MODEL FOR EVALUATION OF THE IMPACT OF CONTAMINATED SOIL ON GROUNDWATER

PHASE II

FINAL REPORT

Submitted to the New Jersey Department of Environmental Protection

by

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Preface

This project entails the development of a one-dimensional contaminant transpo model for layer-heterogeneous, isotropic, and unsaturated soils. The model is t be used by NJDEPE to develop regulatory clean-up levels for contaminants in th unsaturated zone based on an acceptable impact to groundwater.

This is the final report for Phase II of this project. It contains the mathematica development and the method of solution of moisture flow and transport of volatil organic compounds for layer-heterogeneous soils in the unsaturated zone, as well a the mathematical description of the saturated zone mass transport model DILUTE A brief sensitivity analysis is also included.

The following personnel are involved in this project:

Principal Investigators:	Dr. George P. Korfiatis, Stevens
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Chapter 1

Introduction

The flow and contaminant transport mechanisms in layer-heterogeneous soils are examined in this investigation. The work presented herein consists of solutions of the moisture flow and the mass transport equations. Furthermore, a thorough description of a two-dimensional, semi-analytical mass transport model is included for the computation of dilute concentrations within the underlying aquifer.

The unsaturated moisture flow equation is based on Richards' equation [73] which can be expressed either in the moisture content or in the pressure head form. Both formulations have been used extensively by many researchers, and each was found to posses some advantages for certain geological settings and conditions. Hills et al. [40] compared the solutions of the moisture content and the pressure head forms of [illegible] equation by using the implicit finite difference technique. The authors concluded that, despite the inherent difficulties in describing the boundary conditions, the equation based on moisture contents was more advantageous for the following reasons:

- Relatively low mass balance errors are produced in numerical computations;

- Relatively insensitive to dry initial conditions; therefore, adoptable to arid regions;

- Longer time steps can be incorporated in the simulation.

It is, therefore, believed that an algorithm based on the moisture content equation is more desirable for the purposes of the present study.

This study attempts to give a new approach to the formulation of the moisture flow equation in layered soils, similar to the one presented by Hills et al. [40]. The moisture discontinuities that occur on layer interfaces are handled by incorporating additional source and sink terms into the governing moisture transport equation. Real time boundary conditions, using actual daily rainfall data and mean monthly temperatures observed in Northeastern New Jersey, are implemented for the ground surface boundary, accounting for the full cycle of precipitation, evapotranspiration, and runoff events. The resulting non-linear partial differential equations are discretized by using a central difference scheme. The discretized equations are then solved numerically via the implicit finite differences technique, such as the one used by Korfiatis [53, 54]. Several parametric relationships, accounting for soil moisture retention and hydraulic conductivity, are incorporated in the model. The hysteretic behavior of retention properties is not considered within the scope of this study.

The dilute concentrations resulting in different locations within the underlying aquifer due to a strip source located at the top of the water table are calculated by using the semi-analytical solution proposed by Cleary and Ungs (1978) [20]. The saturated zone mass transport model DILUTE is coupled with the unsaturated moisture and mass transport model, and is incorporated into the current version of the IMPACT model (IMPACT v3.0).

Chapter 2

Mathematical Model Formulation

This chapter presents the mathematical formulations of the unsaturated flow and the mass transport processes discussed in the final report for Phase I of the project submitted to NJDEPE earlier. First, the model assumptions are outlined, then the governing moisture flow equation is presented with the appropriate boundary and initial conditions. The unsaturated mass transport equation is also presented in a similar manner. Furthermore, the saturated zone transport equation is formulated along with the appropriate boundary and initial conditions.

2.1 Assumptions

Several assumptions have been made throughout the development of this model. The most important assumptions are summarized below:

1. Soil is layer-heterogeneous (i.e., each layer is assumed to be homogeneous) and isotropic with respect to hydraulic properties;
2. The flow is one-dimensional and isothermal;

3. Contaminant source is assumed to be eliminated, therefore there is no immiscible components of the contaminant present in the soil;
4. Hysteretic behavior in the moisture retention properties is not considered;
5. Hysteretic behavior of the adsorption/desorption processes is neglected;
6. The groundwater table does not fluctuate substantially in comparison with the thickness of the unsaturated zone; therefore, it is assumed to be stationary with respect to time;
7. The groundwater table is assumed to be free of any contamination at the onset of simulation;
8. The air is at the atmospheric pressure and stationary within the soil;
9. Interactions between various chemical constituents and competitive effects are not considered;
10. Biotransformation takes place only in the liquid phase;
11. Oxygen is not a limiting factor for biological growth within the vadose zone;
12. Partitioning of the contaminant mass from one phase to another is assumed to be linear;
13. In the computation of the surface runoff, the cumulative 24-hour rainfall is assumed as a single storm event;
14. Soil existing in the saturated zone (aquifer) is assumed to be homogeneous, isotropic and isothermal;
15. Contaminant transport within the aquifer is assumed to be resulting from a finite length strip source located at the top of the groundwater table;

16. Aquifer is assumed to be free of contamination initially.

2.2 Moisture Flow

The mathematical model formulation is based on the transport mechanisms and the fate processes described in the final report for Phase I of the project. The governing moisture flow equation is solved to provide estimates of volumetric moisture contents and fluxes in one dimension which is taken vertically downward from the soil surface. The flow equation is written in terms of the volumetric moisture content as [73]:

$$\frac{\partial \theta_w}{\partial t} + \frac{\partial K(\theta_w)}{\partial z} - \frac{\partial}{\partial z}\left[D(\theta_w)\frac{\partial \theta_w}{\partial z}\right] = 0 \tag{2.1}$$

where

θ_w = *Volumetric moisture content* $[L^3/L^3]$

t = *Time coordinate* $[T]$

z = *Space coordinate taken positive downward* $[L]$

$K(\theta_w)$ = *Hydraulic conductivity* $[L/T]$

$D(\theta_w)$ = *Soil diffusivity coefficient* $[L^2/T]$

The moisture flux equation is given by Darcy's law as:

$$q_w = K(\theta_w) - D(\theta_w)\frac{\partial \theta_w}{\partial z} \tag{2.2}$$

The following initial and boundary conditions are implemented in the model:

2.2.1 Initial Condition

$$\theta_w(z) = \theta_{w_i}(z) \quad @ \quad t = 0 \tag{2.3}$$

where θ_{w_i} is the moisture content at the onset of the simulation.

2.2.2 Boundary Conditions

A fully transient, real-time simulation of precipitation/evapotranspiration events is incorporated in the upper boundary condition to give the model more flexibility [53].

1. Flux boundary condition during infiltration events:

$$I = K(\theta_w) - D(\theta_w)\frac{\partial \theta_w}{\partial z} \tag{2.4}$$

and

$$\frac{\partial \theta_w}{\partial z} \leq 0 \quad @ \quad z = 0 \quad for \quad 0 \leq t \leq t_p \tag{2.5}$$

$$\begin{aligned}
I &= P - R_s - E_t^* \quad (net\ infiltration\ rate) \quad [L/T] \\
P &= Precipitation\ rate \quad [L/T] \\
E_t^* &= Actual\ evapotranspiration\ rate\ from\ the\ surface \quad [L/T] \\
R_s &= Surface\ runoff\ rate \quad [L/T] \\
t_p &= Time\ required\ for\ the\ surface\ to\ become\ saturated \quad [T]
\end{aligned}$$

2. For the cases where the surface becomes saturated, and the water flux at the upper boundary continues, there are two possibilities:

   a) If $I \geq K_s$, the following boundary condition will be considered:

   $$\theta_w = \theta_s \tag{2.6}$$

   and

   $$\frac{\partial \theta_w}{\partial z} = 0 \quad @ \quad z = 0 \quad for \quad t_p < t \leq t_e \tag{2.7}$$

where

$$K_s = \textit{Saturated hydraulic conductivity} \ [L/T]$$
$$\theta_s = \textit{Saturated moisture content} \ [L^3/L^3]$$
$$t_e = \textit{Time when net precipitation becomes less than } K_s \ [T]$$

b) If $I < K_s$, the flux boundary condition described in Equation (2.4) will be used.

3. During periods of no water flux at the surface, only evapotranspiration will take place. The flux boundary condition for this case can be written as:

$$K(\theta_w) - D(\theta_w)\frac{\partial \theta_w}{\partial z} = -E_t^* \quad @ \quad z = 0 \quad for \ \ t_e' \leq t \leq t_n \tag{2.8}$$

where

$$t_e' = \textit{Time of moisture flux cessation at the surface} \ [T]$$
$$t_n = \textit{Time to initiation of a new moisture flux event or}$$
$$\textit{time required to reach the air} - \textit{dry moisture content} \ [T]$$

4. If the dry period is long enough, the surface moisture content will reach the air-dry value. For this case, the boundary condition becomes:

$$\theta_w = \theta_{ad} \tag{2.9}$$

and

$$\frac{\partial \theta_w}{\partial z} = 0 \quad @ \quad z = 0 \quad for \ \ t_n < t \leq t_c \tag{2.10}$$

where

$$\theta_{ad} = \textit{Air} - \textit{dry moisture content} \ [L^3/L^3]$$
$$t_c = \textit{Time at which a new precipitation event commences} \ [T]$$

When the value of $P - E_t^*$ at a given time step is greater than the saturated hydraulic conductivity of the soil, the excess water will become runoff since it cannot infiltrate into the soil with a rate greater than K_s. The second boundary condition mentioned above for the case of saturation handles this condition implicitly, without having to separate the runoff from the precipitation. This situation may occur if storm events over short periods of time are considered. The soil surface may become saturated immediately after the storm has started, and may remain at saturation as long as $P - E_t^*$ is greater than K_s. If long time periods are simulated, however, the model distributes the actual precipitation rates uniformly over time, reducing the maximum precipitation rate substantially depending on the time increment used. In this situation, the soil surface will not reach saturation. Therefore, the runoff has to be computed and separated explicitly from the precipitation values. This is achieved in the model by the SCS method [77].

The bottom boundary of the simulation domain is the top of the groundwater table. For the purposes of this model, the phreatic surface is assumed to be stationary in time. Two distinct bottom boundary conditions are incorporated in the model. These are:

1. Gravity drainage condition, i.e.

$$\frac{\partial \theta_w}{\partial z} = 0 \quad @ \quad z = z_L \quad for \;\; t > 0 \tag{2.11}$$

   where z_L is the distance from the ground surface to the top of the water table or capillary fringe.

2. Saturation condition, i.e.

$$\theta_w = \theta_s \quad @ \quad z = z_L \quad for \;\; t > 0 \tag{2.12}$$

2.3 Unsaturated Zone Transport

The equilibrium advection-dispersion equation for the transport of contaminants in partially saturated soils was derived by applying continuity principles over an infinitesimal control volume. In this study, transport of the total concentration is expressed in terms of the liquid phase concentration, C_L. The governing mass transport equation is written as:

$$\frac{\partial(\theta_w C_L)}{\partial t} + K_d \rho_b \frac{\partial C_L}{\partial t} + k' \rho_b C_L + \frac{1}{H}\frac{\partial(\theta_a C_L)}{\partial t} + \frac{\partial(q_w C_L)}{\partial z} = \frac{\partial}{\partial z}\left[\left(\theta_w E + \frac{D_a}{H}\right)\frac{\partial C_L}{\partial z}\right] - \theta_w R \tag{2.13}$$

where

C_L = *Liquid phase concentration* $[M/L^3]$

K_d = *Reversible adsorption coefficient* $[L^3/M]$

ρ_b = *Soil bulk density* $[M/L^3]$

k' = *Irreversible adsorption coefficient* $[L^3/MT]$

H = *Henry's constant*

E = *Hydrodynamic dispersion coefficient* $[L^2/T]$

D_a = *Molecular diffusion coefficient in soil air* $[L^2/T]$

R = *Rate of mass loss due to biotransformation* $[M/L^3T]$

Equation (2.13) is similar to that reported by Baehr [9].

If Monod kinetics are assumed, the R term in Equation (2.13) is substituted by the substrate utilization rate which is defined as [27]:

$$R_s = \frac{\mu_m X C_L}{Y(K_m + C_L)} \tag{2.14}$$

where

$$\begin{aligned} R_s &= Substrate\ utilization\ rate\ \ [M/L^3T] \\ \mu_m &= Maximum\ specific\ growth\ rate\ of\ microorganism\ \ [1/T] \\ X &= Microorganism\ concentration\ \ [M/L^3] \\ Y &= Biomass\ yield\ coefficient \\ K_m &= Substrate\ concentration\ at\ 1/2\ of\ \mu_m \end{aligned}$$

In this case, however, a mass balance equation for the microorganisms must be written as follows [27]:

$$\frac{\partial(\theta_w X)}{\partial t} + \frac{\partial(q_w X)}{\partial z} = \frac{\partial}{\partial z}\left[\theta_w \epsilon_w \frac{\partial X}{\partial z}\right] + \theta_w R_s - k_e X \theta_w \tag{2.15}$$

in which

$$\begin{aligned} \epsilon_w &= Mechanical\ dispersion\ coefficient\ \ [L^2/T] \\ k_e &= Endogenous\ decay\ coefficient\ \ [1/T] \end{aligned}$$

Equation (2.15) assumes that the microorganism transport is controlled by advection and mechanical dispersion. The diffusive term is neglected in the equation since it is assumed that advection dominates the transport of microorganisms [27].

Equations (2.13) and (2.15) are fully coupled and must be solved simultaneously. In the present model, the capability is provided to solve the coupled equations. It is, however, believed that the excess computational effort and the non-availability of Monod parameters will render this formulation undesirable. At equilibrium conditions, the microbial concentration becomes constant with respect to time. Therefore, Equation (2.13) is decoupled by using substrate limiting conditions at equilibrium. In this case, the R term in Equation (2.13) is replaced with one of the following:

- For $C_L \gg K_m$

$$R_s = k_0 \tag{2.16}$$

where k_0 is the zeroth order degradation coefficient $[M/L^3T]$;

- For $C_L \ll K_m$

$$R_s = k_1 C_L \tag{2.17}$$

where k_1 is the first order degradation coefficient $[1/T]$.

The first order degradation coefficient can be calculated by using the half-life of the chemical compound of interest, τ $[1/T]$, as follows [47]:

$$k_1 = \frac{\ln(2)}{\tau} \tag{2.18}$$

For nonbiodegradable transport, Equation (2.13) is solved without the R term. Equation (2.13) is similar to that reported by Baehr [9].

2.3.1 Initial Condition

The initial condition is implemented in the form:

$$C_L(z,0) = C_{Li} \quad @ \quad t = 0 \tag{2.19}$$

where C_{Li} is the initial liquid-phase concentration profile.

2.3.2 Boundary Conditions

Two extreme cases are used for the top boundary conditions in the model. The first assumes a no mass flux condition from soil surface to the atmosphere, namely:

$$\frac{\partial C_L(0,t)}{\partial z} = 0 \quad @ \quad z = 0 \tag{2.20}$$

The second top boundary condition assumes an infinite flux from soil surface to the atmosphere, i.e. $C_L = 0$. A comparison of these boundary conditions is given in the sensitivity analysis.

The bottom boundary condition is assumed to be as follows:

$$\frac{\partial C_L}{\partial z} = constant \tag{2.21}$$

therefore

$$\frac{\partial^2 C_L}{\partial z^2} = 0 \quad @ \quad z = z_L \quad for \;\; t > 0 \tag{2.22}$$

The top boundary condition for the microorganisms transport equation is a no-flux condition, similar to the one used for liquid phase mass transport equation.

2.4 Saturated Zone Transport

For a two-dimensional, homogeneous and isotropic, saturated porous medium, the equation governing solute mass transport can be written for stead-state flow conditions as [32]:

$$R_d \frac{\partial C_L}{\partial t} + U \frac{\partial C_L}{\partial x} + V \frac{\partial C_L}{\partial y} = D_x \frac{\partial^2 C_L}{\partial x^2} + D_y \frac{\partial^2 C_L}{\partial y^2} - \lambda R_d C_L \tag{2.23}$$

where

R_d = *Retardation coefficient*

U = *Average linear velocity in x direction* $[L/T]$

V = *Average linear velocity in y direction* $[L/T]$

D_x = *Hydrodynamic dispersion coefficient in x direction* $[L^2/T]$

D_y = *Hydrodynamic dispersion coefficient in y direction* $[L^2/T]$

λ = *First order degradation coefficient* $[1/T]$

The retardation coefficient is computed as [32]

$$R_d = 1 + \frac{\rho_b K_d}{n} \tag{2.24}$$

in which

ρ_b = *Bulk density of the aquifer soil* $[M/L^3]$

K_d = *First order equilibrium adsorption coefficient* $[L^3/M]$

n = *Porosity of the aquifer soil*

The first order equilibrium adsorption (partitioning) coefficient is calculated by using the organic carbon content of the soil (a soil parameter) and the normalized partition coefficient of the chemical with respect to carbon content (a chemical parameter) as:

$$K_d = f_{oc} K_{oc} \tag{2.25}$$

where

f_{oc} = *Organic carbon content of the soil*

K_{oc} = *Normalized partitioning coefficient of the chemical* $[L^3/M]$

Equation (2.23) is a special case of Equation (2.13) in terms of the moisture content, i.e. the coefficients of Equation (2.23) are simplified versions of the coefficients used in Equation (2.13) in the absence of a gaseous phase and for fully saturated conditions.

2.4.1 Initial and Boundary Conditions

A strip source of length $2a$ is assumed to be introduced at the top of the groundwater table at certain instant along the y axis as shown in Figure (2.1).

If the contaminant input concentration diminishes exponentially with time, the initial and boundary conditions for this problem can be written as:

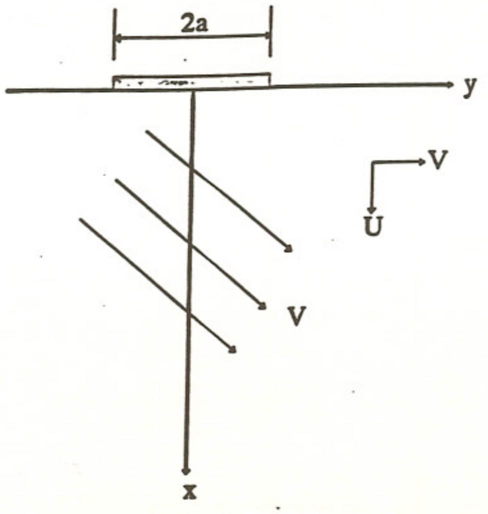


Figure 2.1: Schematic of a Strip Source Forming an Arbitrary Angle with the Flow Field

$$\begin{aligned}
C_L(0,y,t) &= C_0 \exp(-\gamma t) \;\; for \;\; |y| \leq a \; and \; t \geq 0 && (2.26)\\
C_L(0,y,t) &= 0 \;\; for \;\; |y| > a \; and \; t \geq 0 && (2.27)\\
\lim_{x \to \infty} \frac{\partial C_L}{\partial x} &= 0 && (2.28)\\
\lim_{y \to \infty} \frac{\partial C_L}{\partial y} &= 0 && (2.29)
\end{aligned}$$

where C_0 is the initial source concentration and γ is the source decay coefficient.

