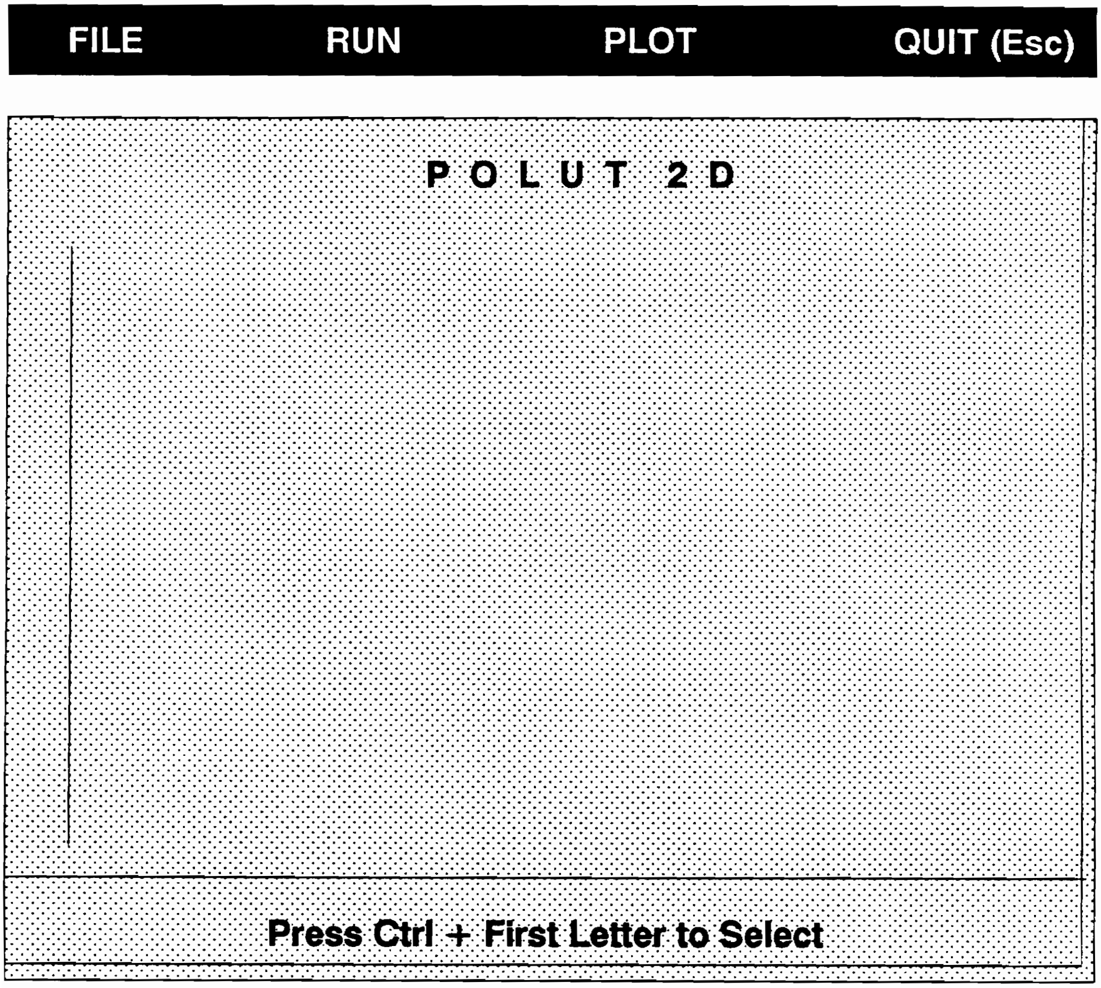
Pre Processor

The purpose of this pre processor is to create and edit data files for the program POLUT2D. The data files include data for nodal coordinates, connectivity, boundary conditions, and material information. Pre - processor is written in "C" language using "CSCAPE" library to create screens. All the screens for data input are interactive, which makes the editing and creating of data for the POLUT2D easier. The screens can be rolled back and and forth, left and right to make any modifications in the data file. The pop up menu screens are useful to select the various categories of operations like Entering the data, Running the Analysis program and Displaying of the results. The user can move around within the input fields of any screen(s) using the <RETURN> or <ENTER> keys. The values in the fields may be changed by using <DEL> or <INS> keys and by pressing <ESC> key, it brings up the next screen after data for a particular section has been entered. The online help messages pertaining to a particular data field are available by taking the cursor to that field and then pressing <F1> key.

Figure A.2 shows the program control screen which comes after the title screen. This screen consists of four different options; FILE, RUN, PLOT and QUIT.

The FILE option refers to the Pre-processor part of the program and it is accessed by pressing <Ctrl> and <F> keys togather. It allows to create, make chnanges or save a data file. The RUN option refers to the Processor part of the program and it is accessed by pressing <Ctrl> and <R> keys togather. It allows to run a data file and the results from analysis are written to specified files. The PLOT option refers to the Post-processor part of the program and it is accessed by pressing <Ctrl> and <P> keys together. It allows to display results obtained by analysis, which includes display of mesh, concentration front and concentration contours at different time levels. The QUIT option allows to exit from the POLUT2D and it can be accessed by pressing <Ctrl> and <Q> keys together or by pressing <Esc> key in the program control screen as shown in figure A.2.

Figure A.3 shows the following four options, which pop up as soon as the FILE option is selected; **Open a New File**, **Edit an Old File**, **View a File**, **Save a File** and **Exit** .



POLUT 2D

Press Ctrl + First Letter to Select

Figure A-2 Program Control Screen

Each of these options can be selected by taking the cursor using arrow keys and then by pressing <Return> or <Enter> key at that position. For Example, **Open a New File** is selected by moving the cursor using arrow keys at that position and then by pressing <Enter> or <Return> key. This option takes the user to main data entry menu as shown in figure A.4. The user can select various categories of data to enter data and in order to exit from the main data entry menu, after data has been entered, by pressing <Esc> key takes the user to a screen where the names of the files in the current directory are shown and then user is prompted for the name of file under which data is to be saved.

Edit an Old File allows to edit an existing file and when this option is selected, the name of the file which already exists is requested. If an old file exists, the main data entry menu is displayed and each category can be accessed separately to make any changes in the file. After editing has been completed, by pressing <Esc> takes the user to a screen where user is asked to overwrite existing file or rename it.

View a File option allows to view a text file such as output results file. The user can move up and down the file using arrow keys.

Save option allows the user to save all the changes to a particular file under a different file name while preserving the original file. **Exit** takes the user to program control screen as shown in figure A.2.

Figure A.4. shows the main data entry menu screen, which consists of ten different categories. Each category can be accessed independently after data for General Parameters has been entered. Any set of consistent units can be used in the POLUT2D and dimensions are shown by the following notations.

$$M = \text{Mass},\ L = \text{Length},\ T = \text{Time}$$

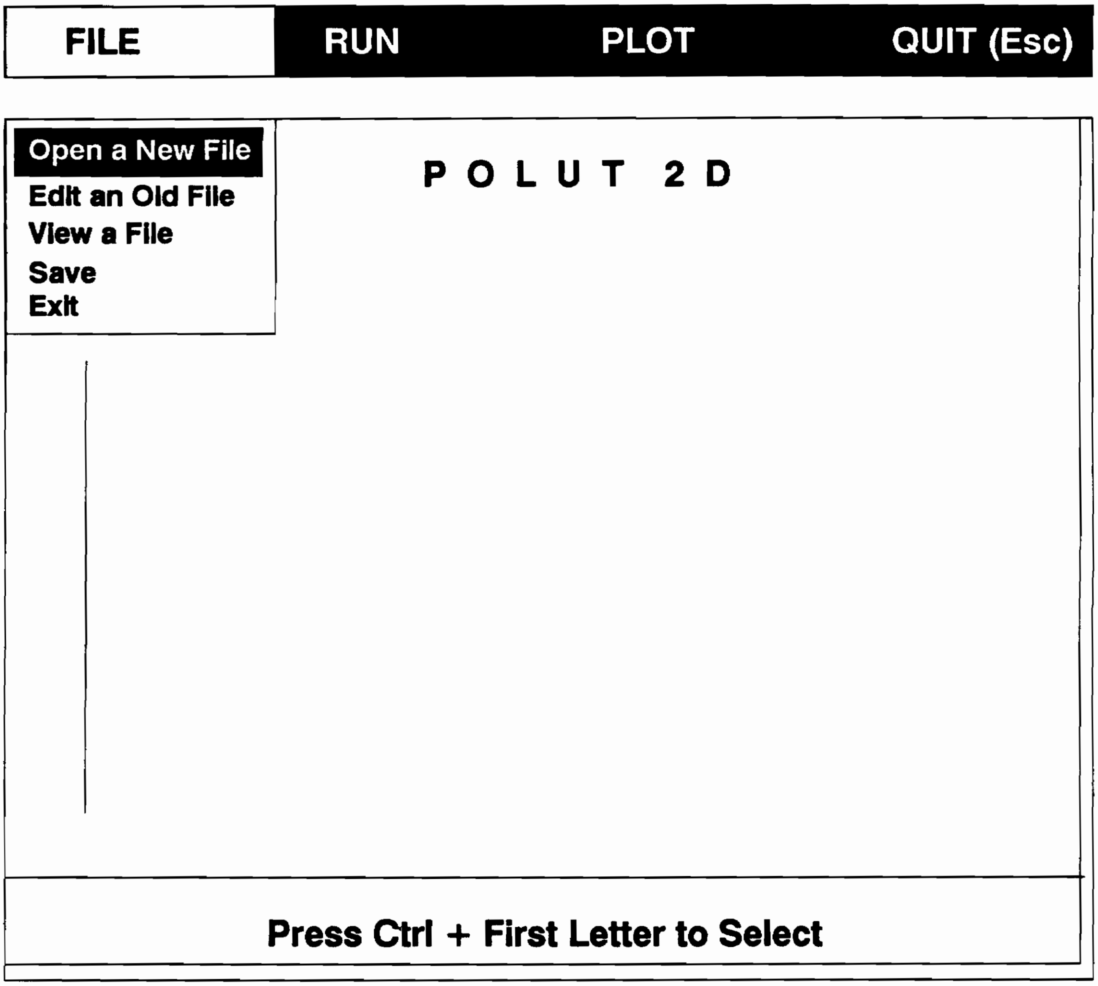


Figure A-3. File menu screen

MAIN MENU FOR DATA ENTRY

The main data entry menu consists of ten different sections.