For the aforementioned conditions, an analytical solution of Equation (2.23) can be written as [20]:

$$\begin{aligned}
C_L(x,y,t) &= \frac{C_0 x}{4\sqrt{\pi D_x}} \exp\left[\frac{Ux}{2D_x} - \gamma t\right] \int_0^{t/R_d} \exp\left[-\left(\lambda R_d - \gamma R_d + \frac{U^2}{4D_x}\right)\tau\right.\\
&- \left.\frac{x^2}{4D_x \tau}\right] \tau^{-3/2} \left\{ \mathrm{erf}\left[\frac{\mathrm{a}-\mathrm{y}}{2\sqrt{\mathrm{D_y}\tau}} + \frac{\mathrm{V}}{2}\left(\frac{\tau}{\mathrm{D_y}}\right)^{1/2}\right] + \mathrm{erf}\left[\frac{\mathrm{a}+\mathrm{y}}{2\sqrt{\mathrm{D_y}\tau}}\right.\right.\\
&- \left.\left.\frac{V}{2}\left(\frac{\tau}{D_y}\right)^{1/2}\right]\right\} d\tau && (2.30)
\end{aligned}$$

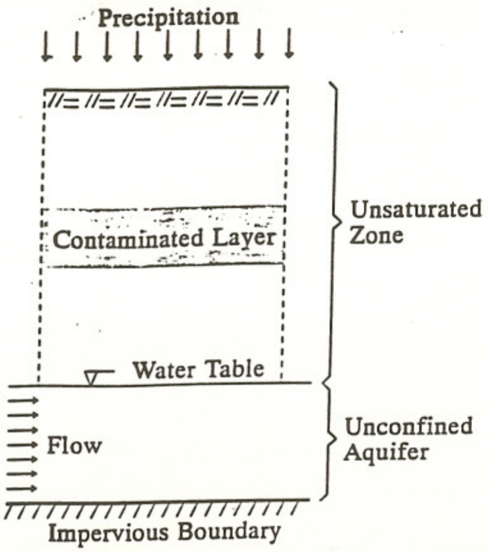


Figure 2.2: Schematic of Contaminated Layer in the Unsaturated Zone Overlying an Unconfined Aquifer

Equation (2.30) is valid for $x > 0$ and for all values of y. It is further stipulated that this equation will describe satisfactorily concentrations very close to the free surface of an unconfined aquifer if the soil gas and pore water above the phreatic surface are uncontaminated at the onset of the event under examination. For the situation depicted in Figure (2.2), the aquifer portion of the problem is restated in Figure (2.3).

In the absence of the impervious boundary, it can be seen that Equation (2.30) would be applicable provided that $U = 0$. However, the presence of the impervious boundary dictates the use of an image source, which is symmetrical to the actual one with respect to the impervious boundary. The actual solution of Equation (2.23) can be written as:

$$C_a(x,y,t) = C_L(x,y,t) + C_L(2b-x,y,t) \tag{2.31}$$

where $C_L(2b-x,y,t)$ is obtained from Equation (2.30) with $2b-x$ in place of x, and b is the aquifer thickness. When the input concentration is a step function, i.e.

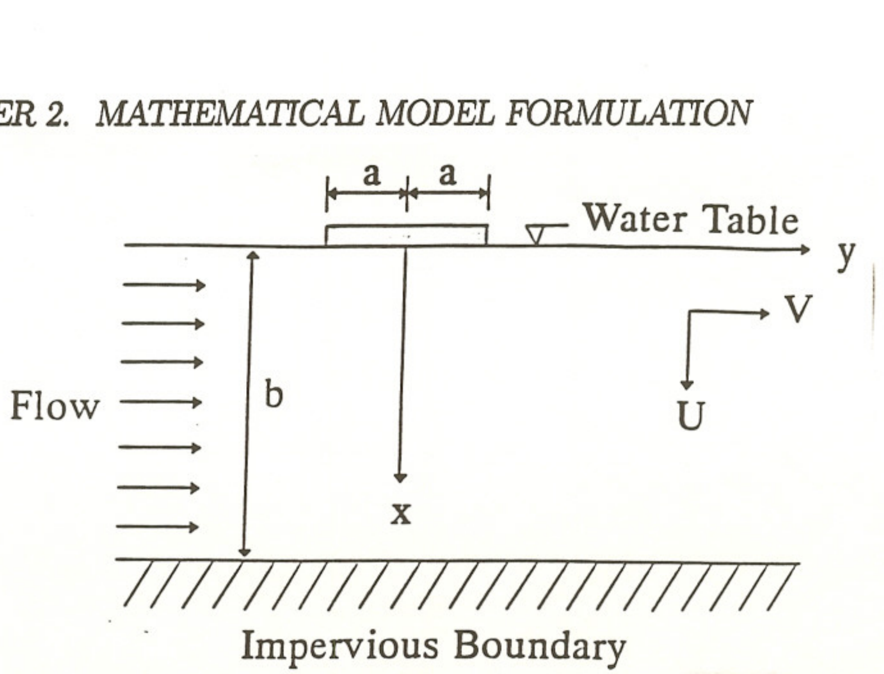


Figure 2.3: Contaminant Strip Source Applied to an Unconfined Aquifer

$\gamma = 0$, the solution for the problem under investigation takes the form:

$$\begin{aligned} C_L(x,y,t) &= \frac{C_0 x}{4\sqrt{\pi D_x}} \int_0^{t/R_d} \exp\left[-\lambda R_d \tau - \frac{x^2}{4 D_x \tau}\right] \tau^{-3/2} \left\{ \mathrm{erf}\left[\frac{\mathrm{a-y}}{2\sqrt{\mathrm{D_y}\tau}} \right.\right. \\ &+ \left.\frac{V}{2}\left(\frac{\tau}{D_y}\right)^{1/2}\right] + \mathrm{erf}\left[\frac{\mathrm{a+y}}{2\sqrt{\mathrm{D_y}\tau}} - \frac{\mathrm{V}}{2}\left(\frac{\tau}{\mathrm{D_y}}\right)^{1/2}\right]\left.\vphantom{\frac{a}{b}}\right\} d\tau \qquad (2.32) \end{aligned}$$

or

$$C_L(x,y,t) = C_0 A(x,y,t) \qquad (2.33)$$

where $A(x,y,t)$ is the right-hand side of Equation (2.32), less the step input concentration, C_0.

Equations (2.32) and (2.31) can be utilized to obtain aquifer concentrations when the input is an arbitrary function of time. Such scheme is numerically developed in Chapter 3.

Chapter 3

Method of Solution

This chapter outlines the solution methods used in the present study for the moisture transport equation in the unsaturated zone for both homogeneous and layer-heterogeneous soils. In addition, the saturated zone mass transport equation is solved by using the semi-analytical solution presented in Chapter 2 for a finite length strip source containing an input concentration condition as an arbitrary function of time.

Since the volumetric moisture content in the unsaturated zone exhibits discontinuities on layer interfaces for heterogeneous soils [40], a different formulation is rendered for the flow equation for layered systems. The discretization of the mass and bioorganism transport equations, however, remain the same for both homogeneous and heterogeneous soils, except for the fact that corresponding soil parameters are used within the equation for different soil layers (see the Final Report for Phase I). Therefore, these solutions are not presented herein.

3.1 Moisture Flow

In the present project, a fully implicit finite differences scheme is used to obtain the solution of the moisture transport equation. The basis of this numerical procedure is the replacement of the partial differential equation by a difference equation which approximately describes the relations of the pertinent variables at a given point of the space-time plane, (z,t), in terms of the values of these variables at neighboring points. The rectangular grid shown in Figure (3.1) represents the (z,t) plane with the space coordinates for $i = 1,\ 2,\ \ldots, n$, and the time coordinates for $k = 1,\ 2,\ \ldots, m$. The grid is considered to be fixed, and is represented by Δz and Δt for space and time increments, respectively.

3.1.1 Homogeneous Soils

The governing moisture flow equation was given in Chapter 2 as follows:

$$\frac{\partial\theta_w}{\partial t} + \frac{\partial K(\theta_w)}{\partial z} - \frac{\partial}{\partial z}\left[D(\theta_w)\frac{\partial\theta_w}{\partial z}\right] = 0 \tag{3.1}$$

The above equation can be written in discretized form:

$$\frac{\Delta\theta}{\Delta t} + \frac{\Delta K}{\Delta z} - \frac{\Delta}{\Delta z}\left[D\frac{\Delta\theta}{\Delta z}\right] = 0 \tag{3.2}$$

Using central differences for an intermediate layer, i, this equation becomes:

$$\left(\frac{\Delta\theta}{\Delta t}\right)_i^{k+1} + \frac{1}{\Delta z}\left(K_{i+1/2}^{k+1} - K_{i-1/2}^{k+1}\right) - \frac{1}{\Delta z}\left[\left(D\frac{\Delta\theta}{\Delta z}\right)_{i+1/2}^{k+1} - \left(D\frac{\Delta\theta}{\Delta z}\right)_{i-1/2}^{k+1}\right] = 0 \tag{3.3}$$

The time derivative is approximated for the i^{th} layer by the implicit finite difference equation of the form:

$$\left(\frac{\Delta\theta}{\Delta t}\right)_i^{k+1} = \frac{\theta_i^{k+1} - \theta_i^k}{\Delta t} \tag{3.4}$$

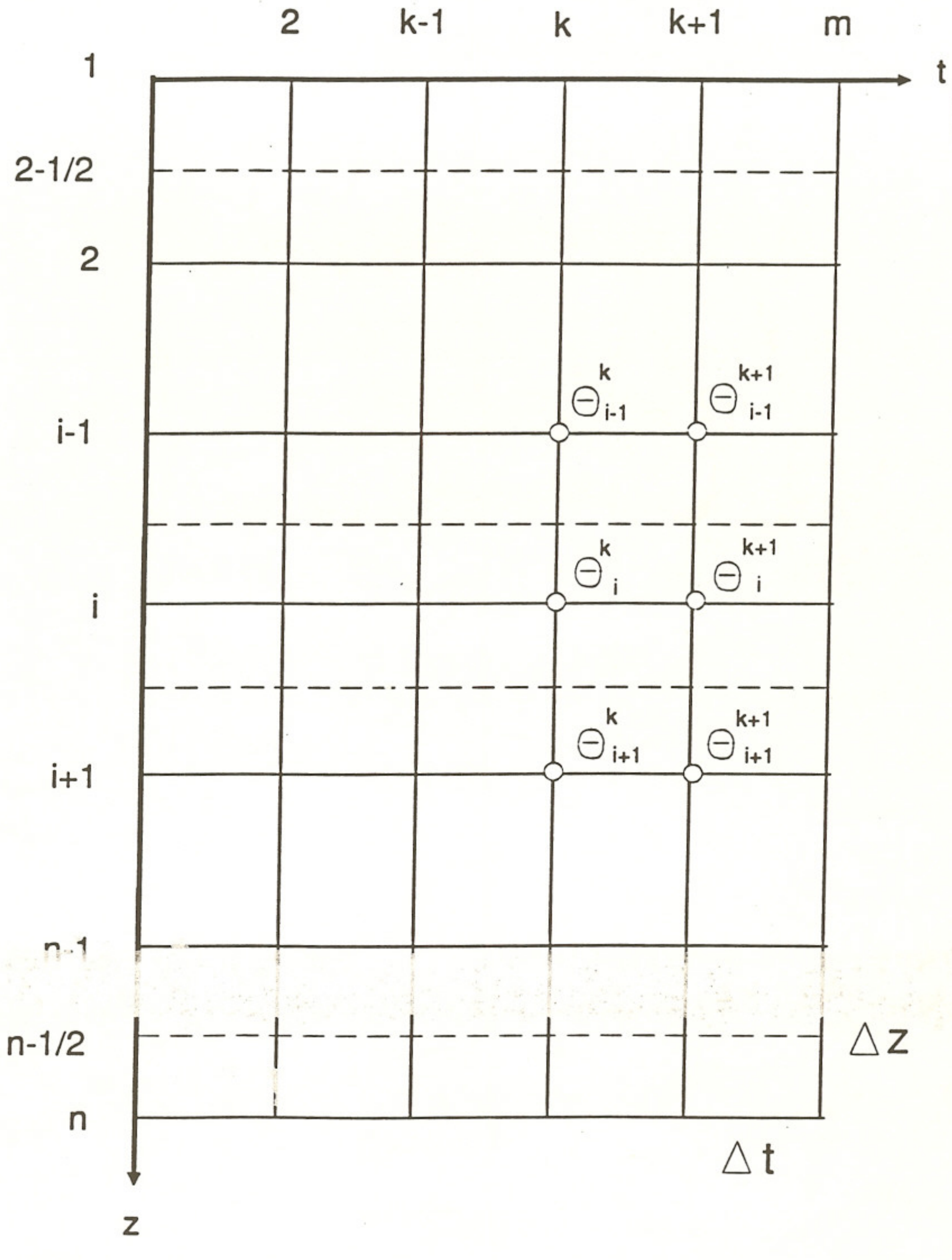


Figure 3.1: Time-space discretization for fully implicit finite differences

similarly, the space discretizations are written

$$\left(\frac{\Delta\theta}{\Delta z}\right)^{k+1}_{i+1/2} = \frac{\theta^{k+1}_{i+1} - \theta^{k+1}_{i}}{\Delta z} \tag{3.5}$$

$$\left(\frac{\Delta\theta}{\Delta z}\right)^{k+1}_{i-1/2} = \frac{\theta^{k+1}_{i} - \theta^{k+1}_{i-1}}{\Delta z} \tag{3.6}$$

The discretized form of the moisture flow equation for the intermediate nodes, $i = 2, \ldots, n-1$, can then be written as follows:

$$\left[-\frac{1}{\Delta z}D^{k+1}_{i-1/2}\right]\theta^{k+1}_{i-1} + \left[\frac{1}{\Delta z}D^{k+1}_{i+1/2} + \frac{1}{\Delta z}D^{k+1}_{i-1/2} + \frac{\Delta z}{\Delta t}\right]\theta^{k+1}_{i} + \left[-\frac{1}{\Delta z}D^{k+1}_{i+1/2}\right]\theta^{k+1}_{i+1} = \frac{\Delta z}{\Delta t}\theta^{k}_{i} - K^{k+1}_{i+1/2} + K^{k+1}_{i-1/2} \tag{3.7}$$

The terms D and K appearing in Equation (3.7) need to be evaluated at the interfaces $i-1/2$ and $i+1/2$ of the i^{th} layer. This is accomplished by discretizing the moisture flux equation for the layer interfaces as follows [53, 26]:

The moisture flux equation, q_w, was written in the following form:

$$q_w = K(\theta_w) - D(\theta_w)\frac{\partial\theta_w}{\partial z} \tag{3.8}$$

The above equation can be discretized for the $i+1/2$ interface by using the upper half layer with a forward difference equation as follows:

$$q^{k+1}_{i+1/2} = K^{k+1}_{i} - D^{k+1}_{i}\frac{\theta^{k+1}_{i+1/2} - \theta^{k+1}_{i}}{\Delta z/2} \tag{3.9}$$

similarly, for the lower half layer with a backward difference equation:

$$q^{k+1}_{i+1/2} = K^{k+1}_{i+1} - D^{k+1}_{i+1}\frac{\theta^{k+1}_{i+1} - \theta^{k+1}_{i+1/2}}{\Delta z/2} \tag{3.10}$$

Superimposing Equations (3.9) and (3.10) reveals:

$$\frac{q_{i+1/2}^{k+1} - K_i^{k+1}}{D_i^{k+1}} + \frac{q_{i+1/2}^{k+1} - K_{i+1}^{k+1}}{D_{i+1}^{k+1}} = -\frac{\theta_{i+1}^{k+1} - \theta_i^{k+1}}{\Delta z/2} \tag{3.11}$$

or

$$q_{i+1/2}^{k+1} = \frac{K_i^{k+1} D_{i+1}^{k+1} + K_{i+1}^{k+1} D_i^{k+1}}{D_i^{k+1} + D_{i+1}^{k+1}} - 2\frac{D_i^{k+1} D_{i+1}^{k+1}}{D_i^{k+1} + D_{i+1}^{k+1}} \left(\frac{\theta_{i+1}^{k+1} - \theta_i^{k+1}}{\Delta z}\right) \tag{3.12}$$

Equation (3.8) can also be discretized by central differences as follows:

$$q_{i+1/2}^{k+1} = K_{i+1/2}^{k+1} - D_{i+1/2}^{k+1} \left(\frac{\theta_{i+1}^{k+1} - \theta_i^{k+1}}{\Delta z}\right) \tag{3.13}$$

By comparing Equations (3.12) and (3.13), it can be deduced that

$$K_{i+1/2}^{k+1} = \frac{K_i^{k+1} D_{i+1}^{k+1} + K_{i+1}^{k+1} D_i^{k+1}}{D_i^{k+1} D_{i+1}^{k+1}} \tag{3.14}$$

$$D_{i+1/2}^{k+1} = 2\frac{D_i^{k+1} D_{i+1}^{k+1}}{D_i^{k+1} + D_{i+1}^{k+1}} \tag{3.15}$$

The above equations are harmonic means. These expressions are physically more sensible than the commonly employed arithmetic means [53].

By the change of variables, for the $i - 1/2$ interface, the hydraulic conductivity and the soil diffusivity terms are discretized as the following:

$$K_{i-1/2}^{k+1} = \frac{K_{i-1}^{k+1} D_i^{k+1} + K_i^{k+1} D_{i-1}^{k+1}}{D_{i-1}^{k+1} + D_i^{k+1}} \tag{3.16}$$

$$D_{i-1/2}^{k+1} = 2\frac{D_{i-1}^{k+1} D_i^{k+1}}{D_{i-1}^{k+1} + D_i^{k+1}} \tag{3.17}$$

3.1.2 Heterogeneous Soils

Layered soils exhibit a special problem in the numerical solution of Richards' moisture flow equation due to the moisture content discontinuities along layer interfaces

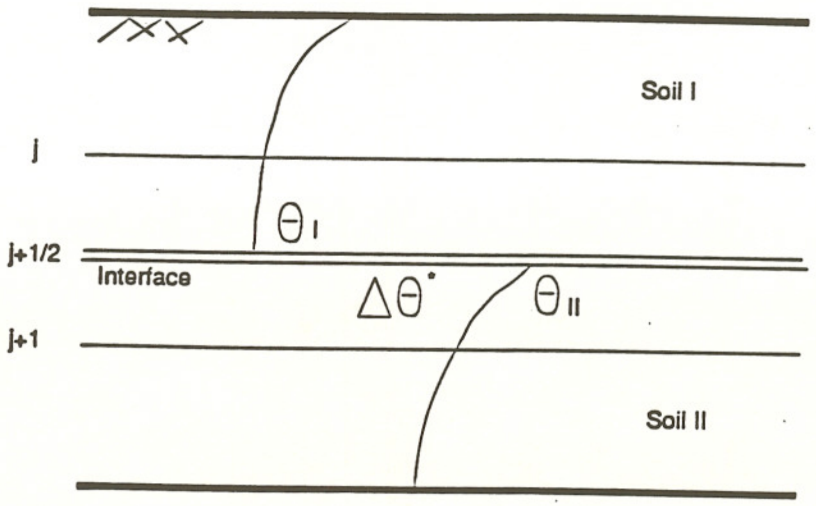


Figure 3.2: Schematic moisture content distribution in a two-layer system

[40]. Therefore, these interfaces have to be treated as intermediate boundaries for the flow equation.

Figure (3.2) represents a schematic moisture profile distribution with respect to depth for a two-layer soil system. The intermediate boundary is chosen to be the mid-layer interface, i.e. $j + 1/2$. The subscripts I and II denote the upper and the lower soil layers, respectively. The discontinuity in the volumetric moisture content is represented by $\Delta\theta^*$. At the interface, $j + 1/2$, the suction head is continuous. Therefore, the moisture flux across the intermediate boundary has to be continuous [40]. Namely,

$$q_I^{k+1} = q_{II}^{k+1} = q_{j+1/2}^{k+1} \tag{3.18}$$

Discretizing the moisture flux equation for the upper half layer with a forward difference equation reveals:

$$q_{j+1/2}^{k+1} = K_j^{k+1} - D_j^{k+1} \frac{\theta_I^{k+1} - \theta_j^{k+1}}{\Delta z/2} \tag{3.19}$$

Similarly, for the lower half layer with a backward difference equation

$$q_{j+1/2}^{k+1} = K_{j+1}^{k+1} - D_{j+1}^{k+1} \frac{\theta_{j+1}^{k+1} - \theta_{II}^{k+1}}{\Delta z/2} \tag{3.20}$$

or, alternatively

$$\frac{q_{j+1/2}^{k+1} - K_j^{k+1}}{D_j^{k+1}} = -2\frac{\theta_I^{k+1} - \theta_j^{k+1}}{\Delta z} \tag{3.21}$$

$$\frac{q_{j+1/2}^{k+1} - K_{j+1}^{k+1}}{D_{j+1}^{k+1}} = -2\frac{\theta_{j+1}^{k+1} - \theta_{II}^{k+1}}{\Delta z} \tag{3.22}$$

By superimposing the above equations, it can be written that

$$\begin{aligned} q_{j+1/2}^{k+1} = {} & \frac{K_j^{k+1} D_{j+1}^{k+1} + K_{j+1}^{k+1} D_j^{k+1}}{D_j^{k+1} + D_{j+1}^{k+1}} - \frac{2D_j^{k+1} D_{j+1}^{k+1}}{D_j^{k+1} + D_{j+1}^{k+1}} \left(\frac{\theta_{j+1}^{k+1} - \theta_j^{k+1}}{\Delta z} \right) \\ & + \frac{2D_j^{k+1} D_{j+1}^{k+1}}{D_j^{k+1} + D_{j+1}^{k+1}} \left(\frac{\theta_{II}^{k+1} - \theta_I^{k+1}}{\Delta z} \right) \end{aligned} \tag{3.23}$$

Using the harmonic means previously defined, Equation (3.23) becomes:

$$q_{j+1/2}^{k+1} = K_{j+1/2}^{k+1} - D_{j+1/2}^{k+1} \left(\frac{\theta_{j+1}^{k+1} - \theta_j^{k+1}}{\Delta z} \right) + D_{j+1/2}^{k+1} \frac{\Delta\theta_{*\,j+1/2}^{k+1}}{\Delta z} \tag{3.24}$$

where $\Delta\theta_{*\,j+1/2}^{k+1}$ is defined as the moisture jump condition along the intermediate boundary, and is equal to $\theta_{II}^{k+1} - \theta_I^{k+1}$. The moisture jump is known *a priori* on the onset of the simulation; however, it has to be determined for each time step throughout the simulation for $t > 0$. A second boundary condition has to be employed in order to determine the value of the moisture jump condition. The continuity of the suction heads along the intermediate boundary will serve this purpose. Namely,

$$\psi_I^{k+1} = \psi_{II}^{k+1} = \psi_{j+1/2}^{k+1} \tag{3.25}$$

Again, discretizing the suction head based moisture flux equation by central differences reveals the following:

$$q^{k+1}_{j+1/2} = K^{k+1}_{j+1/2} + K^{k+1}_{j+1/2}\left(\frac{\psi^{k+1}_{j+1} - \psi^{k+1}_{j}}{\Delta z}\right) \tag{3.26}$$

Equating Equations (3.24) and (3.26) leads:

$$\Delta\theta^{*\,k+1}_{j+1/2} = \theta^{k+1}_{j+1} - \theta^{k+1}_{j} + \frac{K^{k+1}_{j+1/2}}{D^{k+1}_{j+1/2}}(\psi^{k+1}_{j+1} - \psi^{k+1}_{j}) \tag{3.27}$$

For the intermediate nodes within a layer which is assumed to be homogeneous, the discretization of the governing moisture flow equation will be the same as Equation (3.7) for $i = 2, \ldots, j-1$. For the neighboring nodes of intermediate boundaries, however, a sink/source term has to be added to the governing equation to incorporate the moisture jump condition along the boundary. For layers j and $j+1$, the discretization of the moisture flow equation will be accomplished as follows:

For Layer j

The governing flow equation is written in discretized form as follows:

$$\frac{\theta^{k+1}_{j} - \theta^{k}_{j}}{\Delta t} + \frac{1}{\Delta z}\left[q^{k+1}_{j+1/2} - q^{k+1}_{j-1/2}\right] = 0 \tag{3.28}$$

Substituting Equation (3.24) into the above equation leads:

$$\left[-\frac{1}{\Delta z}D^{k+1}_{j-1/2}\right]\theta^{k+1}_{j-1} + \left[\frac{1}{\Delta z}D^{k+1}_{j+1/2} + \frac{1}{\Delta z}D^{k+1}_{j-1/2} + \frac{\Delta z}{\Delta t}\right]\theta^{k+1}_{j} +$$

$$\left[-\frac{1}{\Delta z}D^{k+1}_{j+1/2}\right]\theta^{k+1}_{j+1} = \frac{\Delta z}{\Delta t}\theta^{k}_{j} - K^{k+1}_{j+1/2} + K^{k+1}_{j-1/2} - D^{k+1}_{j+1/2}\frac{\Delta\theta^{*\,k+1}_{j+1/2}}{\Delta z} \tag{3.29}$$

This equation is exactly the same as Equation (3.7) except the last term, which is a sink term representing the moisture jump condition along the intermediate boundary of two soils.

For Layer $j+1$

Similarly, the governing equation is discretized as follows:

$$\frac{\theta_{j+1}^{k+1}-\theta_{j+1}^{k}}{\Delta t}+\frac{1}{\Delta z}\left[q_{j+3/2}^{k+1}-q_{j+1/2}^{k+1}\right]=0 \tag{3.30}$$

and with the use of Equation (3.24),

$$\left[-\frac{1}{\Delta z}D_{j+1/2}^{k+1}\right]\theta_{j}^{k+1}+\left[\frac{1}{\Delta z}D_{j+3/2}^{k+1}+\frac{1}{\Delta z}D_{j+1/2}^{k+1}+\frac{\Delta z}{\Delta t}\right]\theta_{j+1}^{k+1}+$$

$$\left[-\frac{1}{\Delta z}D_{j+3/2}^{k+1}\right]\theta_{j+2}^{k+1}=\frac{\Delta z}{\Delta t}\theta_{j+1}^{k}-K_{j+3/2}^{k+1}+K_{j+1/2}^{k+1}+D_{j+1/2}^{k+1}\frac{\Delta\theta_{*\,j+1/2}^{k+1}}{\Delta z} \tag{3.31}$$

Again, this equation is the same as Equation (3.7) except with a source term representing the moisture jump condition.

3.1.3 Boundary Conditions

The discretized equations given in the sections above are for the intermediate layers, i.e. $i=2,\ \ldots,\ n-1$. For the boundaries, however, the governing equation cannot directly be discretized by central differences. Therefore, for the first layer, a forward difference equation will be utilized to define the top boundary condition. Similarly, a backward difference equation will be used for the last layer, n.

Top Boundary Conditions

1. Flux Boundary Condition

   The governing equation is discretized for the top half layer with a forward difference equation as:

$$\left(\frac{\Delta\theta}{\Delta t}\right)_1^{k+1} + \frac{K_{1+1/2}^{k+1} - K_1^{k+1}}{\Delta z/2} -$$

$$\frac{1}{\Delta z/2}\left[\left(D\frac{\Delta\theta}{\Delta z}\right)_{1+1/2}^{k+1} - \left(D\frac{\Delta\theta}{\Delta z}\right)_1^{k+1}\right] = 0 \tag{3.32}$$

The top boundary condition for the rainfall events was defined as the following:

$$\left(D\frac{\Delta\theta}{\Delta z}\right)_1^{k+1} = K_1^{k+1} - I^{k+1} \tag{3.33}$$

Substituting this condition into the discretized governing equation reveals:

$$\left[\frac{1}{\Delta z}D_{1+1/2}^{k+1} + \frac{\Delta z}{2\Delta t}\right]\theta_1^{k+1} + \left[-\frac{1}{\Delta z}D_{1+1/2}^{k+1}\right]\theta_2^{k+1} =$$

$$\frac{\Delta z}{2\Delta t}\theta_1^k - K_{1+1/2}^{k+1} + I^{k+1} \tag{3.34}$$

2. Saturated and Dry Conditions

When the surface becomes saturated or reaches the air-dry moisture content, the governing equation is discretized for the second layer by a central difference equation:

$$\left(\frac{\Delta\theta}{\Delta t}\right)_2^{k+1} + \frac{K_{2+1/2}^{k+1} - K_{2-1/2}^{k+1}}{\Delta z} -$$

$$\frac{1}{\Delta z}\left[\left(D\frac{\Delta\theta}{\Delta z}\right)_{2+1/2}^{k+1} - \left(D\frac{\Delta\theta}{\Delta z}\right)_{2-1/2}^{k+1}\right] = 0 \tag{3.35}$$

Applying the boundary conditions,

$$\left(D\frac{\Delta\theta}{\Delta z}\right)_{2-1/2}^{k+1} = 0 \tag{3.36}$$

and

$$K_{2-1/2}^{k+1} = K_p^{k+1} \tag{3.37}$$

where

$$K_p^{k+1} = K_s \quad for \quad \theta_1^{k+1} = \theta_s$$

$$K_p^{k+1} = 0 \quad for \quad \theta_1^{k+1} = \theta_a$$

the governing equation then becomes:

$$\left[\frac{\Delta z}{\Delta t} + \frac{1}{\Delta z} D_{2+1/2}^{k+1}\right] \theta_2^{k+1} + \left[-\frac{1}{\Delta z} D_{2+1/2}^{k+1}\right] \theta_3^{k+1} =$$

$$\frac{\Delta z}{\Delta t} \theta_2^k - K_{2+1/2}^{k+1} + K_p^{k+1} \tag{3.38}$$

3. Evaporation Condition

During the times when there is no precipitation, only evapotranspiration will take place. For this case, the governing equation is discretized for the first half layer as has been done for the flux boundary condition. The top boundary condition is written in discretized form as:

$$\left(D\frac{\Delta \theta}{\Delta z}\right)_1^{k+1} = K_1^{k+1} + E_t^{k+1} \tag{3.39}$$

Then, the governing equation becomes:

$$\left[\frac{1}{\Delta z} D_{1+1/2}^{k+1} + \frac{\Delta z}{2\Delta t}\right] \theta_1^{k+1} + \left[-\frac{1}{\Delta z} D_{1+1/2}^{k+1}\right] \theta_2^{k+1} =$$

$$\frac{\Delta z}{2\Delta t} \theta_1^k - K_{1+1/2}^{k+1} - E_t^{k+1} \tag{3.40}$$

Bottom Boundary Conditions

The bottom boundary of the simulation domain is the top of the groundwater table or capillary fringe. In the present study, two conditions are considered as boundary conditions:

1. Gravity drainage condition

   Namely,

   $$\left(D\frac{\Delta\theta}{\Delta z}\right)_n^{k+1} = 0 \quad @ \quad z = z_L \tag{3.41}$$

   The governing equation is discretized for the n^{th} layer by using a backward difference equation of the form:

   $$\left(\frac{\Delta\theta}{\Delta t}\right)_n^{k+1} + \frac{K_n^{k+1} - K_{n-1/2}^{k+1}}{\Delta z/2} -$$
   $$\frac{1}{\Delta z/2}\left[\left(D\frac{\Delta\theta}{\Delta z}\right)_n^{k+1} - \left(D\frac{\Delta\theta}{\Delta z}\right)_{n-1/2}^{k+1}\right] = 0 \tag{3.42}$$

   or

   $$\left[-\frac{1}{\Delta z}D_{n-1/2}^{k+1}\right]\theta_{n-1}^{k+1} + \left[\frac{1}{\Delta z}D_{n-1/2}^{k+1} + \frac{\Delta z}{2\Delta t}\right]\theta_n^{k+1} =$$
   $$\frac{\Delta z}{2\Delta t}\theta_n^k - K_n^{k+1} + K_{n-1/2}^{k+1} \tag{3.43}$$

2. Saturation Condition

   Since $\theta_n = \theta_s$ for all time steps, only $n - 1$ equations will be solved. Therefore, there is no need to discretize the governing equation for this particular boundary condition.

3.1.4 Solution of Finite Difference Equations

Equation (3.7) must be incorporated with the initial and the appropriate boundary conditions in order to obtain a solution of moisture contents on the time-space grid. The discretized equations presented above form a system of order n which can be expressed in matrix form as follows:

$$\mathbf{A}\vec{\theta} = \vec{B} \tag{3.44}$$

where

$$\begin{aligned} \mathbf{A} &= Coefficient\ matrix\ of\ the\ system \\ \vec{\theta} &= Moisture\ vector \\ \vec{B} &= Column\ vector \end{aligned}$$

Replacing the coefficients of θ_{i-1}^{k+1}, θ_i^{k+1}, θ_{i+1}^{k+1}, and θ_i^k by a_i, d_i, c_i, and g_i, respectively, and setting $g_i\theta_i^k = b_i$, Equation (3.44) becomes:

$$\begin{bmatrix} d_1 & c_1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ a_2 & d_2 & c_2 & 0 & \cdots & 0 & 0 & 0 \\ 0 & a_3 & d_3 & c_3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & a_{n-1} & d_{n-1} & c_{n-1} \\ 0 & 0 & 0 & 0 & \cdots & 0 & a_n & d_n \end{bmatrix} \begin{Bmatrix} \theta_1^{k+1} \\ \theta_2^{k+1} \\ \theta_3^{k+1} \\ \vdots \\ \theta_{n-1}^{k+1} \\ \theta_n^{k+1} \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_{n-1} \\ b_n \end{Bmatrix} \tag{3.45}$$

The above equation can now be solved by the Gaussian elimination method as follows [15]:

The second row of the coefficient matrix, **A**, can be written of the form:

$$d_2'\theta_2^{k+1} + c_2\theta_3^{k+1} = b_2' \tag{3.46}$$

where

$$d'_2 = d_2 - \frac{a_2}{d_1}c_1 \tag{3.47}$$

$$b'_2 = b_2 - \frac{a_2}{d_1}b_1 \tag{3.48}$$

These equations can be generalized for the $(n-1)^{th}$ equation as the following:

$$d'_{n-1}\theta_{n-1}^{k+1} + c_{n-1}\theta_n^{k+1} = b'_{n-1} \tag{3.49}$$

where

$$d'_{n-1} = d_{n-1} - \frac{a_{n-1}}{d'_{n-2}}c_{n-2} \tag{3.50}$$

$$b'_{n-1} = b_{n-1} - \frac{a_{n-1}}{d'_{n-2}}b'_{n-2} \tag{3.51}$$

For an intermediate layer, l, the volumetric moisture content is then obtained from the following:

$$\theta_l^{k+1} = \frac{b'_l - c_l\theta_{l+1}^{k+1}}{d'_l} \tag{3.52}$$

where

$$b'_l = b_l - \frac{a_l}{d'_{l-1}}b'_{l-1} \tag{3.53}$$

$$d'_l = d_l - \frac{a_l}{d'_{l-1}}c_{l-1} \tag{3.54}$$

for $l = (n-1), (n-2), \ldots, 1$

For the n^{th} layer, however, the volumetric moisture content is equal to the following:

$$\theta_n^{k+1} = \frac{b'_n}{d'_n} \tag{3.55}$$

Table 3.1: Newton's divided difference method

Point	x	$f[x_0]$	$f[x_0, x_1]$	$f[x_0, x_1, x_2]$
0	z_{i-1}	θ_{i-1}^{k+1}		
			$\frac{\theta_{i-1}^{k+1}-\theta_i^{k+1}}{z_{i-1}-z_i}$	
1	z_i	θ_i^{k+1}		$\frac{(\theta_{i-1}^{k+1}-\theta_i^{k+1})(z_i-z_{i+1})-(\theta_i^{k+1}-\theta_{i+1}^{k+1})(z_{i-1}-z_i)}{(z_{i-1}-z_i)(z_i-z_{i+1})(z_{i-1}-z_{i+1})}$
			$\frac{\theta_i^{k+1}-\theta_{i+1}^{k+1}}{z_i-z_{i+1}}$	
2	z_{i+1}	θ_{i+1}^{k+1}		

3.1.5 Moisture Flux Computation

Once the volumetric moisture contents are computed, the moisture flux for the i^{th} layer is obtained as follows [53]:

$$q_i^{k+1} = K_i^{k+1} - D_i^{k+1} \left(\frac{\Delta\theta}{\Delta z} \right)_i^{k+1} \tag{3.56}$$

Korfiatis [53] evaluated the derivative $\frac{\Delta\theta}{\Delta z}$ in the equation given above by Newton's divided differences technique as follows: A parabola is fitted through three pairs of coordinate points as shown in Figure (3.3). This procedure is outlined below with the use of Table (3.1).