- HEADING DATA
- GENERAL PARAMETERS
- MATERIAL PROPERTIES DATA
- NODAL INFORMATION DATA
- ELEMENT DATA
- FIXED POTENTIAL HEAD DATA
- FIXED CONCENTRATION DATA
- INITIAL POTENTIAL HEAD DATA
- INITIAL CONCENTRATION DATA
- OUTPUT CONTROL INFORMATION DATA

Each section is described here;

1. HEADING DATA

This category of main data entry menu, as shown in figure A.5., consists of title of the problem and number of the problem. This information is printed at the top of the output file.

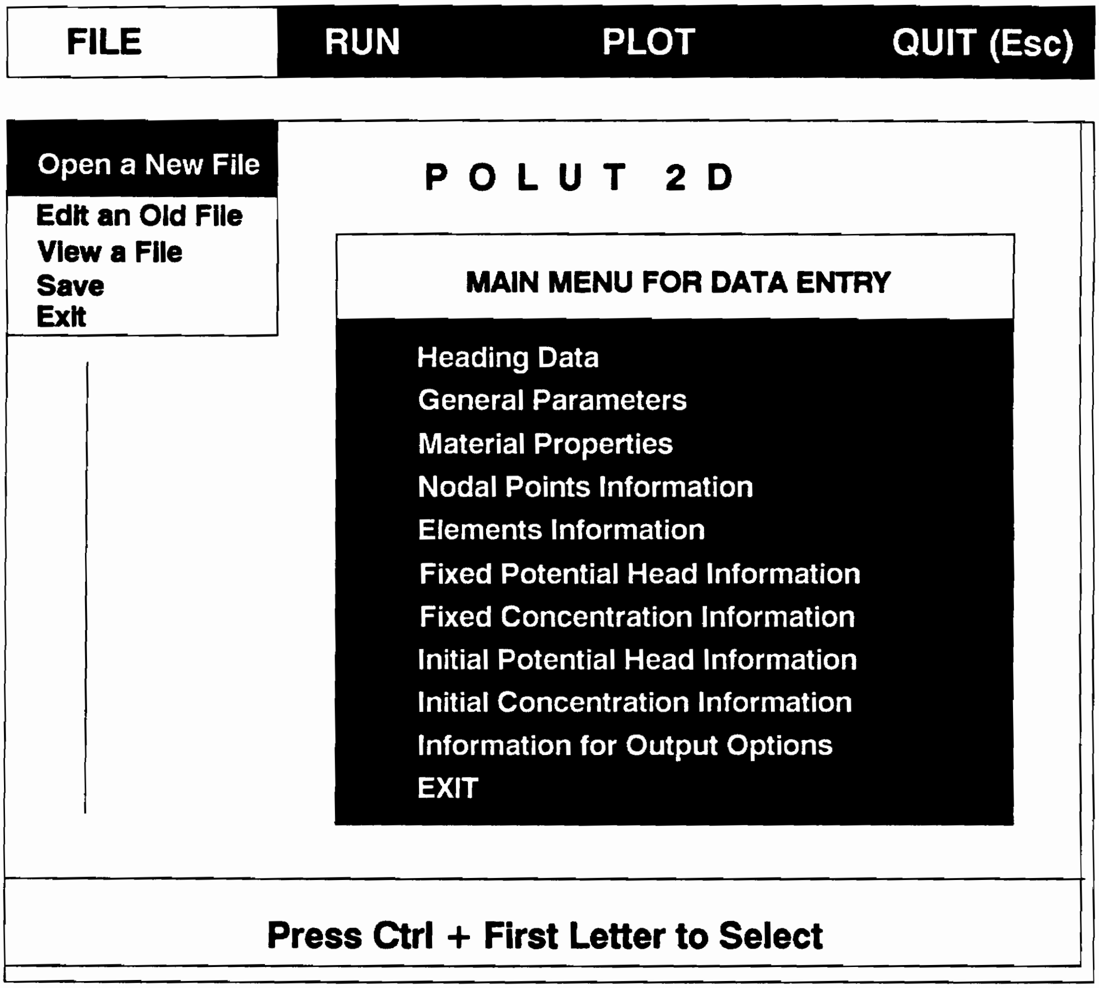
▪ Problem Number

Any Integer value greater than zero is acceptable, It is printed on the top of output file.

▪Problem Title

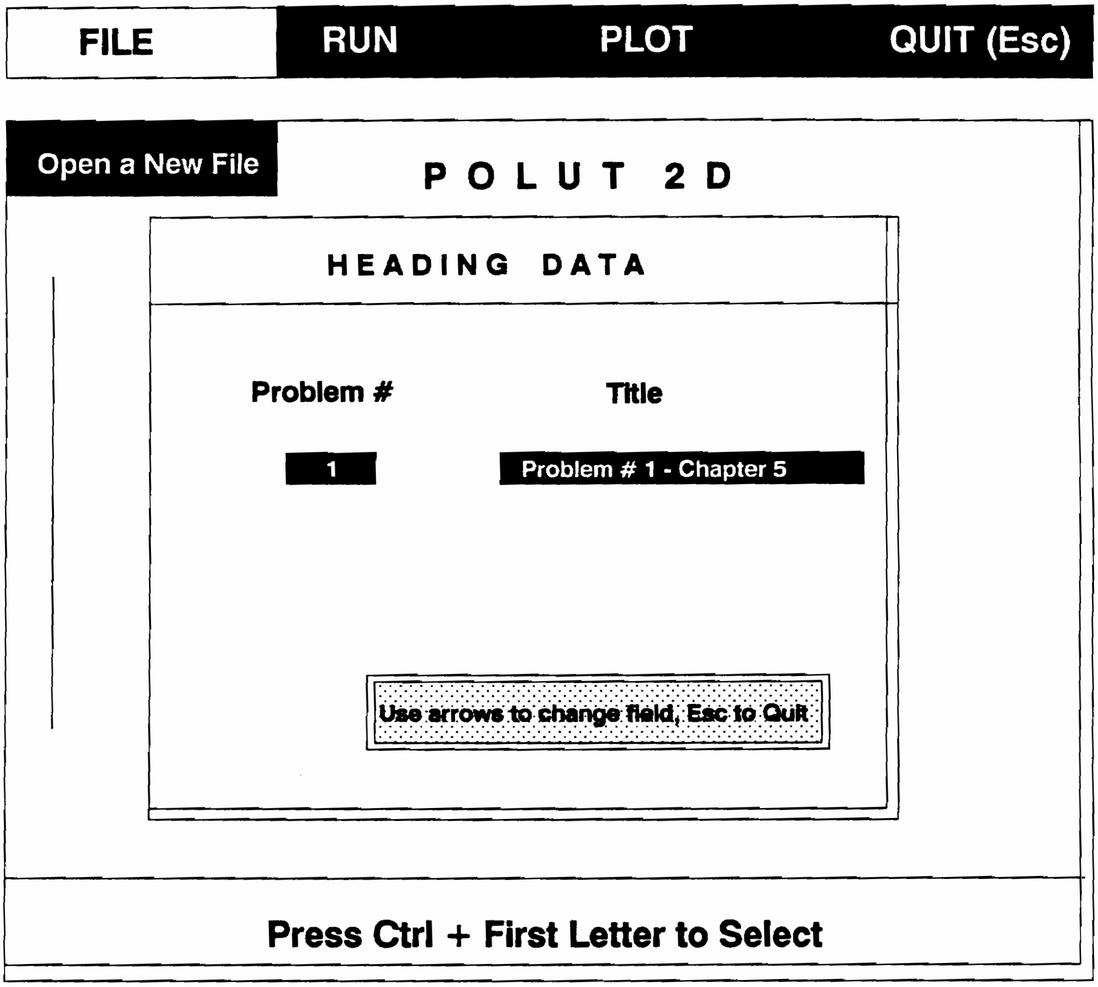
Any combination of upto 60 characters. It is printed at the top of output file.