The volumetric moisture content can be written as a function of depth, z, of the [illegible] form:

$$\theta(z) = f[x_0] + (z - z_{i-1}) f[x_0, x_1] + (z - z_{i-1})(z - z_i) f[x_0, x_1, x_2] \tag{3.57}$$

The derivative of the above equation reveals:

$$\frac{\partial\theta(z)}{\partial z} = f[x_0, x_1] + 2z f[x_0, x_1, x_2] - (z_{i-1} + z_i) f[x_0, x_1, x_2] \tag{3.58}$$

Substituting $z = z_i$ and using the values given in Table (3.1) in the above equation, the final form of Equation (3.56) then becomes:

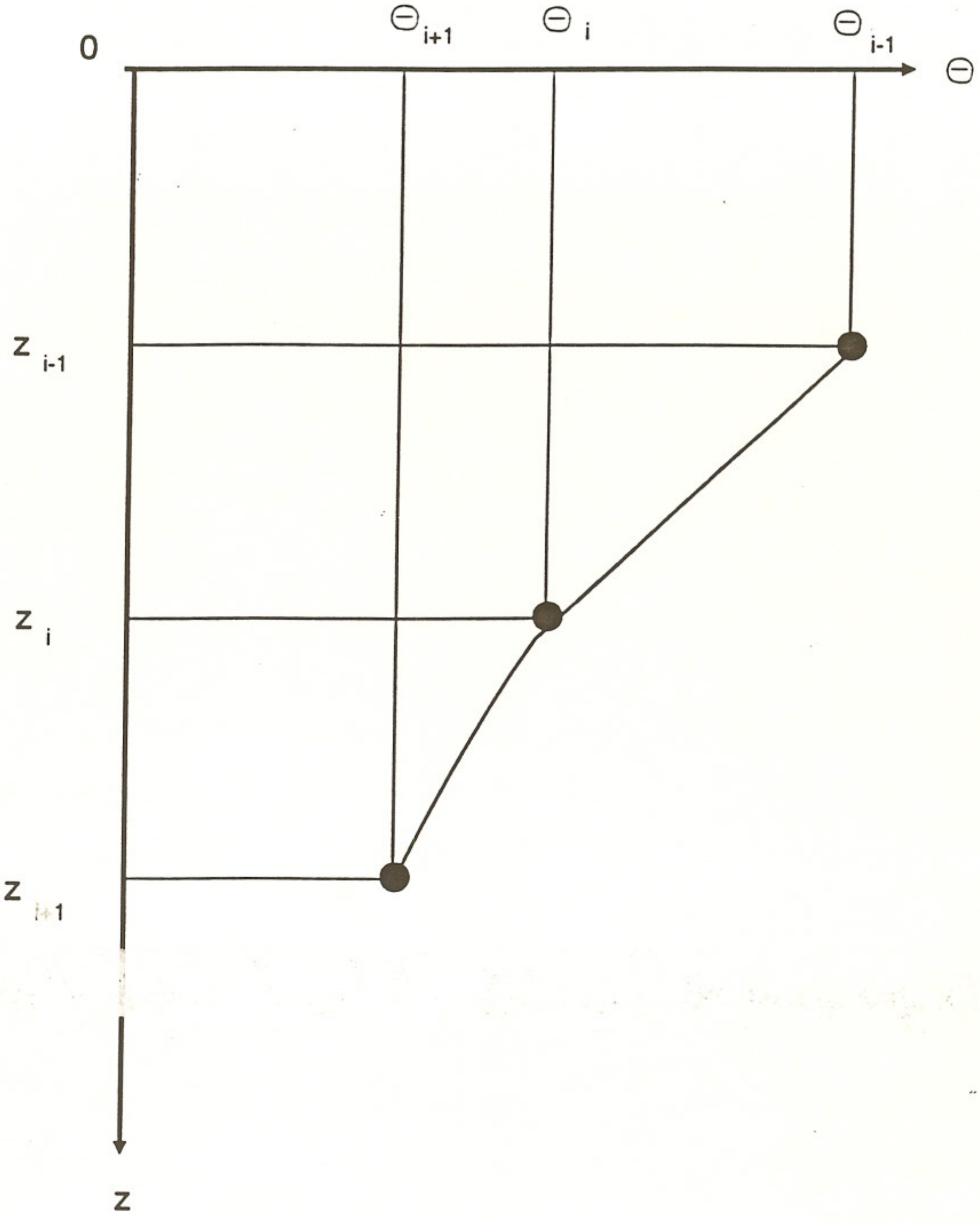


Figure 3.3: Three-point moisture profile for the computation of moisture flux (from Korfiatis, 1984)

$$q_i^{k+1} = K_i^{k+1} - D_i^{k+1} \left\{ 2 \left[\frac{\theta_{i-1}^{k+1}}{(z_{i-1} - z_i)(z_{i-1} - z_{i+1})} + \right. \right.$$

$$\left. \frac{\theta_i^{k+1}}{(z_i - z_{i-1})(z_i - z_{i+1})} + \frac{\theta_{i+1}^{k+1}}{(z_{i+1} - z_{i-1})(z_{i+1} - z_i)} \right] z_i +$$

$$\frac{\theta_{i-1}^{k+1}}{z_{i-1} - z_i} + \frac{\theta_i^{k+1}}{z_i - z_{i-1}} - \left[\frac{\theta_{i-1}^{k+1}}{(z_{i-1} - z_i)(z_{i-1} - z_{i+1})} + \right.$$

$$\left. \left. \frac{\theta_i^{k+1}}{(z_i - z_{i-1})(z_i - z_{i+1})} + \frac{\theta_{i+1}^{k+1}}{(z_{i+1} - z_{i-1})(z_{i+1} - z_i)} \right] (z_i + z_{i-1}) \right\} \tag{3.59}$$

3.1.6 Solution of the Saturated Zone Transport Equation

The analytical solution presented in Chapter 2 for the dilute concentrations in the underlying aquifer is valid for the input concentration which is given as a step function for $t = 0$ to ∞. However, due to a residually contaminated layer located in the unsaturated zone, the input concentration profile for the underlying aquifer is an arbitrary function of time. Such as input concentration history is shown in Figure (3.4). Therein, t^* is used as the time variable for the source function, in order to distinguish from the time of observation. In each time increment, δt^*, the input concentration changes by an increment $(\partial C_0/\partial t^*)$. For a change occurring at time t^*, the result for all future times, due to the incremental change, can be inferred from Equation (2.33) as:

$$\delta c = \frac{\partial C_0}{\partial t^*} \delta t^* A(x, y, t - t^*) \quad for \quad t > t^* \tag{3.60}$$

The total concentration at time t is the sum of the contributions at all prior times, therefore,

$$c(x, y, t) = \int_0^t \frac{\partial C_0}{\partial t^*} A(x, y, t - t^*) dt^* \tag{3.61}$$

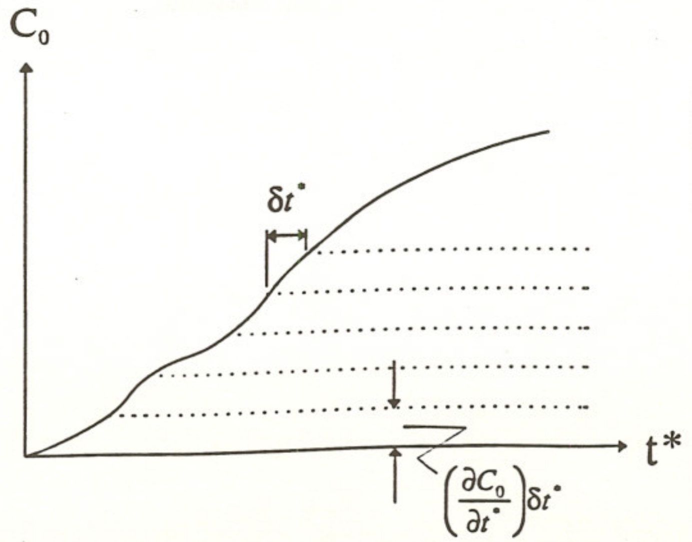


Figure 3.4: Superposition Used to Obtain Solution for a Time Variable Input Concentration

Thus, the actual concentration, accounting for the impervious boundary, can be expressed as:

$$c_a(x, y, t) = c(x, y, t) + c(2b - x, y, t) \tag{3.62}$$

In most practical situations, however, the input concentration history will be available in the form of discrete concentration values at specified time intervals. This is always true when a numerical model, such as IMPACT, is used to generate the input concentration history for the aquifer. Hence, the solution given by Equation (3.61) can be simplified by converting the input concentration history to a histogram form. This can be done in two different ways which both ensure that the total input mass is conserved. In the first approach, the concentration history is converted to a histogram form by averaging concentrations at discrete time instants, while in the second approach, the histogram form is obtained by assuming that concentrations at discrete time instants extend to the midpoints of the neighboring time intervals. Both schemes were tested for accuracy, and no significant deviations were found in terms of the results. Therefore, the first scheme is selected to be included

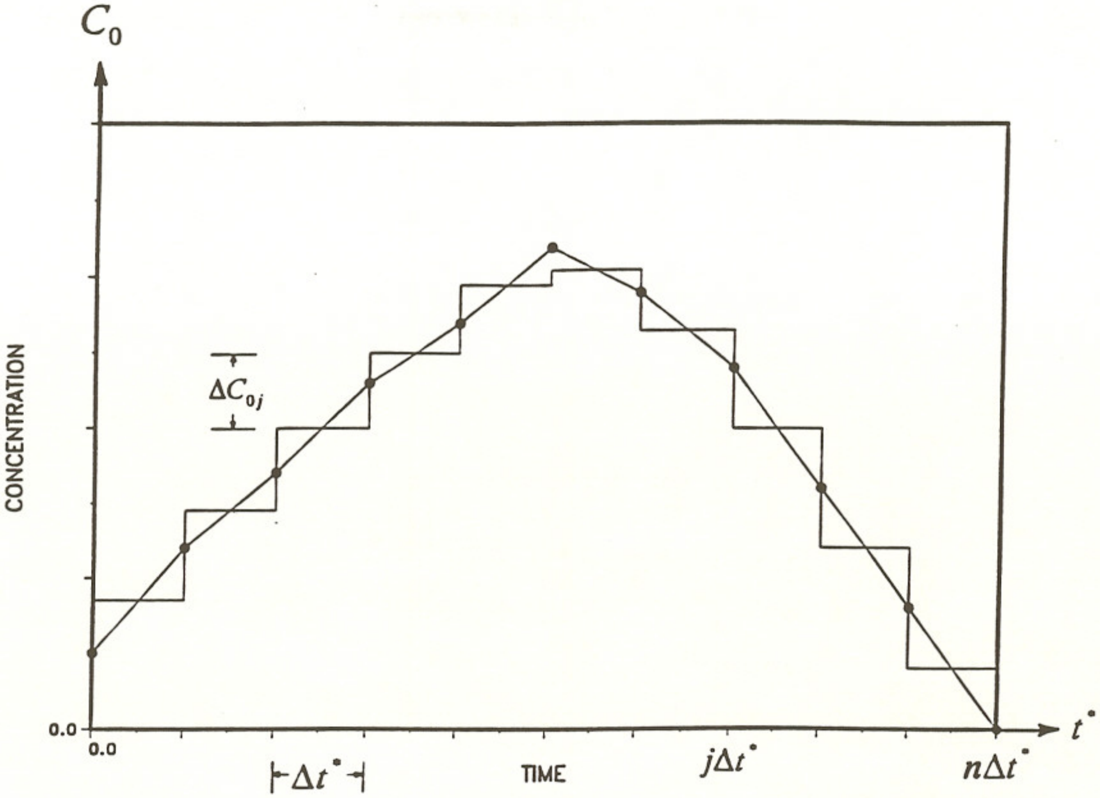


Figure 3.5: Conversion of Input Concentration History to a Histogram Form

in the current version of the model. This scheme is shown in Figure (3.5).

According to the scheme shown in Figure (3.5), Equation (3.61) can be expressed in summation form as:

$$c(x,y,t) = \sum_{j=0}^{J} \Delta C_{0j} A(x,y,t - j\Delta t^*) \tag{3.63}$$

where J is the integer portion of $t/\Delta t^*$ and ΔC_{0j}'s are taken in their algebraic sense. It is apparent that when $t/\Delta t^*$ is greater than n, then J becomes equal to n.

The integral used in $A(x,y,t)$ cannot be evaluated in a closed form by using calculus. Therefore, a numerical approximation scheme is adopted to estimate the value of the integral. For this purpose, a 200-point Gauss-Legendre scheme is employed. Details of this numerical scheme can be found in Press et al. [69].

Chapter 4

Sensitivity Analysis

This chapter presents a brief sensitivity analysis of the model output in layer heterogeneous soils by varying key input parameters. Simulations have been performed for four different soils and three different chemical compounds. The soil were chosen in the range of sand to silty clay. The hydrologic properties of thes soils are shown in Table (4.1) as given by Clapp and Hornberger [19]. In addition t unsaturated zone transport model sensitivity, the aquifer transport model, DILUTE was tested for hypothetical contamination scenarios.

The following default values have been used in all simulations except where indicated otherwise:

- Initial total concentration $C_T = 1$ mg/kg
- Time discretization increment $\Delta t = 1$ day
- Space discretization increment $\Delta z = 1$ ft
- Soil bulk density $\rho_b = 1.65$ gr/cm^3
- Dispersivity $\alpha = 0.2$ ft
- Root zone depth $d_r = 3$ ft

Table 4.1: Hydraulic properties of selected soils (after Clapp and Hornberger, 1978)

Hydraulic Properties	Soil Type			
	Sand	Sandy Loam	Silty Clay Loam	Silty Clay
K_s (ft/day)	49.88	9.83	0.482	0.293
θ_f	0.05	0.10	0.20	0.25
θ_s	0.395	0.440	0.477	0.492
θ_{ad}	0.01	0.05	0.07	0.10
m	11.1	12.8	18.5	23.8
b	4.05	4.9	7.75	10.4
ψ_s (ft)	0.4	0.72	1.17	1.6
θ_{w_i}	0.15	0.20	0.30	0.35
CN	72	82	87	89
θ_{wilt}	0.02	0.07	0.10	0.15

Table 4.2: Chemical properties of selected organic compounds

Chemical Properties	Compound		
	Benzene	TCE	Toluene
Water diffusivity d_w (m^2/day)	6.95×10^{-5}	6.90×10^{-5}	6.23×10^{-5}
Air diffusivity d_a (m^2/day)	0.831	0.609	0.729
Henry's constant K_H	0.233	0.377	0.265
Fugacity coefficient K_{oc} (ml/gr)	83	126	300

- Organic carbon content of the soil $OC = 0.5\%$

Actual rainfall and evapotranspiration data have been used for all sensitivity runs. Thornthwaite's method was used for the evapotranspiration computations. Benzene, toluene and TCE were the chemical compounds selected for the sensitivity analysis. The pertinent properties of these compounds are shown in Table (4.2).

4.1 Layer-Heterogeneous Soils

As mentioned in Chapter 3, layered soils exhibit a numerical difficulty in the solution of the moisture flow equation due to the discontinuities in the moisture content on layer interfaces. Therefore, the most important input parameters affecting the model outputs are the discretization increments. The following sensitivity runs were performed to determine the CFL condition for a four-layer system, consisting of a 5 feet silty clay loam layer at the top, a 15 feet sandy loam layer above a 5 feet silty clay layer in the middle, and a 5 feet sand layer on top of the groundwater table. Figure (4.1) shows the typical moisture content distribution through the unsaturated zone for this four-layer system. This profile has been obtained by using $\Delta z = 0.1$ feet and $\Delta t = 1$ day under the actual climatic input conditions for a total of 1,000

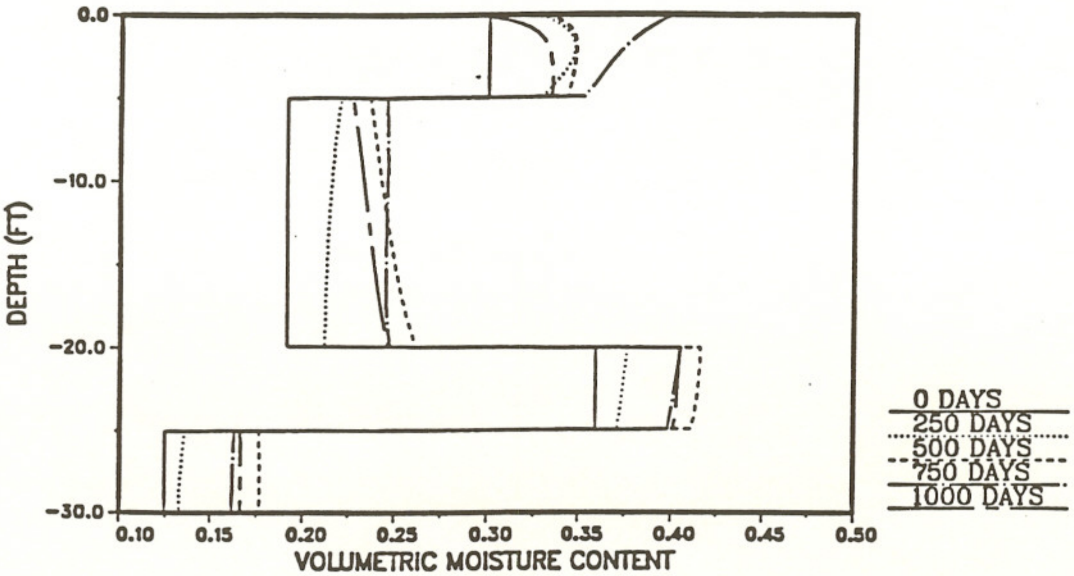


Figure 4.1: Typical moisture content distribution in layered soils

days.

Figure (4.2) shows the effect of different Δz values on the moisture content distribution at 1,000 days for the same geology given above. The differences observed in the moisture contents, especially, along the layer interfaces, were expected since the source/sink term used in the moisture flow equation for heterogenous soils is an indirect function of Δz. Figure (4.3) is the moisture flux history at the groundwater table. The effect of Δz on the moisture fluxes is the same as that observed in the case of homogeneous soils.

The effect of Δt has been examined for the same geology for Δz=1 foot. The results are shown in Figures (4.4) and (4.5) for the moisture content distribution and the moisture fluxes, respectively. As it was shown in the Final Report for Phase I, for the homogeneous soils, the effect of Δt is negligible.