2. GENERAL PARAMETERS



Press Ctrl + First Letter to Select

Figure A-4. Main Data Entry Menu Screen



Problem # 1

Title Problem # 1 - Chapter 5

Use arrows to change field, Esc to Quit

Press Ctrl + First Letter to Select

Figure A-5. Heading Data screen

The data in this section is used to control if, and how many times, subsequent screens are to be displayed. It is recommended that data for this screen be entered first. Figure A.6 displays a screen for General Parameters for an example problem.

■Number of Nodes

Total number of nodes in the mesh. The number of nodes should be less than the maximum value allowed for number of nodes as described in Table A-1.

■Number of Elements

Total number of elements in the mesh. The number of elements should be less than the maximum value allowed for number of elements as described in Table A-1.

■Number of Different Materials

Total number of different materials used in the mesh. The number of elements in the mesh. The number of elements should be less than the maximum value allowed for number of different materials as described in Table A-1.

■Number of Nodes With Fixed Head

The total number of nodes where potential head does not change. It is a fixed boundary condition. The number of nodes with this condition should not exceed the maximum value allowed for number of nodes with fixed head as described in Table A-1.

■Number of Nodes With Fixed Concentration

The total number of nodes where concentration does not change. It is a fixed boundary condition. The number of nodes with this condition should not exceed the maximum value allowed for number of nodes with fixed concentration as described in Table A-1.

■Number of Nodes With Initial Head

The total number of nodes where initial potential head is other than PI. It is a initial boundary condition. The number of nodes with this condition should not exceed the maximum value allowed for number of nodes as described in Table A-1.

■Number of Nodes With Initial Concentration

The total number of nodes where initial concentration is other than CI. It is a initial boundary condition. The number of nodes with this condition should not exceed the maximum value allowed for number of nodes as described in Table A-1.

■Value for Initial Head For Most Nodes (PI)

The value for the initial potential head for most nodes.

■Value for Initial Concentration (CI)

The value for the initial concentration for most nodes.

■Value for Element Source

The value for the element source [1/TL]

▪Percentage of Error

The value for the acceptable percentage of error used in the convergence criterion. The recommended value is 0.05.

▪Number of Iterations

The value for the maximum number of iterations allowed for each time step if solution does not converge. The recommended value is 20.

3. MATERIAL PROPERTIES DATA

This category of data consists of material properties as shown in figure A.7, which includes data for saturated hydraulic conductivities in transverse and vertical directions, back pressure, angle of anisotropy, dispersivity values in X and Y directions, molecular diffusion coefficient, saturated and residual volumetric water contents and van Genuchten parameters M and α. This material properties screen is displayed once for each material, and the material number is displayed at the top of screen.

▪Saturated Hydraulic Conductivity in X - direction

The value for the saturated permeability of the soil in X or longitudinal direction. The dimensions for permeability are [L/T].

▪Saturated Hydraulic Conductivity in Y - direction

The value for the saturated permeability of the soil in Y or transverse direction. The dimensions for permeability are [L/T].

▪Back Pressure

The value for the pressure required for the complete saturation of the soil. The dimensions for back pressure are [M/L*L].

▪Angle of Anisotropy

The value for the angle between principal X axis and mesh coordinate X axis. This value is used only for the permeability values. The value is entered in degrees.

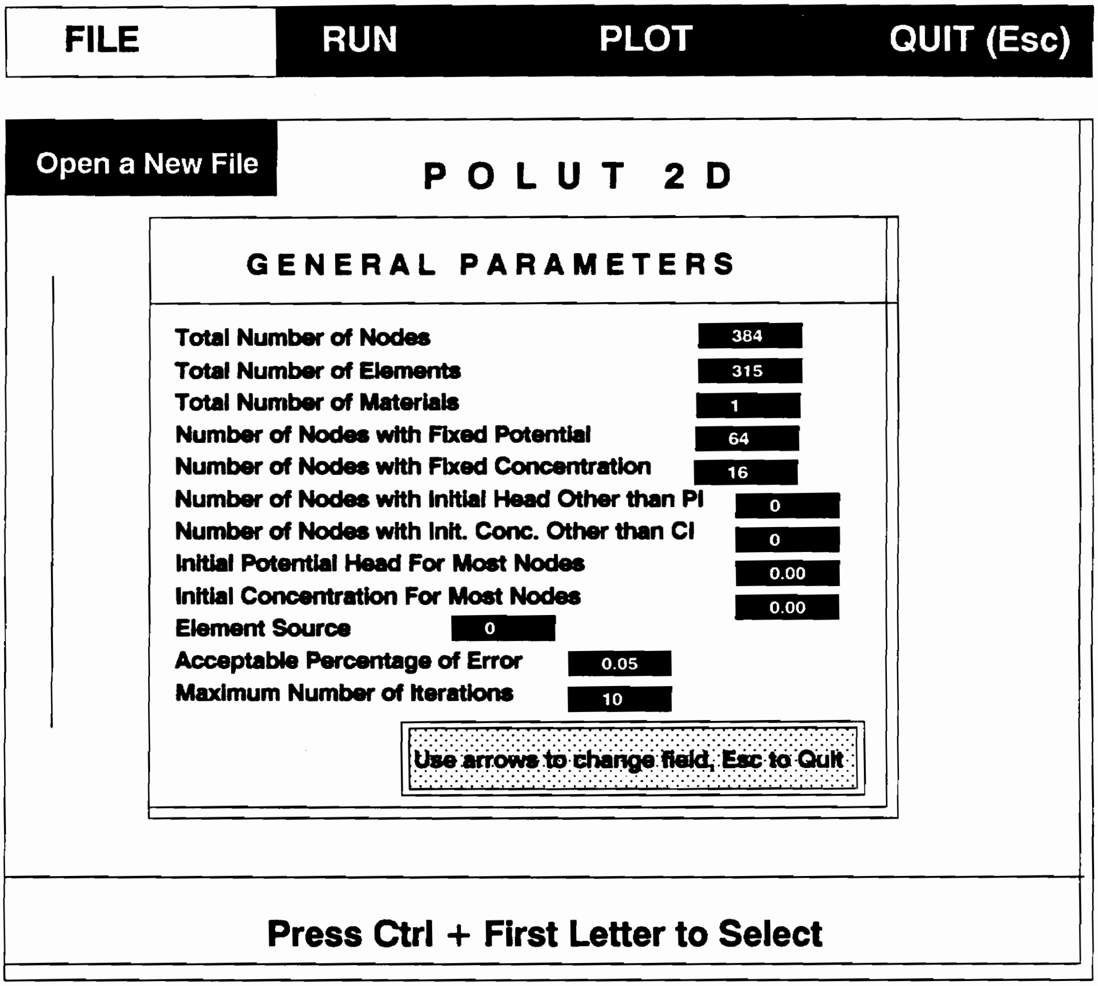
▪Longitudinal Dispersivity

The value for the dispersivity in longitudinal or X axis, in order to calculate dispersion coefficient. The dimension for dispersivity is [L].

▪Transverse Dispersivity

The value for the dispersivity in transverse or Y axis, in order to calculate dispersion coefficient. The dimension for dispersivity is [L].

▪Coefficient of Molecular Diffusion



POLUT 2D

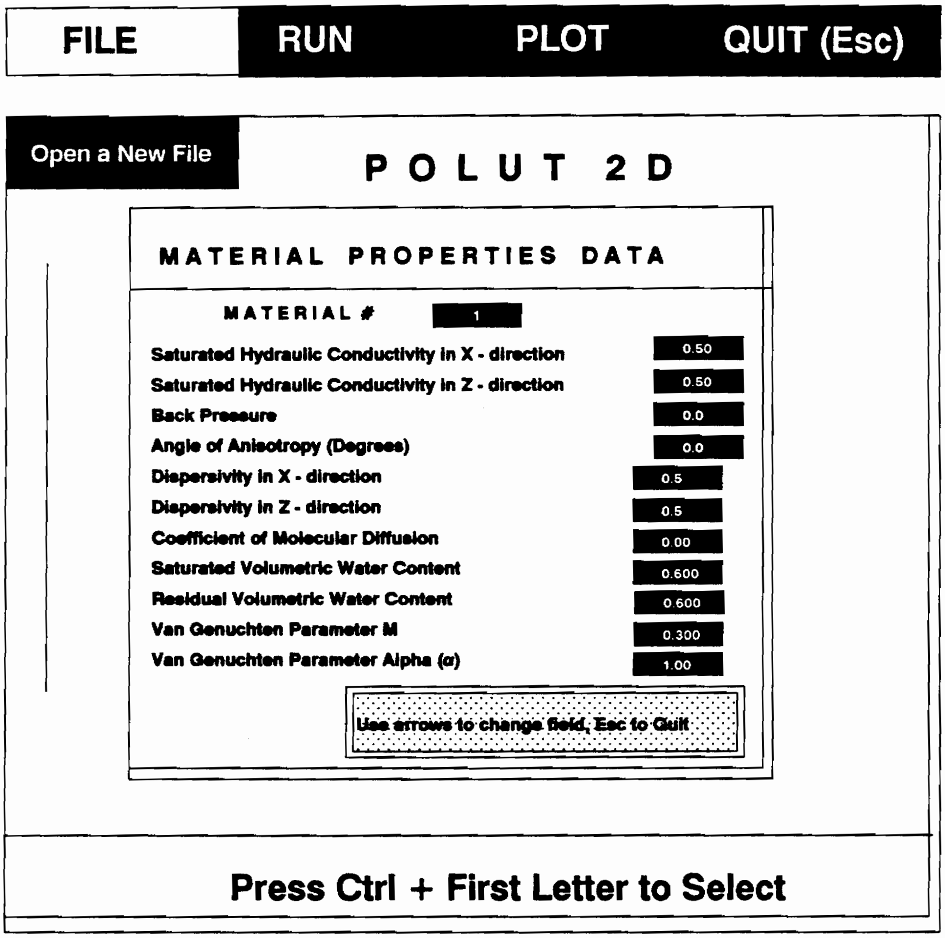
GENERAL PARAMETERS

Total Number of Nodes	384
Total Number of Elements	315
Total Number of Materials	1
Number of Nodes with Fixed Potential	64
Number of Nodes with Fixed Concentration	16
Number of Nodes with Initial Head Other than PI	0
Number of Nodes with Init. Conc. Other than CI	0
Initial Potential Head For Most Nodes	0.00
Initial Concentration For Most Nodes	0.00
Element Source	0
Acceptable Percentage of Error	0.05
Maximum Number of Iterations	10

Use arrows to change field, Esc to Quit

Press Ctrl + First Letter to Select

Figure A-6. General Parameters screen



POLUT 2D

MATERIAL PROPERTIES DATA

MATERIAL #	1
Saturated Hydraulic Conductivity in X - direction	0.50
Saturated Hydraulic Conductivity in Z - direction	0.50
Back Pressure	0.0
Angle of Anisotropy (Degrees)	0.0
Dispersivity in X - direction	0.5
Dispersivity in Z - direction	0.5
Coefficient of Molecular Diffusion	0.00
Saturated Volumetric Water Content	0.600
Residual Volumetric Water Content	0.600
Van Genuchten Parameter M	0.300
Van Genuchten Parameter Alpha (α)	1.00

Use arrows to change field, Esc to Quit

Press Ctrl + First Letter to Select

Figure A-7. Material Properties Data screen

The value for the coefficient of molecular diffusion for pollutant or solute involved, in order to calculate dispersion coefficient. The dimensions for this coefficient are [L*L/T].

■Saturated Volumetric Water Content

The value for the saturated volumetric water content θ_s for the soil, and it is also equal to the porosity when the soil is saturated.

■Residual Volumetric Water Content

The value for the residual volumetric water content θ_r for the soil, and it is value of volumetric water content at very low values of pressure head (high suction), usually near zero.

■van Genuchten Parameter M

The value for the van Genuchten parameter M relating grain size distribution and shape of soil - water retention curve. It has no dimensions.

■van Genuchten Parameter Alpha

The value for the van Genuchten parameter α relating grain size distribution and shape of soil - water retention curve. It has dimensions of [L^{-1}].

4. NODAL INFORMATION DATA

This section of data entry menu consists of X and Y coordinate values for the nodes and it consists of two screens. If the main data entry menu is accessed in the edit mode, the first part of the screen does not come and if the option for creating a new file is used, there are two screens for this category of data as shown in figure A.8. Nodes and coordinates which are skipped can be generated at equal spacing along a line connecting the two nodal points listed before and after the skipped nodes.

■Node Number

The value for the node number and it must be an integer value.

■X-Coordinate

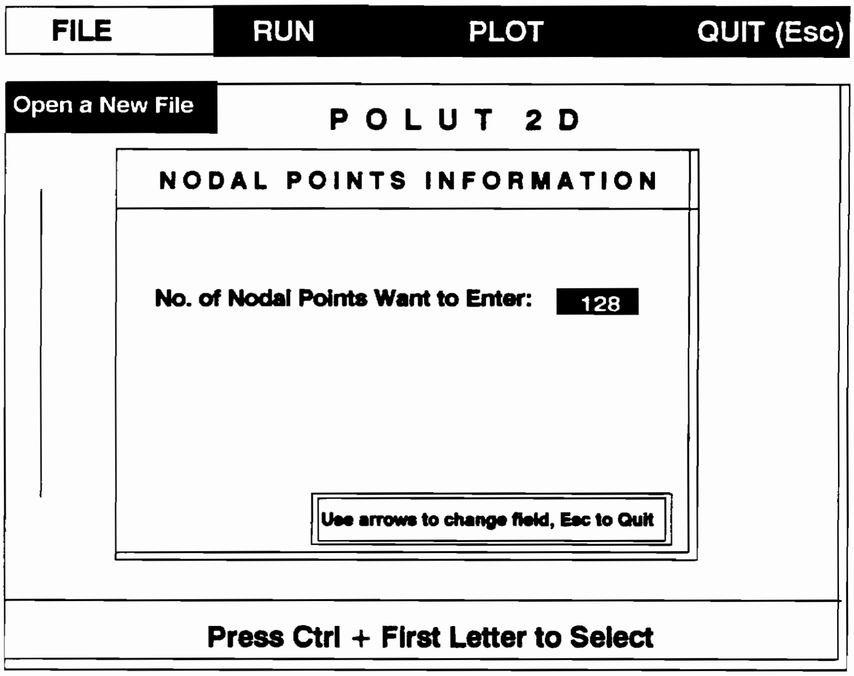
The value for the X - coordinate of the Node.

■Y-Coordinate

The value for the Y - coordinate of the Node.

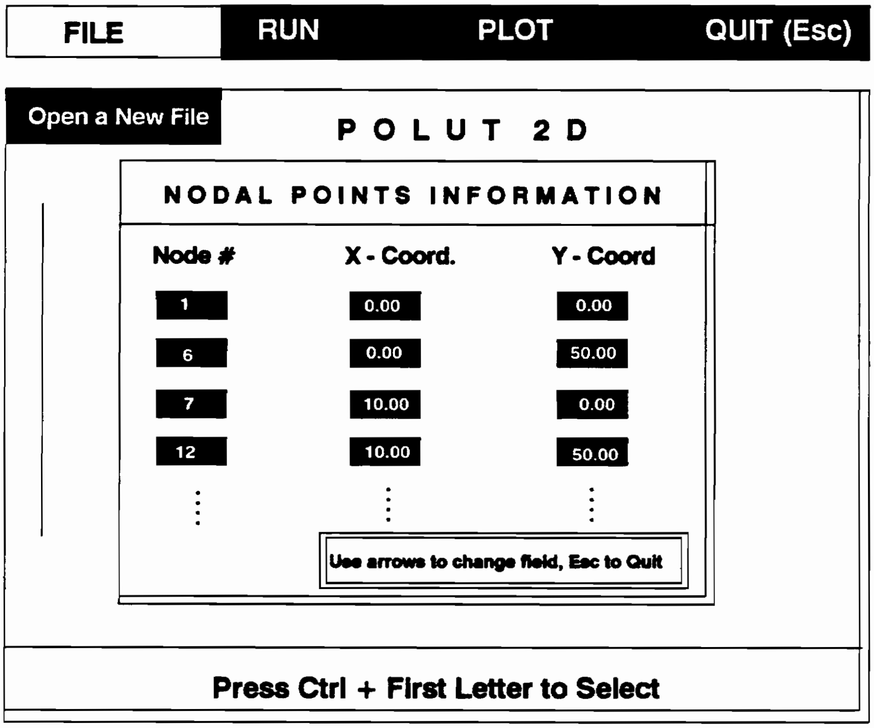
5. ELEMENT INFORMATION DATA

This section of data entry menu consists of element connectivity and values for material type and it consists of two screens. If the main data entry menu is accessed in the edit mode, the first part of the screen does not come and if the option for creating a new file is used, there are two screens



No. of Nodal Points Want to Enter: 128

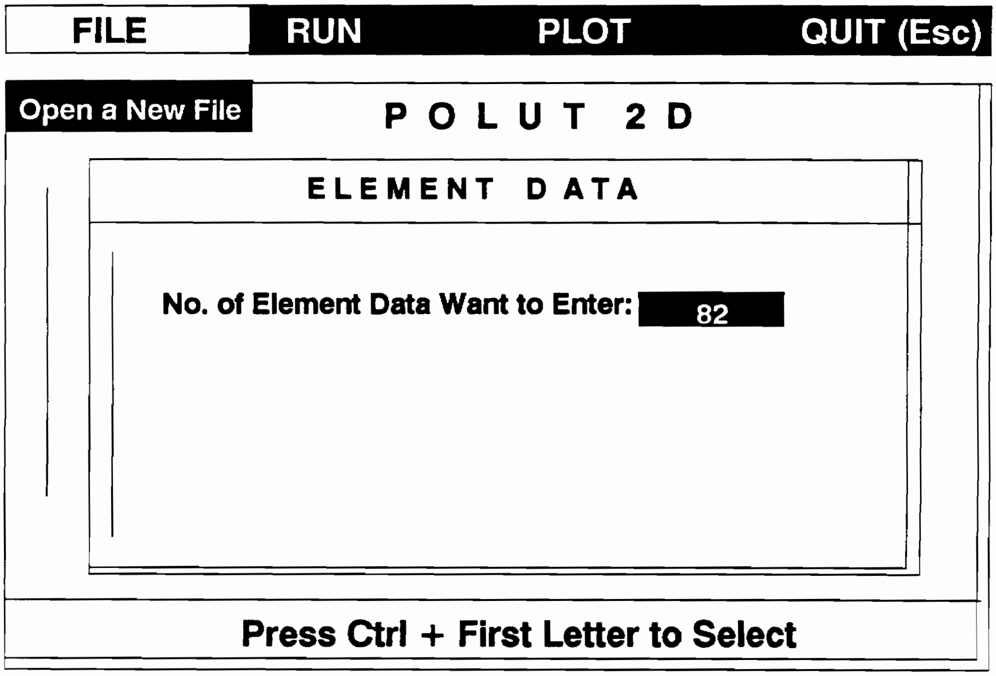
(PART - A)