Next, the soil layout configuration was investigated for a two-layer system contaminated with benzene. The top 6 feet of a 30 feet thick sand layer was alternated with different types of soil using Δz=2 feet and Δt=1 day for 2,000 days. The

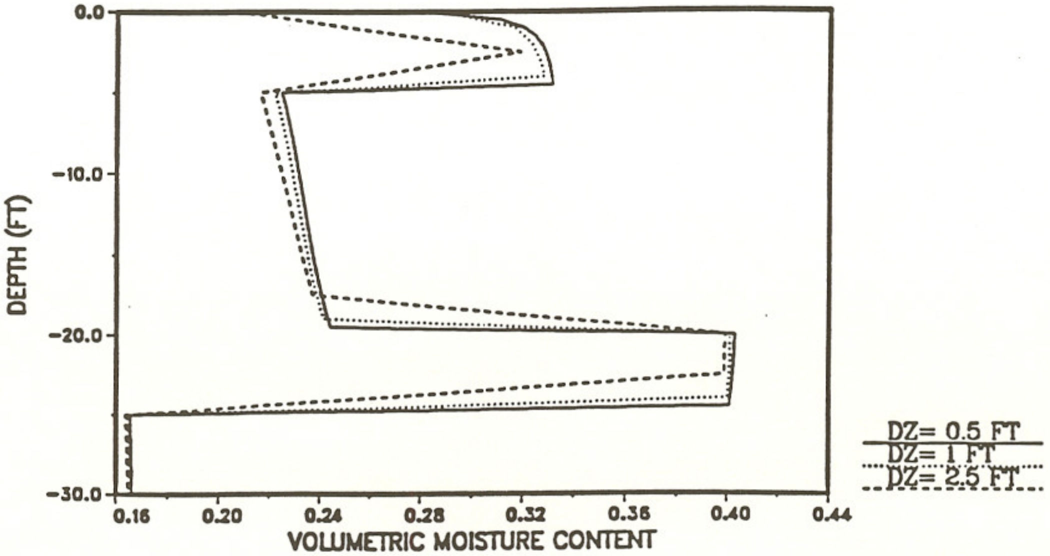


Figure 4.2: Effect of Δz on moisture content distribution of a four-layer soil

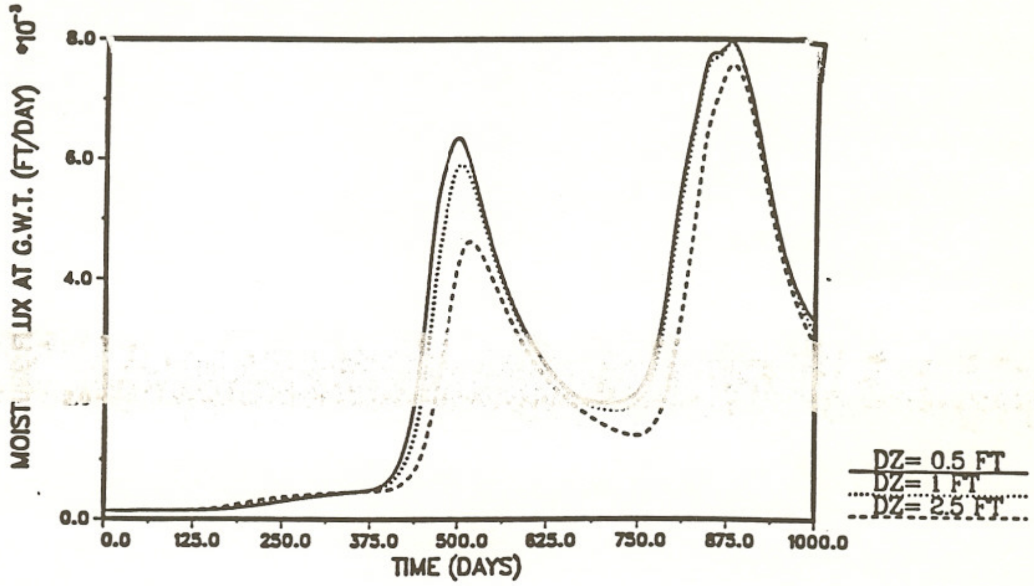


Figure 4.3: Effect of Δz on moisture fluxes at g.w.t. for a four-layer soil

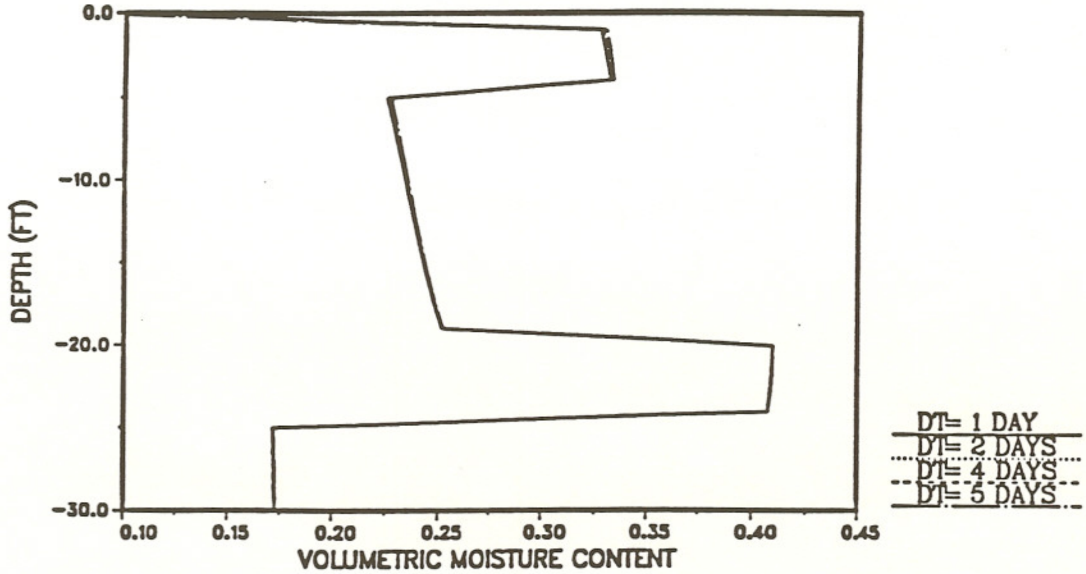


Figure 4.4: Effect of Δt on moisture content distribution of a four-layer soil

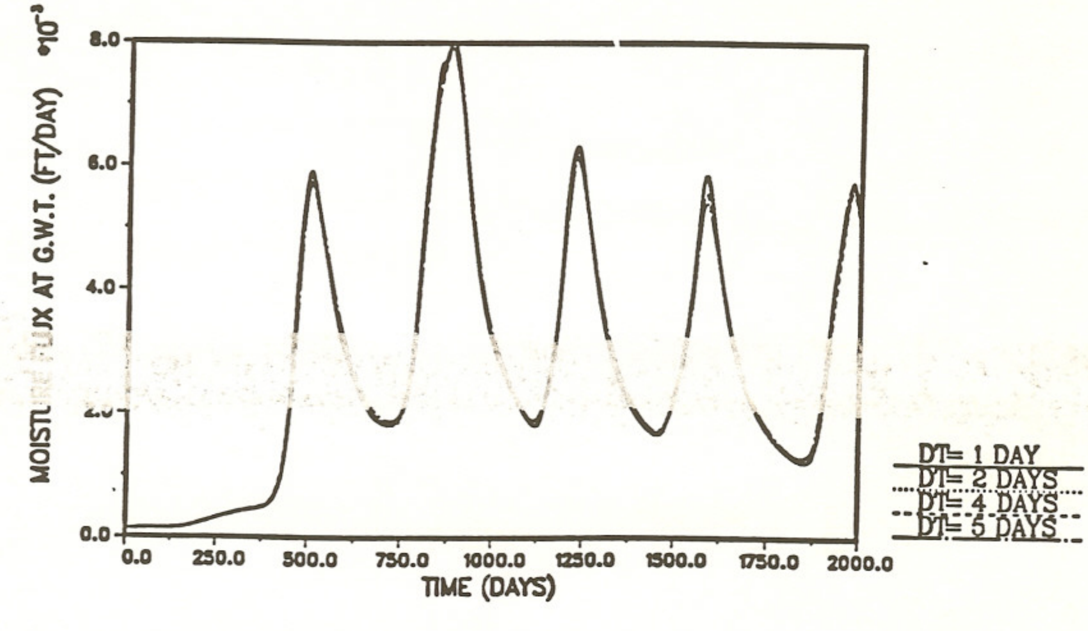


Figure 4.5: Effect of Δt on moisture fluxes at g.w.t. for a four-layer soil

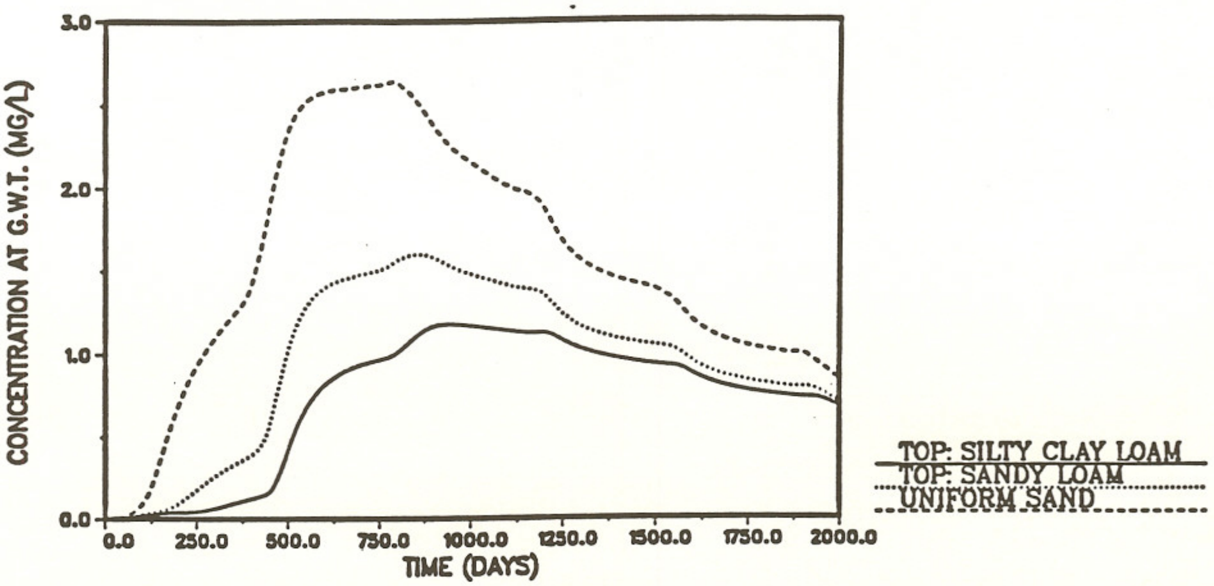


Figure 4.6: Effect of different types of soil cover on liquid phase concentrations at g.w.t.

effect of the soil cover on the liquid phase concentration at the groundwater table is shown in Figure (4.6). It is observed that the maximum concentration value is decreased drastically when clayey soils are used as the top layer. Figure (4.7) shows the moisture flux history at the groundwater table for different types of soil covers.

Lastly, the effect of the soil cover on the gaseous phase mass fluxes at the surface has been examined. The simulation was performed with Δz=0.5 feet and Δt=1 day for 2,000 days for a 30 feet thick sand layer with the first 6 feet covered with silty clay loam. The vapor flux history at the surface is shown in Figure (4.8). A close observation of Figure (4.8) reveals that the silty clay loam surface cover reduces the gaseous concentration values very close to the surface by more than two orders of magnitude in comparison with the case which does not contain a surface cover (see the Final Report for Phase I submitted to NJDEPE earlier).

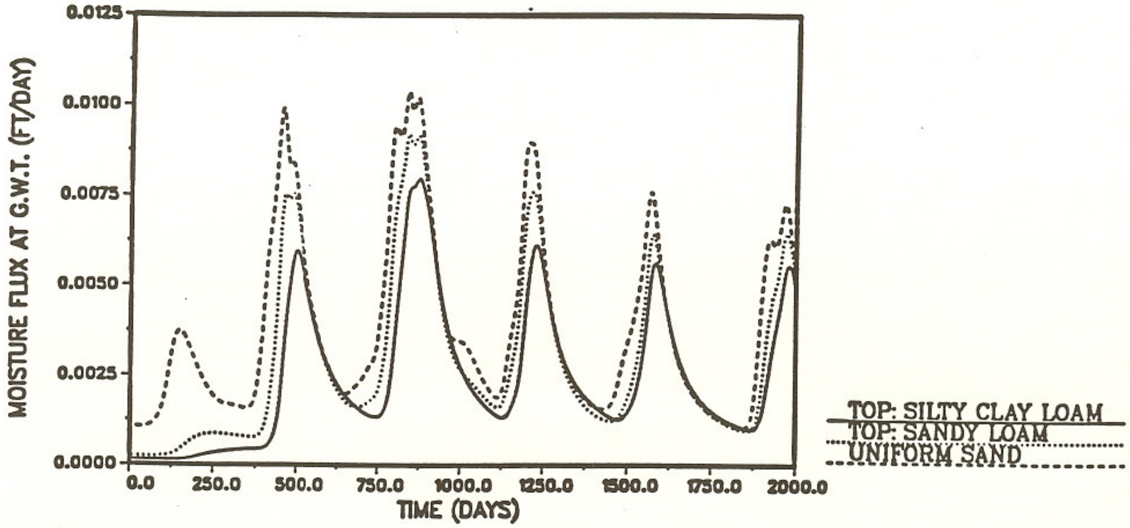


Figure 4.7: Effect of different types of soil cover on moisture fluxes at g.w.t.

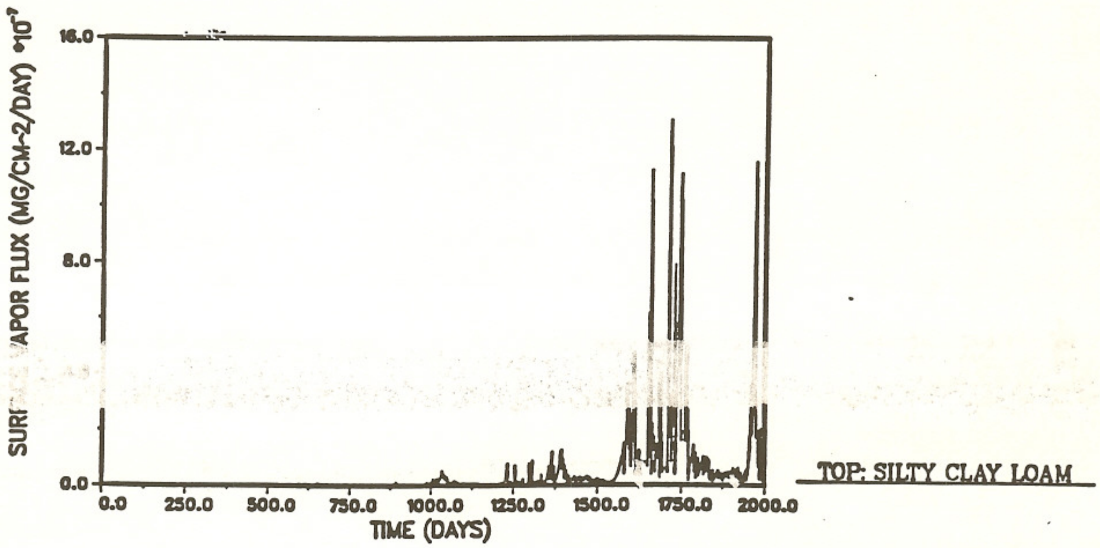


Figure 4.8: Effect of silty clay loam soil cover on gaseous phase fluxes at the surface of a sand layer

4.2 Aquifer Transport

In order to check the accuracy and efficiency of the numerical solution of Equation (2.33), two integration schemes were employed in this study, namely Romberg and 200-point Gauss-Legendre schemes [69]. The pertinent values of the parameters used were obtained from Javandel et al. [45] as follows: $U = 0.1\ m/day$, $a = 50\ m$, $D_x = 1\ m^2/day$, $D_y = 0.1\ m^2/day$, $R_d = 1$, and $\gamma = \lambda = 0$. The comparisons which are not shown herein proved that the Gauss-Legendre scheme is superior to the Romberg technique; therefore, all subsequent runs reported in this section were performed via the former approach.

A concentration history obtained from IMPACT was used as an input to the present model. Concentrations were computed at a distance of 20 m normal to the midpoint of the strip source ($x = 20\ m,\ y = 0\ m$). Discretization was performed for values of Δt equal to 1, 2, 4, 5 and 10 days. The agreement was very good; for $\Delta t = 1$ day, the output concentration is shown in Figure (4.9) as well as typical results corresponding to Δt of 4 and 10 days.

The present model qualitatively compared to the results of Pickens and Lennox [68], which are based on a finite element solution of the governing equations. It must be pointed out that direct comparisons cannot be made, because many of the parameters had to be approximated from information available in their paper. They first solved the steady-state flow problem in an approximately 50 m thick unconfined aquifer. Close observation of their results reveals that the flow field is approximately horizontal, especially downgradient from the input source. From their figures, it was roughly estimated that the head gradient of the flow field is 0.0122 and the length of the strip source is 160 m ($a = 80\ m$). The authors also provide other pertinent parameters as follows: hydraulic conductivity $K = 0.5\ m/day$, porosity $n = 0.3$ and bulk density $\rho_b = 1.8\ gr/cm^3$. Based on the above, it was estimated that the aquifer

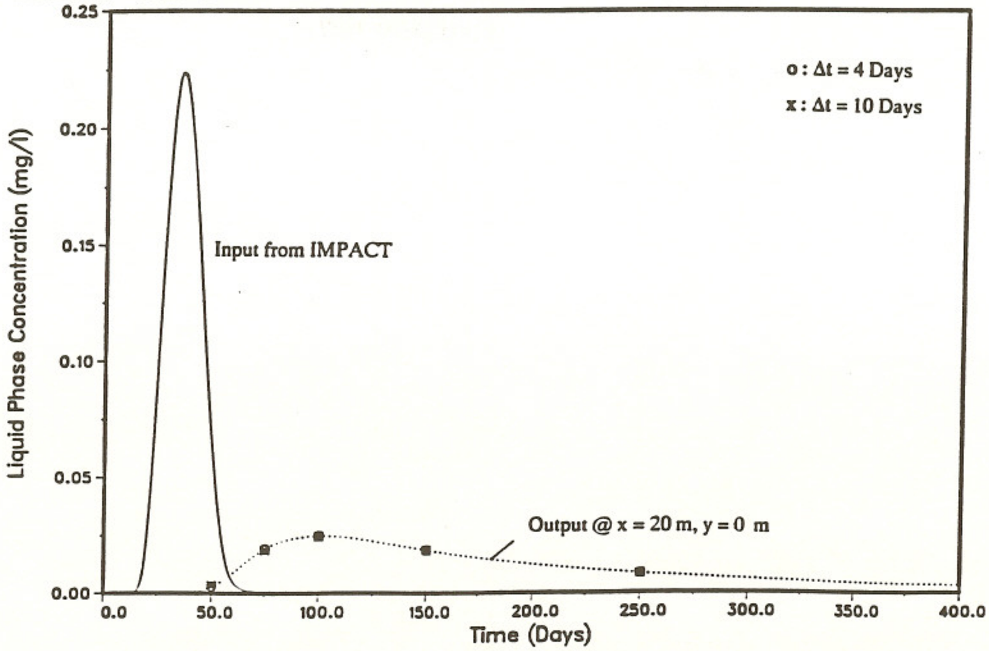


Figure 4.9: Output Concentration History for an Arbitrary Input Source

flow velocity at steady-state is $V = 0.0203\ m/day$. Furthermore, the hydrodynamic dispersion coefficients are defined, neglecting molecular diffusion, therein as:

$$D_L = \alpha_L V \tag{4.1}$$

$$D_T = \alpha_T V \tag{4.2}$$

where α is the soil dispersivity, and the subscripts L and T stand for longitudinal and transverse directions, respectively.

The aquifer portion of the present model was executed for the above values of the parameters and for a normalized step input. The results are shown in Figures (4.10) through (4.13). The qualitative agreement between the two solutions is satisfactory, although the present model underestimates concentrations near the phreatic surface due to the differences in the top boundary conditions of the two models.

Pickens and Lennox [68] also performed a simulation for variable input concentration as shown in Figure (4.14). The results obtained with the present model is shown in Figure (4.15). It is found that for $t = 20$ years, the qualitative agreement is also satisfactory.