Node #	X - Coord.	Y - Coord
1	0.00	0.00
6	0.00	50.00
7	10.00	0.00
12	10.00	50.00
⋮	⋮	⋮

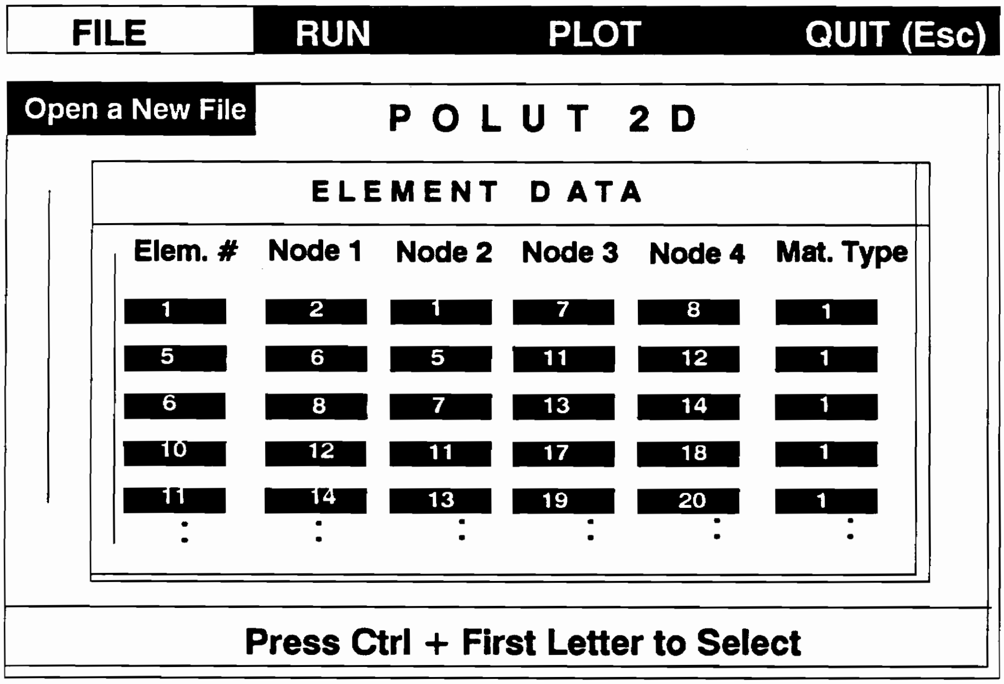
(PART B)

Figure A-8. Nodal Points Information Screen



No. of Element Data Want to Enter: 82

(PART A)



Elem. #	Node 1	Node 2	Node 3	Node 4	Mat. Type
1	2	1	7	8	1
5	6	5	11	12	1
6	8	7	13	14	1
10	12	11	17	18	1
11	14	13	19	20	1
:	:	:	:	:	:

(PART B)

Figure A-9. Element Data Screen

for this category of data as shown in figure A.9. Any skipped elements are generated by adding one to the node numbers of the previous element. The material number of skipped elements will be set equal to that of last element entered. The four nodes of each element must be specified in a counterclockwise direction. A triangular element can also be used by equation node 4 and node 3 of a element.

6. FIXED POTENTIAL HEAD DATA

This category of main data entry menu, as shown in figure A.10., consists of data for fixed potential head for the node. It displays the number of blank fields equal to the value entered in the General Parameters screen.

■Node Number

The node number where potential head is fixed.

■Potential Head

The value for the potential head for a partcular node and the dimensions for potential head are [L].

7. FIXED CONCENTRATION DATA

This category of main data entry menu, as shown in figure A.11., consists of data for fixed concentration for the node. It displays the number of blank fields equal to the value entered in the General Parameters screen.

■Node Number

The node number where input concentration is fixed.

■Concentration

The value for the input concentration at that particular node.

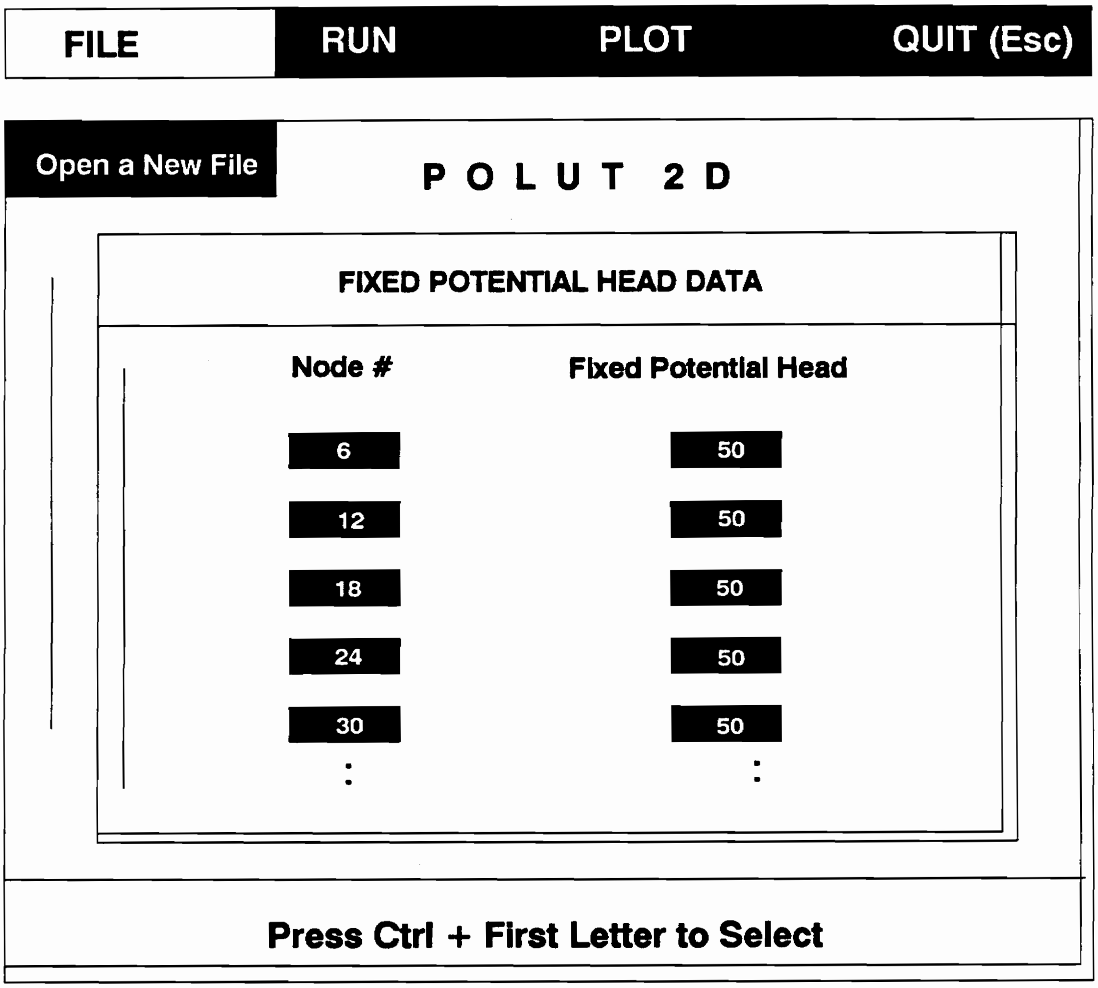
8. INITIAL POTENTIAL HEAD DATA

This category of main data entry menu, consists of data for initial potential head for the node. It displays the number of blank fields equal to the value entered in the General Parameters screen. It shows a screen similar to the one as shown in figure A.10.

■Node Number

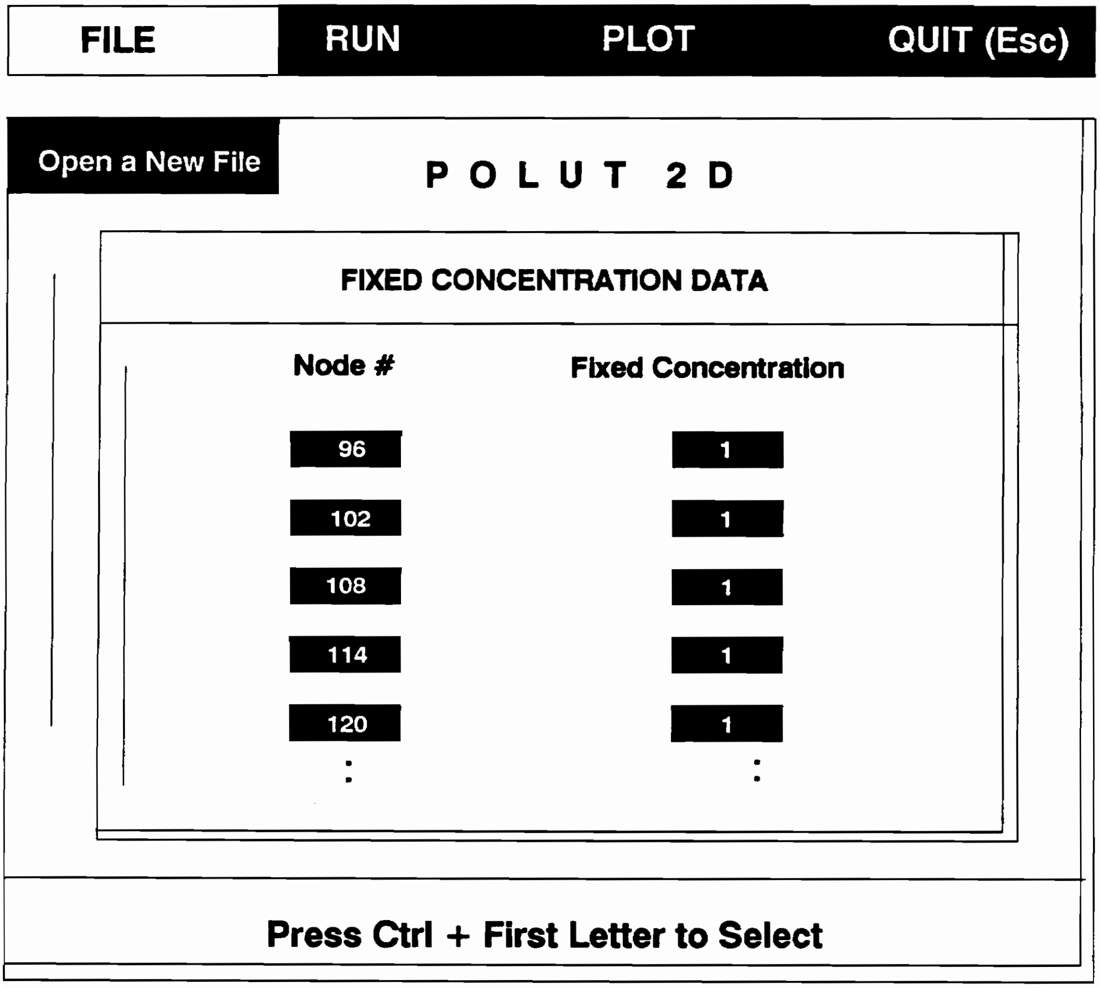
The node number where initial head is known.

■Initial Head



Node #	Fixed Potential Head
6	50
12	50
18	50
24	50
30	50
:	:

Figure A-10. Fixed Potential Head Data Screen



POLUT 2D

FIXED CONCENTRATION DATA

Node #	Fixed Concentration
96	1
102	1
108	1
114	1
120	1
:	:

Press Ctrl + First Letter to Select

Figure A-11. Fixed Concentration Data Screen

The value for the initial potential head at a particular node and the dimensions for potential head are [L].

9. INITIAL CONCENTRATION DATA

This category of main data entry menu, consists of data for initial concentration for the node. It displays the number of blank fields equal to the value entered in the General Parameters screen. It displays a screen similar to the one as shown in figure A.11.

▪Node Number

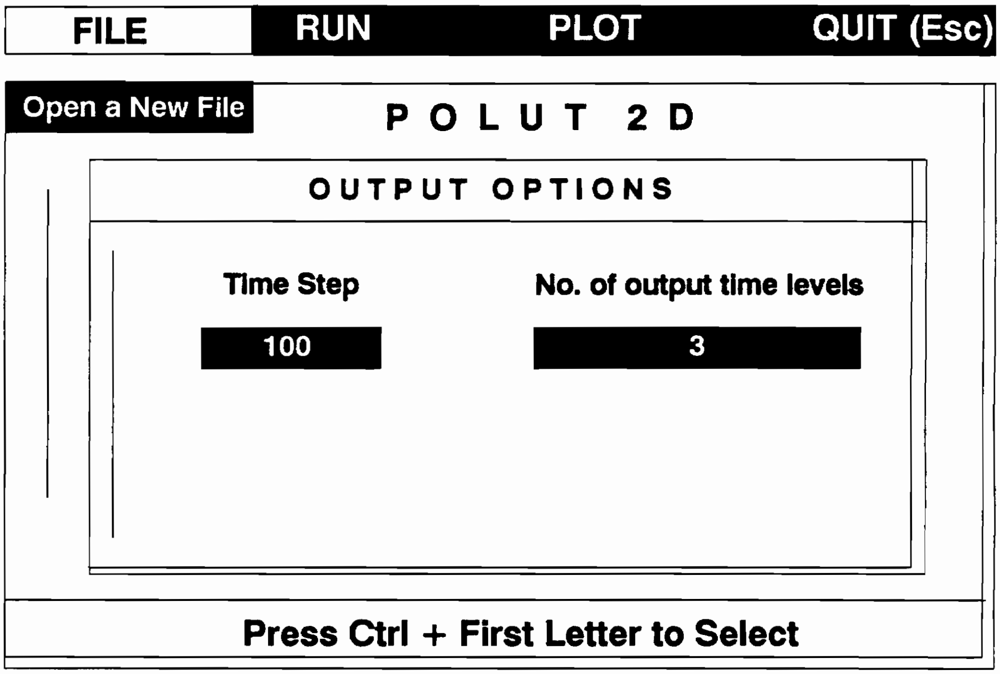
The node number where input concentration is known.

▪Concentration

The value for the initial concentration at that particular node.

10. OUTPUT CONTROL DATA

This category of main data entry menu, as shown in figure A.12., consists of two screens. On the first screen user specifies time increment Δt and the number of times in which program output is desired. The specific output times are entered on the second screen. The units of time must be the same as the permeability. The time increment Δt remains the same for the first 10 time steps, after which it is increased by 1.4x. This is done to reduce the computational time required to solve a problem. For most cases the stability of the problem will increase after first several time steps, allowing a larger value of Δt. The time increment then remains the same until 10x the new Δt, when it is increased by 1.4x again. The process continues until the maximum time is reached. Results are output at the times closest to the specified output times.



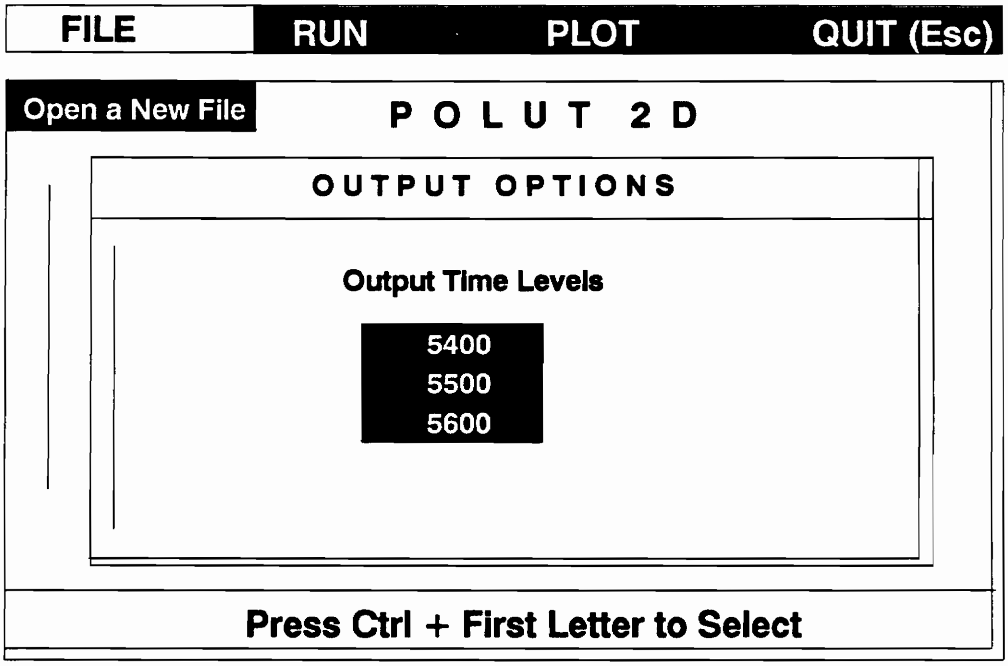
Time Step

100

No. of output time levels

3

(PART A)



Output Time Levels

5400
5500
5600

(PART B)

Figure A-12 Output Control Data Screen

Table A-1. Limits on the size of problem

Category	Maximum Value
Number of Nodes	500
Number of Elements	400
Number of Different Materials	10
Number of Nodes with Fixed Potential Head	100
Number of Nodes with Fixed Concentration	100
Number of Nodes with Initial Potential Head	100
Number of Nodes with Initial Concentration	100
Bandwidth of the problem	50

Processor program

The processor or the analysis part of the program reads input data file created by the pre processor and then computes results, which include concentration and potential head at various time levels. It is written in FORTRAN 77. The program first computes the nodal values of pressure head h and mean water pore velocity by solving 2-D Unsaturated flow equation using van Genuchten model. In the second stage, it solves mass transport equation with advection and dispersion and obtains concentration spread at various time steps. The flow chart of the processor part of the program is displayed as figure A.13.