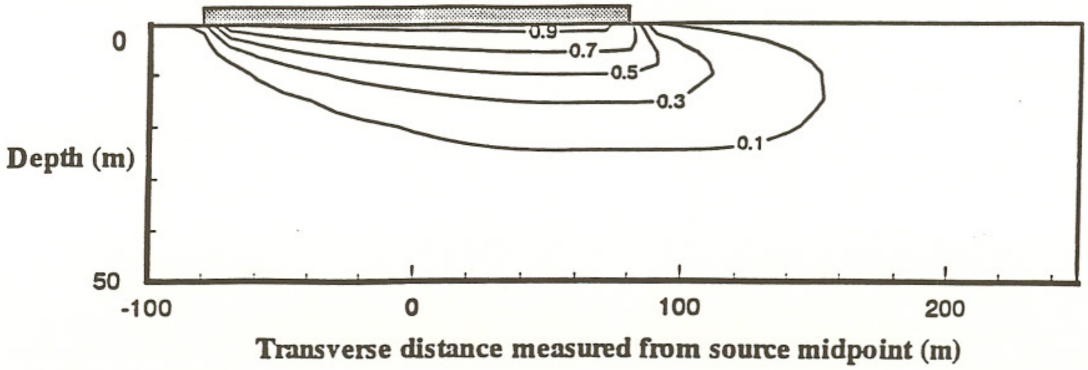


Figure 4.10: Concentration Distribution at $t = 15$ years. $\alpha_L = \alpha_T = 1\ m$

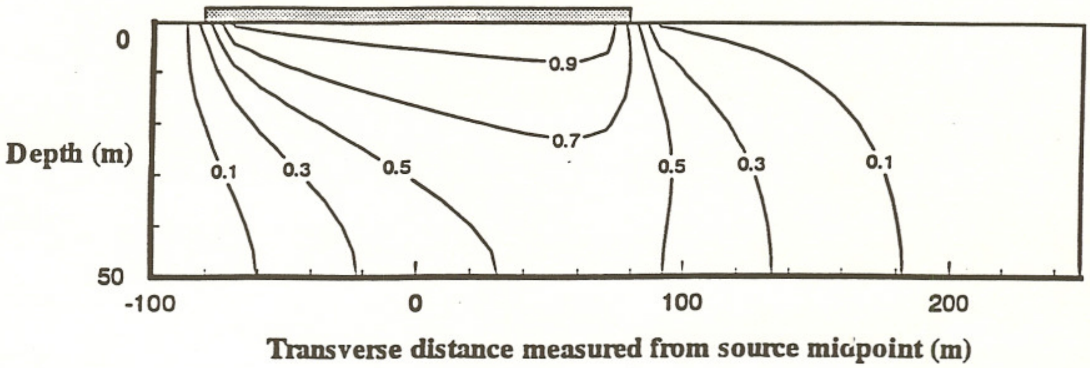


Figure 4.11: Concentration Distribution at $t = 15$ years. $\alpha_L = \alpha_T = 10\ m$

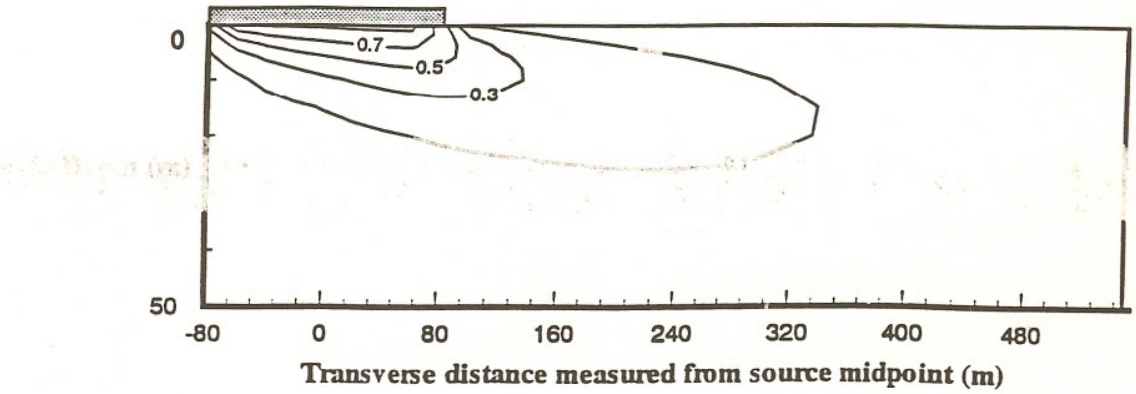


Figure 4.12: Concentration Distribution at $t = 60$ years. $\alpha_L = 10\ m, \alpha_T = 0.5\ m$ and, $K_d = 0\ cm^3/gr$

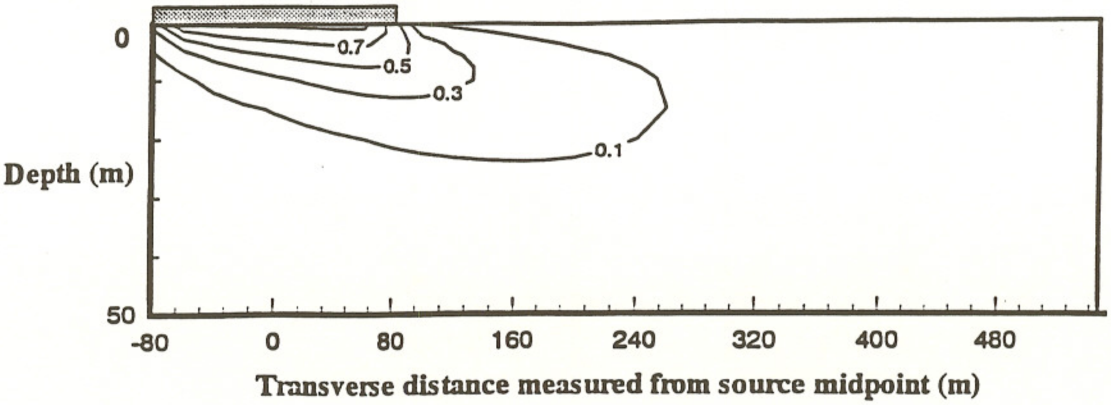


Figure 4.13: Concentration Distribution at $t = 60$ years. $\alpha_L = 10\ m, \alpha_T = 0.5\ m$, and, $K_d = 0.1\ cm^3/gr$

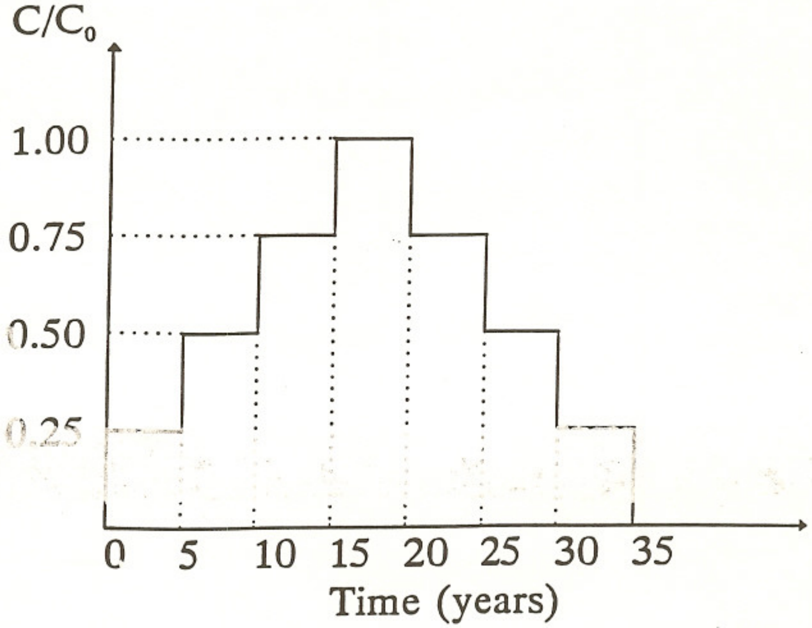


Figure 4.14: Variable Input Concentration History (after Pickens and Lennox, 1976)

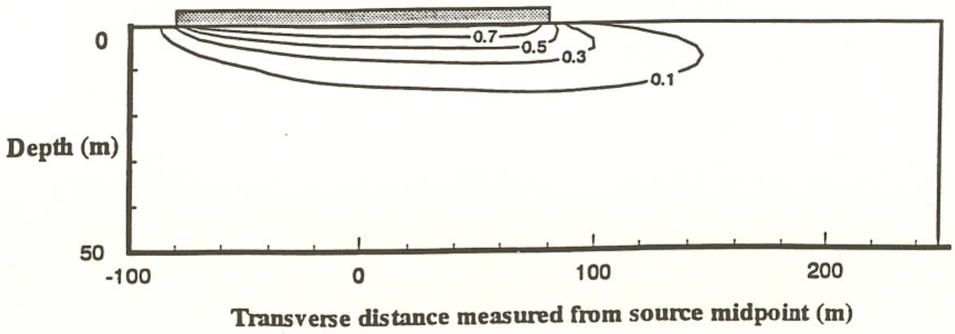


Figure 4.15: Concentration Distribution for $t = 20$ years, $\alpha_L = 10$ m, $\alpha_T = 0.5$ m

Based on the maximum allowable concentrations in any location of the aquifer the model can be used to determine maximum levels of residual contaminant concentrations for a layer located in the unsaturated zone. The current version of the IMPACT model has the capability of computing ultimate soil clean-up levels on the basis of the maximum concentrations observed either at the groundwater table or any arbitrary location(s) in the underlying aquifer. The latter is more realistic and gives higher levels of clean-up standards, since the concentrations will be diluted once the contaminant reaches the aquifer.

Chapter 5

Model Operation

5.1 Sample Run

The following sample run represents a contamination scenario where the first ten feet underneath the ground surface and the bottom ten feet above the groundwater table are initially free of contamination, and the middle ten feet of sand is contaminated with a total concentration of 0.5 mg/kg of TCE. It is further assumed that the first 5.75 feet of sand from the ground surface is excavated and replaced with silty clay loam liner to form a two-layer system.

The relevant hydrogeological and chemical input data are taken directly from Tables (4.1) and (4.2). The organic carbon content of the soil is assumed to be 0.5 %, and no biodegradation is considered. The simulation is performed for a total of [illegible] days. The spatial discretization of the 30 feet thick vadose zone is achieved with the increments of 0.5 foot. Similarly, the time marching scheme is established with one day intervals, and the actual climatic data are used throughout the simulation. The results are printed every 500 days.

```
PROGRAM IMPACT v1.3


 TYPE ONE OF THE FOLLOWING:

    A- RUN PROGRAM INTERACTIVELY

    B- RUN PROGRAM IN BATCH MODE

    E- EXIT

Enter A or B or E : A

ENTER THE FILE NAME TO BE CREATED FOR BATCH INPUT : SAMPLE.DAT

ENTER RUN NUMBER     <IRUN> : 1

         DATA COMPLETED - ANY CHANGES? [N]:

ENTER PROBLEM TITLE <TITLE> : SAND WITH SILTY CLAY LOAM LINER

         DATA COMPLETED - ANY CHANGES? [N]:

ENTER

    1: IF <FT-DAY>   UNITS ARE USED

    2: IF <M-DAY>    UNITS ARE USED

    3: IF <INCH-DAY> UNITS ARE USED

    4: IF <CM-DAY>   UNITS ARE USED

<IUN> : 1

         DATA COMPLETED - ANY CHANGES? [N]:

ENTER ONE OF THE FOLLOWING:

    1 : FOR MOISTURE BALANCE MODEL ONLY

    0 : FOR BOTH MASS TRANSPORT AND MOISTURE BALANCE MODELS

<ICI> : 0

         DATA COMPLETED - ANY CHANGES? [N]:



                    INPUT FLAGS

ENTER

    0: IF SOIL IS HOMOGENEOUS
```

```
    1: IF SOIL IS HETEROGENEOUS
<ISOIL> : 1
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER NUMBER OF LAYERS [MAX 4]  <ILAYER> : 2
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER NODE NUMBER IMMEDIATELY ABOVE
THE INTERFACE BETWEEN SOIL 1 AND SOIL 2    <JINT(1)> : 12
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER
    0: IF PRECIPITATION RATE IS VARIABLE W.R.T. TIME
    1: IF PRECIPITATION RATE IS CONSTANT W.R.T. TIME
    2: IF PRECIPITATION RATE WILL BE COMPUTED BY SUBROUTINE PREP
<IFL4> : 2
         DATA COMPLETED - ANY CHANGES? [N]:
ENTER
    0: IF EVAPOTRANSPIRATION RATE IS VARIABLE W.R.T. TIME
    1: IF EVAPOTRANSPIRATION RATE WILL BE COMPUTED BY SUBROUTINE EVAP
    2: IF EVAPOTRANSPIRATION RATE IS CONSTANT W.R.T. TIME
<IFL6> : 1
         DATA COMPLETED - ANY CHANGES? [N]:
ENTER
    0: IF MOISTURE FLUX WILL BE PRINTED AT EACH TIME STEP
    1: IF MOISTURE FLUX WILL NOT BE PRINTED
<IFL7> : 1
         DATA COMPLETED - ANY CHANGES? [N]:
```

```
ENTER
    0: IF CONSTITUENT IS BIODEGRADABLE
    1: IF CONSTITUENT IS NONBIODEGRADABLE
<INDEX> : 1
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER TYPE OF TOP B.C. FOR MASS TRANSPORT EQUATION
    0: ZERO LIQUID PHASE CONCENTRATION [CL=0]
    1: NO MASS FLUX CONDITION          [d(CL)/d(Z)=0]
<IFL11> : 0
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER
    0: IF INITIAL TOTAL CONCENTRATION IS CONSTANT W.R.T. SPACE
    1: IF INITIAL TOTAL CONCENTRATION IS VARIABLE W.R.T. SPACE
<IFL8> : 1
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER
    0: IF CONCENTRATION REDUCTION SCHEME IS NOT EXERCISED
    1: IF CONCENTRATION REDUCTION SCHEME IS EXERCISED
<IFL12> : 0
         DATA COMPLETED - ANY CHANGES? [N]:


          INPUT PARAMETERS FOR SOIL 1
ENTER
    THE VALUE OF SATURATED HYDRAULIC CONDUCTIVITY    <AKS(1)>
    THE VALUE OF FIELD CAPACITY MOISTURE CONTENT     <THF(1)>
    THE VALUE OF SATURATION MOISTURE CONTENT         <THS(1)>
```

```
    THE VALUE OF AIR-DRY MOISTURE CONTENT           <THAD(1)>
RESPECTIVELY : 0.482 0.20 0.477 0.07
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE EXPONENT M IN CAMPBELL'S K-THETA EXPRESSION  <AM(1)> : 18.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER
    THE COEFFICIENT b AND                                      <B(1)>
    THE SATURATION SUCTION HEAD IN CAMPBELL'S EXPRESSION   <PSIR(1)>
RESPECTIVELY : 7.75 1.17
         DATA COMPLETED - ANY CHANGES? [N]:

          INPUT PARAMETERS FOR SOIL 2
ENTER
    THE VALUE OF SATURATED HYDRAULIC CONDUCTIVITY    <AKS(2)>
    THE VALUE OF FIELD CAPACITY MOISTURE CONTENT     <THF(2)>
    THE VALUE OF SATURATION MOISTURE CONTENT         <THS(2)>
    THE VALUE OF AIR-DRY MOISTURE CONTENT           <THAD(2)>
RESPECTIVELY : 49.88 0.05 0.395 0.01
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE EXPONENT M IN CAMPBELL'S K-THETA EXPRESSION  <AM(2)> : 11.1
         DATA COMPLETED - ANY CHANGES? [N]:
ENTER
    THE COEFFICIENT b AND                                      <B(2)>
    THE SATURATION SUCTION HEAD IN CAMPBELL'S EXPRESSION   <PSIR(2)>
RESPECTIVELY : 4.05 0.4
         DATA COMPLETED - ANY CHANGES? [N]:
```

```
ENTER
    DEPTH INCREMENT    <DZ>
    TIME INCREMENT     <DT>
RESPECTIVELY : 0.5 1
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF PRINTOUT FREQUENCY (TIME INTERVAL)  <INT> : 500
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF ITERATION CONVERGENCE CRITERION     <EPS> : 0.001
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER
    NUMBER OF NODES OR LAYER INTERFACES          <N>
    NUMBER OF TIME STEPS                         <M>
RESPECTIVELY : 61 1000
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE CONSTANT VALUE OF INITIAL MOISTURE CONTENT  <THOL(1)> : 0.30
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE SCS SOIL CURVE NUMBER    <CN> : 87
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER TYPE OF CONSTITUENT CONSIDERED  <UNT> : TCE
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
```

```
AT DEPTH    0.50 FT                         <CTOTAL(  2)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    1.00 FT                         <CTOTAL(  3)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    1.50 FT                         <CTOTAL(  4)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    2.00 FT                         <CTOTAL(  5)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    2.50 FT                         <CTOTAL(  6)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    3.00 FT                         <CTOTAL(  7)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    3.50 FT                         <CTOTAL(  8)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    4.00 FT                         <CTOTAL(  9)> : 0
```

```
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   4.50 FT                         <CTOTAL( 10)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   5.00 FT                         <CTOTAL( 11)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   5.50 FT                         <CTOTAL( 12)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   6.00 FT                         <CTOTAL( 13)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   6.50 FT                         <CTOTAL( 14)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   7.00 FT                         <CTOTAL( 15)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   7.50 FT                         <CTOTAL( 16)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:
```

```
ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   8.00 FT                          <CTOTAL( 17)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   8.50 FT                          <CTOTAL( 18)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   9.00 FT                          <CTOTAL( 19)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   9.50 FT                          <CTOTAL( 20)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   10.00 FT                          <CTOTAL( 21)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   10.50 FT                          <CTOTAL( 22)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   11.00 FT                          <CTOTAL( 23)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:
```

```
ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    11.50 FT                          <CTOTAL( 24)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    12.00 FT                          <CTOTAL( 25)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    12.50 FT                          <CTOTAL( 26)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    13.00 FT                          <CTOTAL( 27)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    13.50 FT                          <CTOTAL( 28)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    14.00 FT                          <CTOTAL( 29)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH    14.50 FT                          <CTOTAL( 30)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
```

```
AT DEPTH   15.00 FT                          <CTOTAL( 31)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   15.50 FT                          <CTOTAL( 32)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   16.00 FT                          <CTOTAL( 33)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   16.50 FT                          <CTOTAL( 34)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   17.00 FT                          <CTOTAL( 35)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   17.50 FT                          <CTOTAL( 36)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   18.00 FT                          <CTOTAL( 37)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   18.50 FT                          <CTOTAL( 38)> : 0.5
```

```
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   19.00 FT                          <CTOTAL( 39)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   19.50 FT                          <CTOTAL( 40)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   20.00 FT                          <CTOTAL( 41)> : 0.5
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   20.50 FT                          <CTOTAL( 42)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   21.00 FT                          <CTOTAL( 43)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   21.50 FT                          <CTOTAL( 44)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   22.00 FT                          <CTOTAL( 45)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:
```

```
ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   22.50 FT                             <CTOTAL( 46)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   23.00 FT                             <CTOTAL( 47)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   23.50 FT                             <CTOTAL( 48)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   24.00 FT                             <CTOTAL( 49)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   24.50 FT                             <CTOTAL( 50)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   25.00 FT                             <CTOTAL( 51)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   25.50 FT                             <CTOTAL( 52)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:
```

```
ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   26.00 FT                          <CTOTAL( 53)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   26.50 FT                          <CTOTAL( 54)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   27.00 FT                          <CTOTAL( 55)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   27.50 FT                          <CTOTAL( 56)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   28.00 FT                          <CTOTAL( 57)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   28.50 FT                          <CTOTAL( 58)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   29.00 FT                          <CTOTAL( 59)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:

ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
```

```
AT DEPTH   29.50 FT                          <CTOTAL( 60)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN [MG/KG]
AT DEPTH   30.00 FT                          <CTOTAL( 61)> : 0
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER
    BULK WATER DIFFUSION COEFFICIENT IN [M^2/DAY]    <DDW>
    BULK AIR   DIFFUSION COEFFICIENT IN [M^2/DAY]    <DDA>
    HENRY'S CONSTANT [GASEOUS/LIQUID]                <HENRY>
    FUGACITY COEFFICIENT IN [ML/GR]                  <AKOC>
RESPECTIVELY : 6.90E-5 0.609 0.377 126
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER
    DESORPTION COEFFICIENT OF SOIL 1 IN [ML/GR/DAY]  <AKPR(1)>
    ORGANIC CARBON CONTENT OF SOIL 1 IN [%]            <OC(1)>
    DISPERSIVITY OF SOIL 1                           <ALAM(1)>
    BULK DENSITY OF SOIL 1 IN [GR/CM3]                <RHO(1)>
RESPECTIVELY : 0 0.5 0.2 1.65
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER
    DESORPTION COEFFICIENT OF SOIL 2 IN [ML/GR/DAY]  <AKPR(2)>
    ORGANIC CARBON CONTENT OF SOIL 2 IN [%]            <OC(2)>
    DISPERSIVITY OF SOIL 2                           <ALAM(2)>
    BULK DENSITY OF SOIL 2 IN [GR/CM3]                <RHO(2)>
RESPECTIVELY : 0 0.5 0.2 1.65
```

```
         DATA COMPLETED - ANY CHANGES? [N]:


ENTER ONE OF THE FOLLOWING:

    0: IF THORNTHWAITE'S EQUATIONS ARE USED

    1: IF PENMAN'S       EQUATIONS ARE USED

<IFLE> : 0

         DATA COMPLETED - ANY CHANGES? [N]:


ENTER

    0: IF MONTHLY MEAN TEMPERATURES ARE SUPPLIED BY USER

    1: IF THE AVERAGE VALUES OF THE LAST 30 YEARS ARE USED

<IFLT>: 1

         DATA COMPLETED - ANY CHANGES? [N]:


ENTER WILTING POINT OF THE SOIL IN [%] <THW> : 10

         DATA COMPLETED - ANY CHANGES? [N]:


ENTER THE DEPTH OF ROOT ZONE <DRZ> : 3

         DATA COMPLETED - ANY CHANGES? [N]:


TOTAL ITERATIONS IN YGRA=   2670


         END OF EXECUTION
```