The program uses four-noded, two dimensional quadrilateral element and a general β method for the time integration scheme. The solution procedure involves iterations by Picard's method to handle the non-linearities.

The processor program reads an input data file and if there are no errors found in the input data file, it writes results to two files with extensions as ".out" and ".plt". The ".out" is the output result file and it can be printed and ".plt" is a file created for the use in graphics or the post processing programs. The ".out" or output file consists echo of detailed form of input data, nodal values for the concentration and head, and values for the velocity in transverse and longitudinal directions for each element at various time steps. The ".plt" or graphics file contains data for mesh generation, nodal concentration values at various time steps.

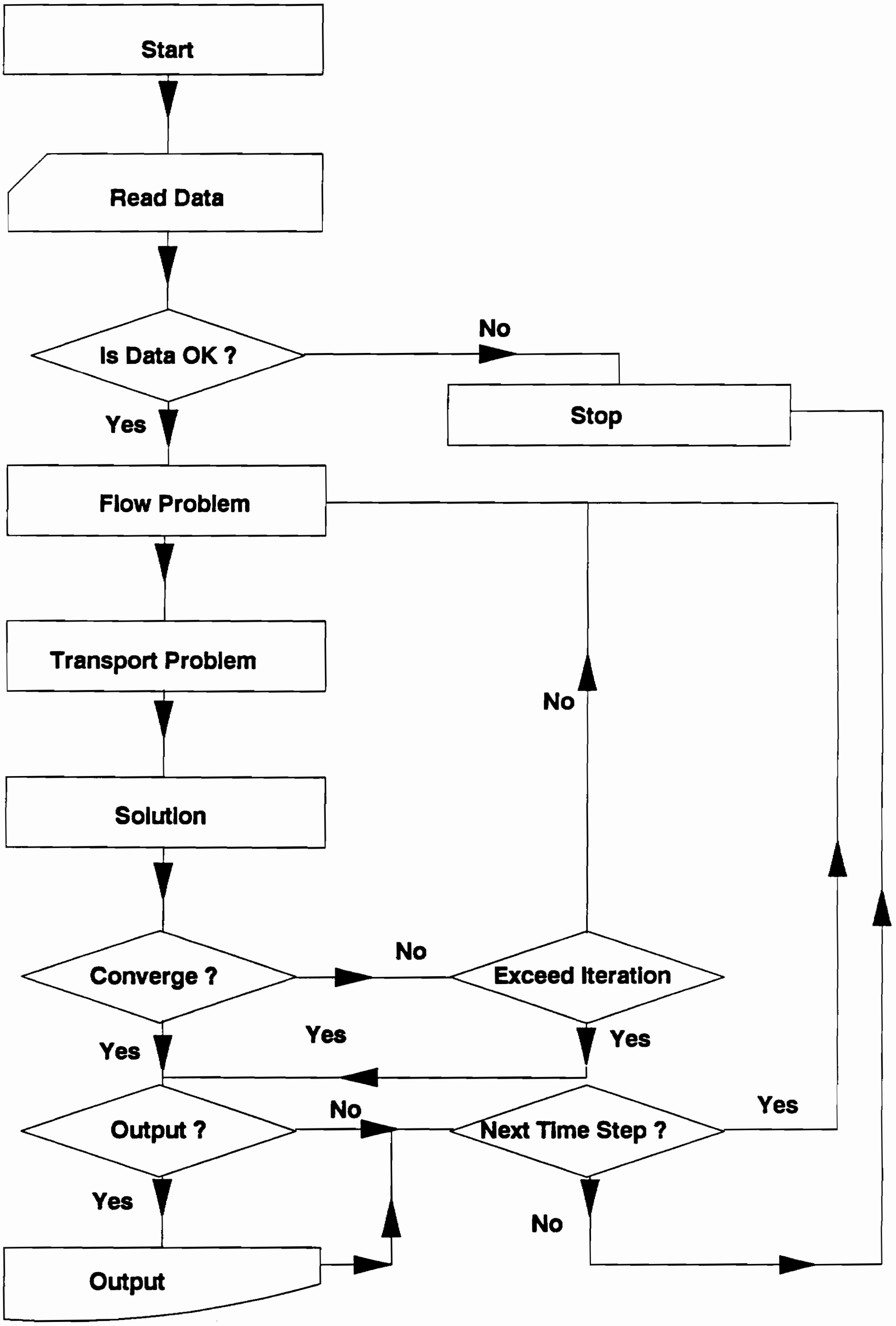


Figure A-13. Flow chart for the Analysis program

Post Processor

The post processing stage deals with the presentation of results. There are three different types of graphics, as shown in figure A-1, which can be used to graphically verify results;

- Mesh Plot
- Concentration Front
- Concentration Contours

Mesh plot displays a two dimensional finite element mesh by reading data from ".plt" or graphics file, which is created by the processor part of the program. The different materials used in the mesh are displayed by using color codes. There is a zoom option which allows to enlarge selected areas of the mesh. Figure A.14 illustrates a typical mesh as displayed by the program.

Concentration Front option allows to show the concentration front at various time steps. It requires the input of time step and concentration level, in addition to the data from ".plt" file. This option, first generates mesh and then shows concentration front on it with the help of color codes. Figure A.15 shows a typical concentration front plot.

Concentration contour option allows to create color coded concentration contour levels at different time values. It generates contours by reading data from ".plt" file and the values for concentration contours are computed by dividing the range of concentration into equal sections. The number of sections depend upon the graphics capability of the hardware. Figure A.16 illustrates a typical concentration contour plot.

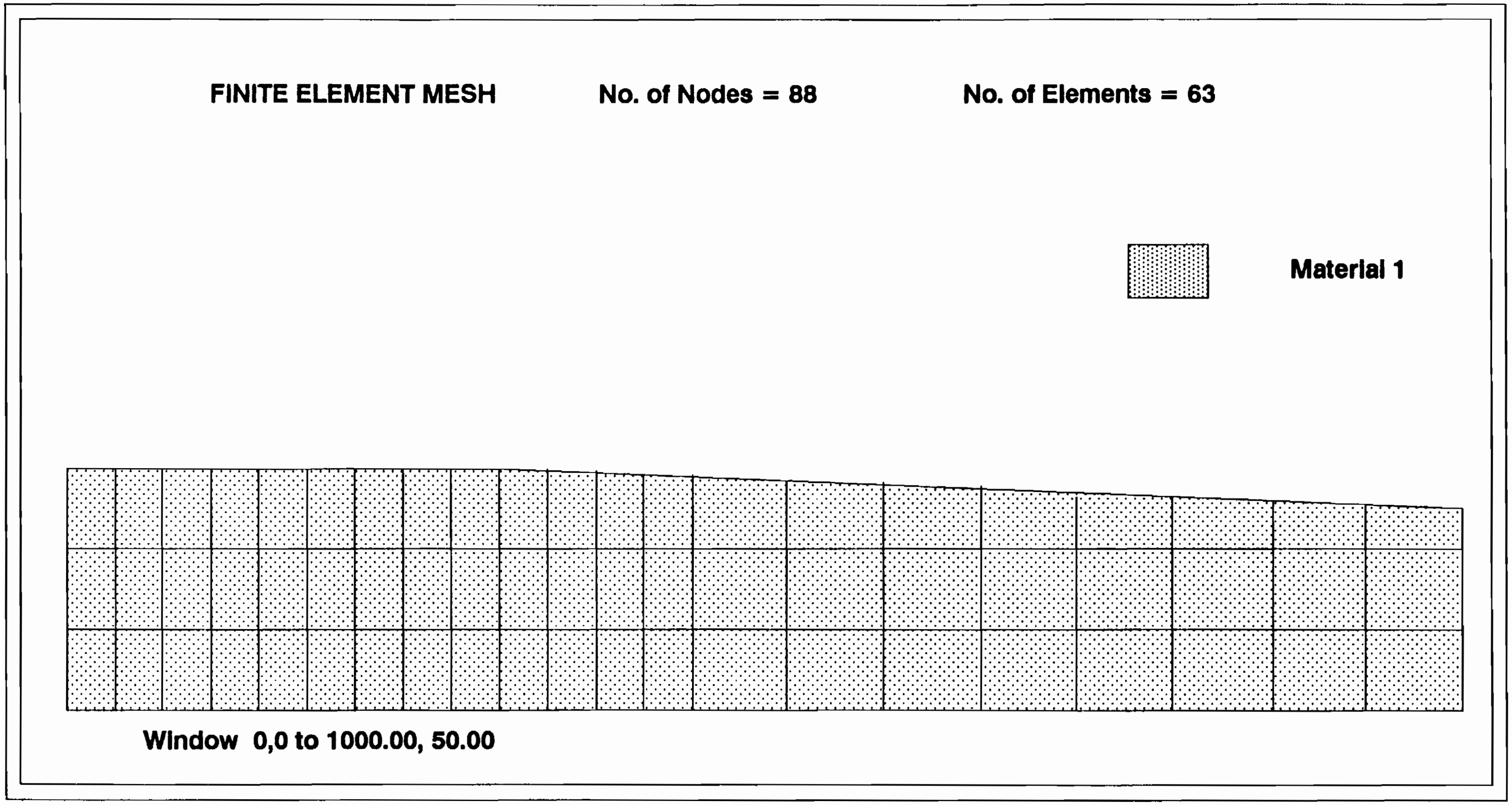


Figure A-14. Finite Element Mesh Plot Screen

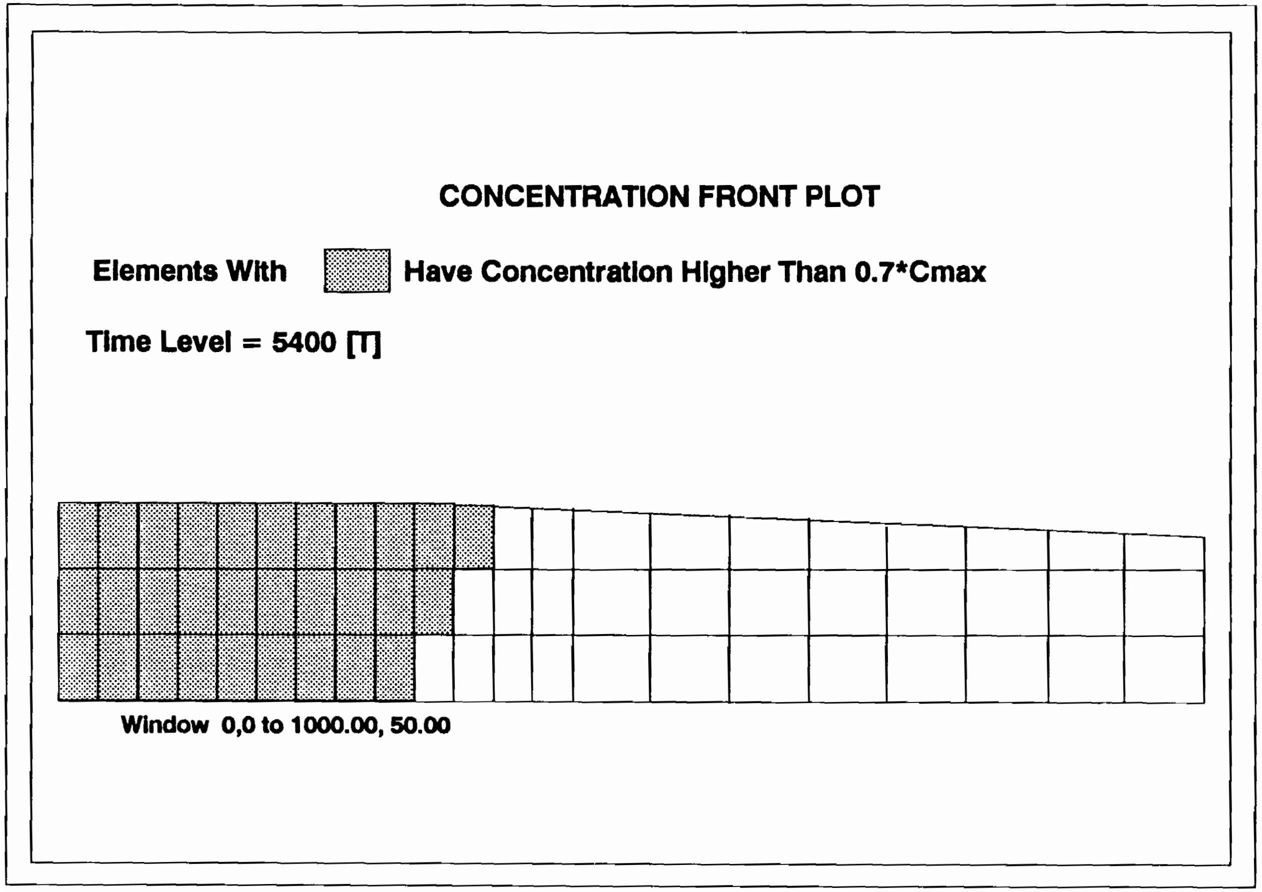
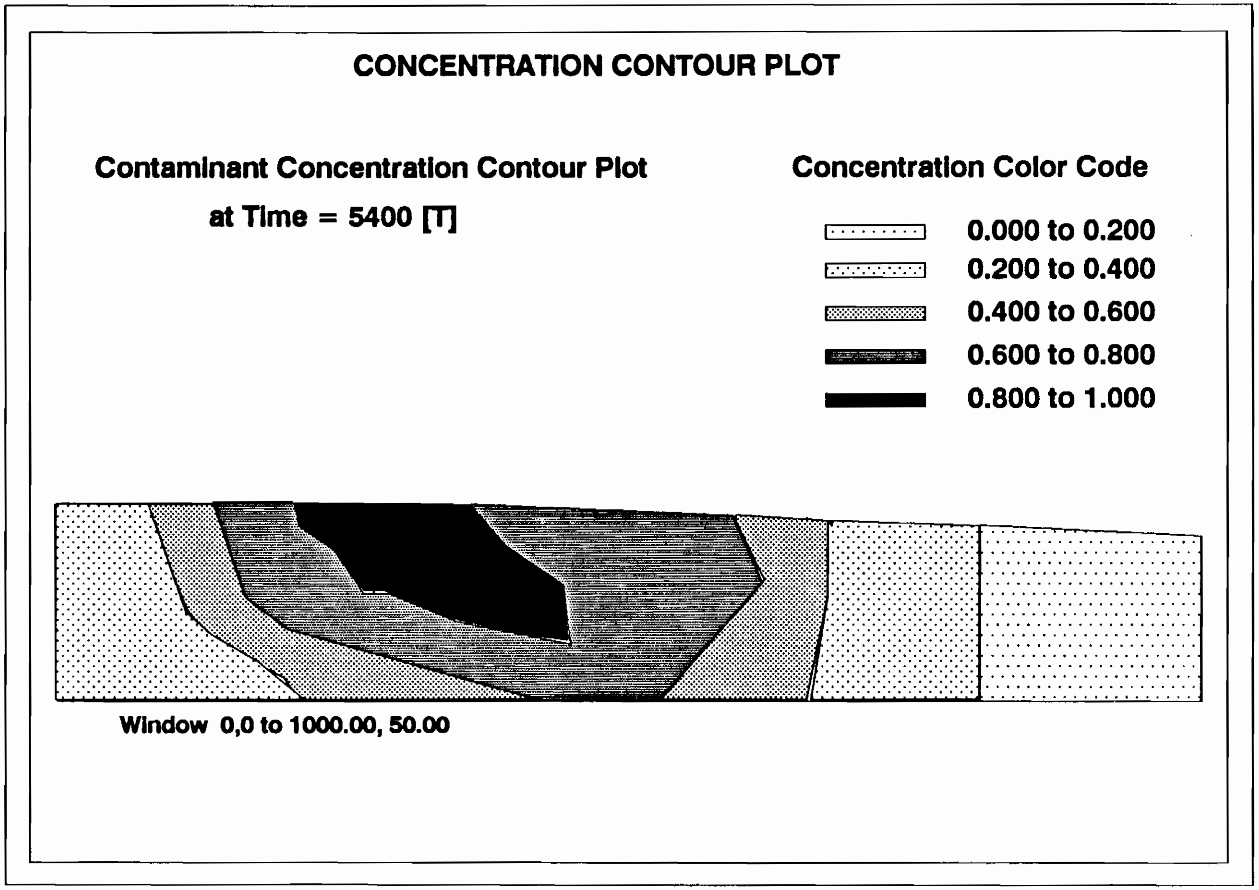


Figure A-15 Concentration Front Plot



CONCENTRATION CONTOUR PLOT

Contaminant Concentration Contour Plot
at Time = 5400 [T]

Concentration Color Code

░ 0.000 to 0.200
░ 0.200 to 0.400
▒ 0.400 to 0.600
▓ 0.600 to 0.800
█ 0.800 to 1.000

Window 0,0 to 1000.00, 50.00

Figure A-16. Concentration Contour Plot Screen

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Vita

The author was born on October 28, 1967 in Lahore, Pakistan. He did his secondary and higher secondary education in Oman. In September 1985, he entered at West Virginia Institute of Technology as a freshman and graduated with B.S in Civil Engineering in May 1988. He is currently completing the requirements for the degree of Master of Science in Civil Engineering (Geotechnical) and is a member of Tau Beta Pi , American Society of Civil Engineers and American Geophysical Union.