The following output file lists a more detailed set of results for all iterations:

```
        SAND WITH SILTY CLAY LOAM LINER


        RUN NO : 1




         THIS IS A SIMULATION FOR BOTH MOISTURE AND SOLUTE TRANSPORT




                   ****** INPUT DATA FOR SUBPROGRAM YGRA *****
                          .............................


  FLAG1 = 1     FLAG2 = 1     FLAG3 = 0     FLAG4 = 2

  FLAG5 = 1     FLAG6 = 1     FLAG7 = 1     FLAG8 = 1

  FLAG9 = 1     FLAG10= 0     FLAG11= 0     FLAG12= 0




         HYDRAULIC PROPERTIES AND SIMULATION PARAMETERS

         .............................................




           SOIL 1


  SATURATED HYDRAULIC CONDUCTIVITY =    0.4820  FT/DAY


  FIELD CAPACITY MOISTURE CONTENT  =    0.2000  FT3/FT3
```

```
SATURATION MOISTURE CONTENT       =   0.4770  FT3/FT3

AIR-DRY MOISTURE CONTENT          =   0.0700  FT3/FT3

COEFFICIENT <AM>                  =  18.5000

COEFFICIENT <B>                   =   7.7500

SATURATION SUCTION HEAD           =   1.1700  FT

          SOIL 2

SATURATED HYDRAULIC CONDUCTIVITY =  49.8800  FT/DAY

FIELD CAPACITY MOISTURE CONTENT  =   0.0500  FT3/FT3

SATURATION MOISTURE CONTENT      =   0.3950  FT3/FT3

AIR-DRY MOISTURE CONTENT         =   0.0100  FT3/FT3

COEFFICIENT <AM>                 =  11.1000

COEFFICIENT <B>                  =   4.0500

SATURATION SUCTION HEAD          =   0.4000  FT


DEPTH INCREMENT                  =   0.5000  FT
```

```
TIME INCREMENT                   =    1.0000  DAYS



   *** OUTPUT PRINTED EVERY   500 TIME INCREMENTS ***



EPSILON                          =     0.001000

NUMBER OF LINES                  =    61

NUMBER OF TIME STEPS             =  1000



                    ***** INPUT DATA FOR MASS TRANSPORT MODEL *****
                          ...................................


                    THIS IS A SIMULATION FOR NONBIODEGRADABLE MATTER


        PRINTOUT FREQUENCY                    =  500

        NATURE OF THE SUBSTRATE               = TCE
```

```
          SOIL 1

FUGACITY COEFFICIENT                   =   0.1260E+03  ML/GR

SOIL DISPERSIVITY                      =   0.2000   FT

FIRST ORDER ADSORPTION COEFFICIENT     =   0.6300E+00  ML/GR

FIRST ORDER DESORPTION COEFFICIENT     =   0.0000E+00  ML/GR/DAY

BULK WATER DIFFUSION COEFFICIENT       =   0.6900E-04  M2/DAY

BULK  AIR  DIFFUSION COEFFICIENT       =   0.6090E+00  M2/DAY

HENRY'S CONSTANT                       =   0.3770

SOIL BULK DENSITY                      =   0.1650E+01  GR/CM3

          SOIL 2

FUGACITY COEFFICIENT                   =   0.1260E+03  ML/GR

SOIL DISPERSIVITY                      =   0.2000   FT

FIRST ORDER ADSORPTION COEFFICIENT     =   0.6300E+00  ML/GR

FIRST ORDER DESORPTION COEFFICIENT     =   0.0000E+00  ML/GR/DAY
```

```
          BULK WATER DIFFUSION COEFFICIENT      =     0.6900E-04   M2/DAY


          BULK  AIR  DIFFUSION COEFFICIENT      =     0.6090E+00   M2/DAY


          HENRY'S CONSTANT                      =     0.3770


          SOIL BULK DENSITY                     =     0.1650E+01   GR/CM3



                        INITIAL TOTAL CONCENTRATION   (MG/KG)
                        ...........................

0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00
0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00
0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00
0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00
0.5000E+00     0.5000E+00     0.5000E+00     0.5000E+00     0.5000E+00
0.5000E+00     0.5000E+00     0.5000E+00     0.5000E+00     0.5000E+00
0.5000E+00     0.5000E+00     0.5000E+00     0.5000E+00     0.5000E+00
0.5000E+00     0.5000E+00     0.5000E+00     0.5000E+00     0.5000E+00
0.5000E+00     0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00
0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00
0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00
0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00
0.0000E+00


                        INITIAL LIQUID PHASE CONCENTRATION   (MG/L)
```

```
0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00
0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00
0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00
0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00
0.6516E+00      0.6516E+00      0.6516E+00      0.6516E+00      0.6516E+00
0.6516E+00      0.6516E+00      0.6516E+00      0.6516E+00      0.6516E+00
0.6516E+00      0.6516E+00      0.6516E+00      0.6516E+00      0.6516E+00
0.6516E+00      0.6516E+00      0.6516E+00      0.6516E+00      0.6516E+00
0.6516E+00      0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00
0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00
0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00
0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00
0.0000E+00




                                    ***** RESULTS *****

                     ..............................................



                               MONTHLY MEAN TEMPERATURES (F)

                               .............................


    JAN    FEB    MAR    APR    MAY    JUN    JUL    AUG    SEP


  30.20  32.80  41.70  52.30  62.90   71.90  77.10  75.90  68.30
```

```
  OCT    NOV    DEC
57.00  46.90   35.80

CN  =  87.
THF =  20.00 (%)
THW =  10.00 (%)
DRZ =   3.00 (FT)

                       SUMMARY OF WATER BALANCE METHOD
                          (All results are in [mm])
                       ..............................

            JAN      FEB      MAR      APR      MAY      JUN      JUL      AUG

       P   84.93    78.55    98.06    95.70    97.94    75.92   113.09    96.55
  RUNOFF   13.80    11.90    18.75    19.33    19.19    12.02    28.27    24.72
       I   71.13    66.65    79.31    76.37    78.75    63.90    84.82    71.83
     PET    0.00     0.36    15.00    45.62    91.94   132.71   160.15   143.27
   I-PET   71.13    66.29    64.31    30.75   -13.19   -68.81   -75.34   -71.45
S(I-PET)    0.00     0.00     0.00     0.00    13.19    82.00   157.34   228.79
      ST   91.44    91.44    91.44    91.44    78.68    36.76    16.77     7.78
     dST    0.00     0.00     0.00     0.00   -12.76   -41.92   -19.99    -8.99
     AET    0.00     0.36    15.00    45.62    91.51   105.82   104.81    80.82
    PERC   71.13    66.29    64.31    30.75     0.00     0.00     0.00     0.00


            SEP      OCT      NOV      DEC      ANNUAL TOTALS
```

```
       P    92.57   74.49  100.11   89.34         1097.25

  RUNOFF    24.14   15.80   17.58   14.12          219.62

       I    68.44   58.69   82.53   75.22          877.63

     PET    96.69   52.86   22.09    3.16          763.87

   I-PET   -28.25    5.83   60.43   72.05

S(I-PET)   257.04    0.00    0.00    0.00

      ST     5.62   11.45   91.44   91.44          705.70

     dST    -2.16    5.83   79.99    0.00            0.00

     AET    70.59   52.86    2.54    3.16          573.10

    PERC     0.00    0.00    0.00   72.05          304.53


AVERAGE DAILY EVAP. FOR TIME STEP 500 = 0.9685E-02  FT/DAY ( 5/14/1960)



                    CONCENTRATION DISTRIBUTION AT   500.  DAYS MG/L


0.0000E+00     0.1211E-06     0.7901E-06     0.4343E-05     0.2142E-04

0.9775E-04     0.4133E-03     0.1644E-02     0.6847E-02     0.3662E-01

0.2195E+00     0.2018E+00     0.2000E+00     0.1964E+00     0.1971E+00

0.2031E+00     0.2136E+00     0.2278E+00     0.2447E+00     0.2632E+00

0.2827E+00     0.3024E+00     0.3219E+00     0.3408E+00     0.3587E+00

0.3753E+00     0.3905E+00     0.4033E+00     0.4142E+00     0.4226E+00

0.4284E+00     0.4316E+00     0.4320E+00     0.4296E+00     0.4245E+00

0.4167E+00     0.4066E+00     0.3942E+00     0.3798E+00     0.3637E+00

0.3462E+00     0.3274E+00     0.3078E+00     0.2876E+00     0.2671E+00

0.2465E+00     0.2260E+00     0.2059E+00     0.1864E+00     0.1674E+00

0.1493E+00     0.1319E+00     0.1154E+00     0.9973E-01     0.8489E-01

0.7083E-01     0.5745E-01     0.4467E-01     0.3237E-01     0.2041E-01
```

```
0.8628E-02


AVERAGE DAILY EVAP. FOR TIME STEP 1000= 0.7720E-02  FT/DAY ( 9/26/1961)




                    CONCENTRATION DISTRIBUTION AT  1000.  DAYS MG/L


0.0000E+00    0.2531E-05    0.1454E-04    0.6601E-04    0.2436E-03

0.8633E-03    0.3070E-02    0.1123E-01    0.4153E-01    0.1407E+00

0.3764E+00    0.3524E+00    0.3496E+00    0.3409E+00    0.3277E+00

0.3160E+00    0.3063E+00    0.2991E+00    0.2943E+00    0.2919E+00

0.2918E+00    0.2936E+00    0.2970E+00    0.3016E+00    0.3072E+00

0.3133E+00    0.3196E+00    0.3259E+00    0.3319E+00    0.3374E+00

0.3422E+00    0.3462E+00    0.3491E+00    0.3510E+00    0.3517E+00

0.3512E+00    0.3495E+00    0.3464E+00    0.3421E+00    0.3365E+00

0.3296E+00    0.3216E+00    0.3125E+00    0.3023E+00    0.2912E+00

0.2793E+00    0.2666E+00    0.2532E+00    0.2393E+00    0.2249E+00

0.2102E+00    0.1951E+00    0.1799E+00    0.1645E+00    0.1491E+00

0.1335E+00    0.1180E+00    0.1025E+00    0.8698E-01    0.7148E-01

0.5599E-01


MAX. CONCENTRATION AT G.W.T. : 0.5599E-01 MG/L AT  1000 DAYS



                    EFFLUENT CONCENTRATION AT WATER TABLE

                    .....................................


                       AT EVERY  500 TIME STEPS
```

```
                    ....................................



TIME DAYS           DISCHARGE FT/DAY          CHEMICAL CONC. MG/L


  500.                  0.6800E-02                0.8628E-02

  1000.                 0.3024E-02                0.5599E-01


                    DISCHARGE AND CUMM. VOL. AT WATER TABLE

                    ....................................

                          AT EVERY  500 TIME STEPS


                    ....................................



TIME DAYS DISCHARGE CUBIC FT/DAY  VOLUME CUBIC FT CUMM. VOLUME CUBIC FT


 500.       0.6800E-02                0.6817E-02       0.5435E+00

 1000.      0.3024E-02                0.3032E-02       0.2681E+01
```

5.2 Input Preprocessor

The current version of the IMPACT model contains a preprocessor for creating input files for the model in a spreadsheet environment. The preprocessor is written in Microsoft Excel © version 4.0 by using macros linked with dialog boxes.

The preprocessor, like a template, helps users to select appropriate model parameters via interactive dialog boxes and mouse operation. The preprocessor is equipped with several easy to update soil and chemical databases. Particular databases are built into the corresponding macro sheets, and permanent values of variables are hard-coded.

Appendix A contains a practical user's guide for preprocessor operation.

5.2.1 Soil and Chemical Databases

Pertinent values of the properties of four different soils, ranging from silty clay to sand, are built into a database which can be used in preprocessor operation. Similarly, Properties of 19 chemical compounds are supplied in a separate database which is also implemented in the preprocessor. Appendix B contains the chemical properties built into the chemical database. The aforementioned databases can easily be updated by users. The procedure for updating the databases is outlined in the preprocessor user's guide given in Appendix A.

Bibliography

[1] Abbott, M. B. *Computational Hydraulics.* Pitman Publ., London, U.K., 1979.

[2] Abriola, L. M. and G. F. Pinder. "A Multiphase Approach to the Modeling of Porous Media Contamination by Organic Compounds, 1. Equation Development". *Water Resources Research*, 21(1):11–18, 1985.

[3] Abriola, L. M. and G. F. Pinder. "A Multiphase Approach to the Modeling of Porous Media Contamination by Organic Compounds, 2. Numerical Simulation". *Water Resources Research*, 21(1):163–186, 1985.

[4] Ahlert, W. K., C. G. Uchrin. "Movement of Selected Organic Compounds in Soil Columns". In *Geotechnical and Geohydrological Aspects of Waste Management*, pages 223–232, Fort Collins, February 1986. Colorado State University.

[5] Ahlert, W. K., C. G. Uchrin. "Rapid and Secondary Sorption of Benzene and Toluene by Two Aquifer Solids". *Journal of Hazardous Materials*, 23:317–330, 1990.

[6] Ahlert W. K., J. Katz, and C. G. Uchrin. "On the Validity of Partition Coefficients". In R. Khanbilvardi and J.Fillos, editors, *Pollution, Risk Assessment, and Remediation in Groundwater*, pages 295–320. Scientific Publications Co., Washington, D.C., 1987.

[7] Akratanakul, S., L. Boersma, and G. O. Klock. "Sorption Processes as Influenced by Pore Water Velocity, 1. Theory". *Soil Science*, 135:267–274, 1983.

[8] Allen, M. B., III. "Numerical Modeling of Multiphase Flow in Porous Media". *Adv. Water Resources*, 8:163–186, 1985.

[9] Baehr, A. L. "Selective Transport of Hydrocarbons in the Unsaturated Zone Due to Aqueous and Vapor Phase Partitioning". *Water Resources Research*, 23(10):1926–1938, 1987.

[10] Baehr, A. L. and M. Y. Corapcioglu. "A Compositional Multiphase Model for Groundwater Contamination by Petroleum Products, 2. Numerical Solution". *Water Resources Research*, 23(1):201–213, 1987.

[11] Bear, J. *Dynamics of Fluids in Porous Media.* American Elsevier, New York, NY, 1972.

[12] Bosen, J. F. "A Formula for Approximation of the Saturation Vapor Pressure over Water". *Mon. Weather Review*, 88, 1960.

[13] Bras, R. L. *Hydrology, An Introduction to Hydrologic Science.* Addison-Wesley, New York, 1990.

[14] Campbell, G. S. "A Simple Method for Determining Unsaturated Conductivity from Moisture Retention Data". *Soil Science*, 117:311–314, 1974.

[15] Carnahan, B., H. A. Luther, J. O. Wilkes. *Applied Numerical Methods.* John Wiley and Sons, New York, NY, 1969.

[16] Carslaw, H. S. and J. C. Jaeger. *Conduction of Heat in Solids.* Clarendon Press, Oxford, U.K., 1988.

[17] Celia, M. A., J. S. Kindred, and I. Herrera. "Contaminant Transport and Biodegradation, 1. A Numerical Model for Reactive Transport in Porous Media". *Water Resources Research*, 25(6):1141–1148, 1989.

[18] Chow, V. T. *Handbook of Applied Hydrology.* McGraw-Hill, New York, 1964.

[19] Clapp, R. B., G. M. Hornberger. "Empirical Equations for Some Soil Hydraulic Properties". *Water Resources Research*, 14(4):601–604, 1978.

[20] Cleary, R. W. and M. J. Ungs. "Groundwater Pollution and Hydrology, Mathematical Models and Computer Programs". Report 78-WR-15, Water Resources Program, Princeton University, Princeton, NJ, 1978.

[21] Corapcioglu, M. Y. and A. Haridas. "Transport and Fate of Microorganisms in Porous Media: A Theoretical Investigation". *Journal of Hydrol.*, 72:149–169, 1984.

[22] Corapcioglu, M. Y. and A. Haridas. "Microbial Transport in Soils and Groundwater: A Numerical Model". *Adv. Water Resources*, 8:188–200, 1985.

[23] Corapcioglu, M. Y. and A. L. Baehr. "A Compositional Multiphase Model for Groundwater Contamination by Petroleum Products, 1. Theoretical Considerations". *Water Resources Research*, 23(1):191–200, 1987.

[24] Crank, J. *The Mathematics of Diffusion.* Oxford University Press, New York, 1956.

[25] Dass, P., G. R. Tamke, and C. M. Stoffel. "Leachate Production at Sanitary Landfill Sites". *ASCE Journal of Environmental Engineering*, 103(EE6):981–988, 1977.

[26] Demetracopoulos, A. C., G. P. Korfiatis, E. L. Bourodimos, and E. G. Nawy. "Unsaturated Flow Through Solid Waste Landfills: Model and Sensitivity Analysis". *Water Resources Bulletin*, 22(3):601–609, 1986.

[27] Demetracopoulos, A. C., L. Sehayek, H. Erdogan. "Modeling Leachate Production from Municipal Landfills". *ASCE Journal of Environmental Engineering*, 112(5):849–866, 1986.

[28] DiToro, D. M. and L. M. Horzempa. "Reversible and Resistant Components of PCB Adsorption-Desorption". *Environmental Science Technology*, 16:594, 1982.

[29] Enderby, J. A. "The Domain Model of Hysteresis, I. Independent Domains". *Trans. Faraday. Soc.*, 51:835–848, 1955.

[30] Everett, D. H. "A General Approach to Hysteresis, 3. A Formal Treatment of the Independent Domain Model of Hysteresis". *Trans. Faraday Soc.*, 50:1077–1096, 1954.

[31] Freeze, R. A. "Three-Dimensional, Transient, Saturated-Unsaturated Flow in a Groundwater Basin". *Water Resources Research*, 7:347–366, 1971.

[32] Freeze, R. A. and J. A. Cherry. *Groundwater*. Prentice Hall, New Jersey, 1979.

[33] Gardner, W. R. and M. S. Mayhugh. "Solutions and Tests on the Diffusion Equation for the Movement of Water in Soil". *Proc. Soil Sci. Soc. Amer.*, 22:197–201, 1958.

[34] Gray, D. M. *Handbook on the Principles of Hydrology.* Water Information Center, Port Washington, New York, 1973.

[35] Green, R. E. "Pesticide-Organic Matter Interactions". In W. D. Guenzi, editor, *Pesticides in Soil and Water.* Soil Science Society of America, Madison, WI, 1974.

[36] Hamaker, J. W. and J. M. Thompson. "Adsorption". In C. A. Goring and J. W. Hamaker, editors, *Organic Chemicals in the Soil Environment.* Marcel-Dekker, Inc., New York, NY, 1972.

[37] Hartley, G. S. "Evaporation of Pesticides". *Adv. Chem. Series*, 86:115–134, 1969.

[38] Hern, S. C. and S. M. Melancon. *Vadose Zone Modeling of Organic Pollutants.* Lewis Publishers, Inc., Chelsea, MI, 1986.

[39] Hillel, D. *Applications of Soil Physics.* Academic Press, New York, 1980.

[40] Hills, R. G., I. Porro, D. B. Hudson, and P. J. Wierenga. "Modeling One-Dimensional Infiltration into Very Dry Soils: I- Model Development and Evaluation". *Water Resources Research*, 25(6):1259–1269, 1989.

[41] Hills, R. G., I. Porro, D. B. Hudson, and P. J. Wierenga. "Modeling One-Dimensional Infiltration into Very Dry Soils: II- Estimation of the Soil Water Parameters and Model Predictions". *Water Resources Research*, 25(6):1271–1282, 1989.

[42] Huyakorn, P. S., B. G. Jones, and P. F. Andersen. "Finite Element Algorithms for Simulating Three-Dimensional Groundwater Flow and Solute Transport in Multilayer Systems". *Water Resources Research*, 22(3):361–374, 1986.

[43] Huyakorn, P. S., G. F. Pinder. *Computational Methods in Subsurface Flow.* Academic Press, San Diego, CA, 1983.

[44] Jaffe, P. R. "Modeling Sorbing Chemicals: Considering the Nonsingular Adsorption-Desorption Isotherm". *Journal of Environmental Science and Health*, A21(1):55–69, 1986.

[45] Javandel, I., C. Doughty and C-F. Tsang. "Groundwater Transport: Handbook of Mathematical Models". Water Resources Monograph Series 10, American Geophysical Union, Washington, DC, 1984.

[46] Jury, W. A. "Volatilization from Soil". In Hern and Melancon, editors, *Vadose Zone Modeling of Organic Pollutants*, pages 159–176. Lewis Publishers, Inc., Chelsea, MI, 1986.

[47] Jury, W. A., A. D. Russo, G. Streile, and H. El Abd. "Evaluation of Volatilization by Organic Chemicals Residing Below the Soil Surface". *Water Resources Research*, 26(1):13–20, 1990.

[48] Jury, W. A., W. F. Spencer, and W. J. Farmer. "Use of Models for Assessing Relative Volatility, Mobility, and Persistence of Pesticides and Other Trace Organics in Soil Systems". In J. Saxena, editor, *Hazard Assessment of Chemicals.* Academic Press, New York, NY, 1983.

[49] Karickhoff, S. W. "Semi-Empirical Estimation of Sorption of Hydrophobic Pollutants on Natural Sediments". *Chemisphere*, 10:833–846, 1981.

[50] Karickhoff, S. W. "Organic Pollutant Sorption in Aquatic Systems". *ASCE Journal of Hydraulic Engineering*, 110(6):707–735, 1984.

[51] Kindred, J. S. and M. A. Celia. "Contaminant Transport and Biodegradation, 2. Conceptual Model and Test Simulations". *Water Resources Research*, 25(6):1149–1159, 1989.

[52] Klute, A. "A Numerical Method for Solving the Flow of Water in Unsaturated Materials". *Soil Science*, 73:105–116, 1952.

[53] Korfiatis, G. P. *Modeling the Moisture Transport through Solid Waste Landfills.* PhD thesis, Rutgers University, 1984.

[54] Korfiatis, G. P., A. C. Demetracopoulos, E. L. Bourodimos, and E. G. Nawy. "Moisture Transport in a Solid Waste Column". *ASCE Journal of Environmental Engineering*, 110(4):780–796, 1984.

[55] Metcalfe, D. J. and G. F. Farquhar. "Modeling Gas Migration Through Unsaturated Soils from Waste Disposal Sites". *Water Air Soil Pollut.*, 32:247–259, 1987.

[56] Millington, R. J. and J. M. Quirk. "Permeability of Porous Solids". *Trans. Faraday Society*, 57:1200–1207, 1961.

[57] Monod, J. "The Growth of Bacterial Cultures". *Ann. Rev. Microb.*, 3:371–394, 1949.

[58] Mualem, Y. "A New Model for Predicting the Hydraulic Conductivity of Unsaturated Porous Media". *Water Resources Research*, 12:513–522, 1976.

[59] Mualem, Y. "Hydraulic Conductivity of Unsaturated Porous Media: Generalized Macroscopic Approach". *Water Resources Research*, 14(2):325–331, 1978.

[60] Mualem Y. A. "A Modified Dependent Domain Theory of Hysteresis". *Soil Science*, 137:283–291, 1984.

[61] Nielsen, D. R., M. Th. van Genuchten, and J. W. Biggar. "Water Flow and Solute Transport Processes in the Unsaturated Zone". *Water Resources Research*, 22(9):89S–108S, 1986.

[62] Nielson, K. K., V. C. Rogers, and G. W. Gee. "Diffusion of Radon through Soils". *Soil Scientific Society of America Journal*, 48:482–487, 1984.

[63] Oweis I. S. and R. P. Khera. *Geotechnology of Waste Management.* Butterworths, London, UK, 1990.

[64] Penman, H. L. "Gas and Vapour Movements in the Soil, 1- The Diffusion of Vapours through Porous Solids". *Journal of Agricultural Science*, 30:437–462, 1940.

[65] Penman, H. L. "Natural Evaporation from Open Water, Bare Soil, and Grass". *Proceedings of Royal Society London*, 193:120–145, 1948.

[66] Perrier, E. R. and A. C. Gibson. *Hydrologic Simulation on Solid Waste Disposal Sites.* EPA-SW-868, USEPA, Cincinatti, Ohio, 1980.

[67] Pickens, J. F. and R. W. Gillham. "Finite Element Analysis of Solute Transport under Hysteretic Unsaturated Flow Conditions". *Water Resources Research*, 16(6):1070–1078, 1980.

[68] Pickens, J. F. and W. C. Lennox. "Numerical Simulation of Waste Movement in Steady Groundwater Flow Systems". *Water Resources Research*, 12(12):171–180, 1976.

[69] Press, W. H., B. P. Flannery, S. A. Teukolsky and W. T. Vetterling. *Numerical Recipes, The Art of Scientific Computing, FORTRAN Version.* Cambridge University Press, Cambridge, UK, 1990.

[70] Ragab, R., J. Feyen, and D. Hillel. "Comparative Study of Numerical and Laboratory Methods for Determining the Hydraulic Conductivity Function of a Sand". *Soil Science*, 131(5):375–388, 1981.

[71] Rao, P. S. C. and J. M. Davidson. "Estimation of Pesticide Retention and Transformation Parameters". In M. R. Overcash and J. M. Davidson, editors, *Environmental Impact of Nonpoint Source Pollution.* Ann Arbor Science Publications, Ann Arbor, MI, 1980.

[72] Reeves, M. and R. M. Cranwell. "User's Manual for the Sandia Waste-Isolation Flow and Transport Model (SWIFT)". Technical Report CR-2324, U.S. Nuclear Regulatory Commision, Washington, D.C., 1981.

[73] Richards, L. A. "Capillary Conduction of Liquids through Porous Medium". *Physics*, 1:318–333, 1931.

[74] Richie, J. T. "Model for Predicting Evaporation from a Raw Crop with Incomplete Cover". *Water Resources Research*, 8(5):1204–1213, 1972.

[75] Rubin, J., R. Steinhardt. "Soil Water Relations During Rain Infiltration: I. Theory". In *Soil Science Society Proceedings*, pages 246–251, 1963.

[76] Selim, H. M., J. M. Davidson, and R. S. Mansell. "Evaluation of a Two-Site Adsorption-Desorption Model for Describing Solute Transport in Soils". In *Summer Computer Simulation Conference Proceedings*, Washington, D.C., July 1976. National Science Foundation.

[77] Soil Conservation Service. *National Engineering Handbook–Hydrology Section 4.* U.S. Department of Agriculture, Washington, D.C., March 1985.

[78] Sleep, B. E. and J. F. Sykes. "Modeling the Transport of Volatile Organics in Variably Saturated Media". *Water Resources Research*, 25(1):81–92, 1989.

[79] Spencer, W. F., W. J. Farmer, and M. M. Cliath. "Pesticide Volatilization". *Residue Rev.*, 49:1–47, 1973.

[80] Spencer, W. F., W. J. Farmer, and W. A. Jury. "Review: Behavior of Organic Chemicals at Soil, Air, Water Interfaces as Related to Predicting the Transport and Volatilization of Organic Pollutants". *Environ. Toxicol. Chem.*, 1:17–26, 1982.

[81] Sykes, J. F., S. B. Pahwa, R. B. Lantz, and D. S. Ward. "Numerical Simulation of Flow and Contaminant Migration at an Extensively Monitored Landfill". *Water Resources Research*, 18(6):1687–1704, 1982.

[82] Talimcioglu, N. M. *A Model for Evaluation of the Impact of Contaminated Soil on Groundwater.* PhD thesis, Stevens Institute of Technology, 1991.

[83] Taylor, S. W. and P. R. Jaffe. "Substrate and Biomass Transport in a Porous Medium". *Water Resources Research*, 26(9):2181–2194, 1990.

[84] Thornthwaite, C. W. "An Approach Toward a Rational Classification of Climate". *American Geographical Review*, 38:55–94, 1948.

[85] Thornthwaite, C. W. and J. R. Mather. "Instructions and Tables for Computing Potential Evapotranspiration and the Water Balance". In *Publications in Climatology*, volume 10/3, pages 185–311. Drexel Institute, New Jersey, 1957.

[86] Trescott, P. C. "Documentation of Finite Difference Model for Simulation of Three-dimensional Groundwater Flow". Technical report, U.S. Geological Survey, July 1976.

[87] Uchrin, C. G. "Sorption Kinetics and Equilibria of Organic Chemicals to Soils". In R. Khanbilvardi and J. Fillos, editors, *Groundwater Hydrology, Contamination, and Remediation*, pages 323–338. Scientific Publications Co., Washington, DC, 1986.

[88] Uchrin, C. G., T. E. Lewis. "Modelling Sorption and Degradation of Toxic and Hazardous Substances in Ground Water Systems". In Pawlowski et al., editor, *Chemistry for Protection of the Environment 1987*, pages 153–167. Elsevier, New York, 1988.

[89] Vaccari, D. A. "Modeling Hysteretic Adsorption-Desorption". In *International Conference on Physiochemical and Biological Detoxification of Hazardous Wastes*, Atlantic City, New Jersey, May 1988.

[90] Vaccari, D. A. and M. Kaouris. "A Model for Irreversible Adsorption Hysteresis". *Journal of Environmental Science and Health*, A28(8):797–822, 1988.

[91] Valentine R. L. and J. L. Schnoor. "Biotransformation". In Hern and Melancon, editors, *Vadose Zone Modeling of Organic Pollutants*, pages 191–222. Lewis Publishers, Inc., Chelsea, MI, 1986.

[92] van Genuchten, M. Th. "A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils". *Soil Scientific Society of America Journal*, 44:892–898, 1980.

[93] van Genuchten, M. Th. "A Comparison of Numerical Solutions of the One-Dimensional Unsaturated-Saturated Flow and Mass Transport Equations". *Adv. Water Resources*, 5:47–55, 1982.

[94] van Genuchten, M. Th. "An Hermitian Finite Element Solution of the Two-Dimensional Saturated-Unsaturated Flow Equation". *Adv. Water Resources*, 6:106–111, 1983.

[95] van Genuchten, M. Th. and R. W. Cleary. "Movement of Solutes in Soil". In G. H. Bolt, editor, *Developments in Soil Science*, pages 349–386. Elsevier Scientific Pub. Co., Amsterdam, Holland, 1979.

[96] Viessman, W. Jr., J. W. Knapp, G. L. Lewis, and T. E. Harbaugh. *Introduction to Hydrology.* Harper & Row Inc., 1977.

[97] Willis, R., W. W-G. Yeh. *Groundwater Systems Planning and Management.* Prentice Hall, New Jersey, 1987.

Appendix A

Microsoft Excel © Input Preprocessor

IMPACT v3.0

Worksheet for Data Input

IMPACT v3.0 Preprocessor is a Microsoft Excel Worksheet that can be used to create an input data file for the **IMPACT** model. This worksheet, like a template, is linked with various macros to help users in implementing data entry with Buttons and Dialog Boxes

The worksheet consists of three major regions:

1. Variable descriptions;
2. Buttons;
3. Data values.

Upon execution of the preprocessor, the initial cell (F9) is automatically selected in the data region. Unless otherwise specified, Buttons are used to record values of variables in the data area. To ensure data integrity, users must follow Buttons 1 through 43 in a sequence, and must ALWAYS use the EXIT button to save data or quit from the worksheet. Data entry by direct typing into the data region is also allowed in the worksheet, but has a potential danger of violating data integrity. Therefore, the following precautions must be taken for data entry by direct typing.

The worksheet is color-coded for random data entry, if desired. If the user does not wish to follow all the buttons in a sequence, he/she may change data in any random order by using the **BLUE** coded buttons, provided that all **YELLOW** coded buttons are executed again prior to the EXIT button. This is required because the YELLOW coded buttons hide or unhide certain rows in the worksheet according to the flow chart branching. The **RED** buttons insert or delete rows from the worksheet according to the values they take. Therefore, it is not recommended that users change data by direct typing into the data region for any of the RED coded buttons.

Buttons
Dialog Boxes
List of Macro Sheets
Databases

Buttons

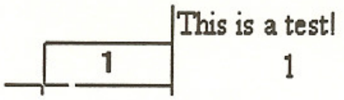
The template worksheet contains a total of 45 dynamic buttons to help users accomplish data entry in an automated fashion. Every button in the worksheet has a particular macro sheet attached to it. Each time the button is pressed, the corresponding macro sheet is called and executed. In turn, the built-in Dialog Boxes are displayed to prompt the user to select appropriate values for the variables. Once the selection is complete and the "OK" option is pressed, the values are recorded into the data region.

The first button in the worksheet is labeled as "HELP" which provides an introductory information about the preprocessor. The rest of the buttons in the worksheet are labeled with numbers from 1 to 43 followed by an "EXIT" button. All buttons are color-coded to aid users in random data entry. The following color codes are used for buttons to represent:

BLUE: These buttons have no effect on the worksheet structure, except recording values into the data region.
RED: These buttons insert or delete rows in the worksheet.
YELLOW: These buttons hide or unhide rows in the worksheet.

IMPORTANT NOTE: When a button is pressed, the cell adjacent to the button in the data region is selected. If, for any reason, some other cell is selected, the data file created for the model IMPACT will not work properly in model execution. If this happens, the user should quit the worksheet, and start over again.

A typical button looks like:

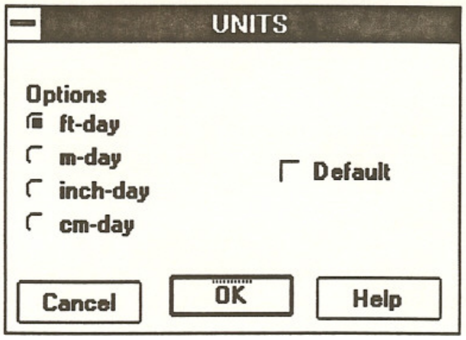


List of Macro Sheets

Button # 1
Button # 2
Button # 3
Button # 4
Button # 5
Button # 6
Button # 7
Button # 8
Button # 9
Button # 10
Button # 11
Button # 12
Button # 13
Button # 14
Button # 15
Button # 16
Button # 17
Button # 18
Button # 19
Button # 20
Button # 21
Button # 22
Button # 23
Button # 24
Button # 25
Button # 26
Button # 27
Button # 28
Button # 29
Button # 30
Button # 31
Button # 32
Button # 33
Button # 34
Button # 35
Button # 36
Button # 37
Button # 38
Button # 39
Button # 40
Button # 41
Button # 42
Button # 43
EXIT

Dialog Boxes

Almost every macro sheet in the preprocessor has at least one dialog box implemented in it. The dialog boxes are standard Microsoft Windows dialog boxes which are used in all Windows applications. All dialog boxes in this preprocessor contain an "OK" button, a "Cancel" button, and a "Help" button. Some of the dialog boxes have group options from which only one of the listed options can be selected. Some of the dialog boxes have check boxes, namely a "Default" option, when pressed a pre-set selection is made for the user. In addition, tex number, and integer edit lists as well as pull-down lists are used in combination with other options wherever appropriate. The selection made within a dialog box is only implemented into the worksheet when the "OK" button is pressed. If the "Cancel" button is pressed, however, the recent selections will be ignored. A typical dialog box looks like:



Options
● ft-day
○ m-day
○ inch-day
○ cm-day

☐ Default

List of Macro Sheets Used

The following is the list of macro sheets used in the template worksheet:

Button Number	Macro Sheet Assigned	Databas
1	UNITS.XLM	NO
2	MODELS.XLM	NO
3	SOILTYPE.XLM	NO
4	KT.XLM	NO
5	DT.XLM	NO
6	IMC.XLM	NO
7	PRECIP.XLM	NO
8	EVAPOT.XLM	NO
9	PRINT1.XLM	NO
10	PRINT2.XLM	NO
11	BBC.XLM	NO
12	TC.XLM	NO
13	TBC.XLM	NO
14	ICP.XLM	NO
15	DILUTE.XLM	NO
16	TD.XLM	NO
17	CRS.XLM	NO
18	SPAR.XLM	YES
19	DISCR1.XLM	NO
20	PFR.XLM	NO
21	CONV.XLM	NO
22	DISCR2.XLM	NO
23	RMOIS.XLM	NO
24	RAIN.XLM	NO
25	SCS1.XLM	YES
26	ET.XLM	NO
27	CHN.XLM	YES
28	TCONC.XLM	NO
29	CPAR.XLM	YES
30	SCPAR.XLM	NO
31	BIOD.XLM	YES
32	SCS2.XLM	YES
33	ETC.XLM	NO
34	SDATE.XLM	NO
35	TEMP.XLM	NO
36	WPT.XLM	NO
37	RZONE.XLM	NO
38	DISCR3.XLM	NO
39	VC.XLM	NO
40	HC.XLM	NO
41	ST.XLM	NO
42	AQP.XLM	NO
43	AQC.XLM	NO
EXIT	ZSAVE.XLM	NO
HELP	HELP.XLM	NO

Databases

This preprocessor is equipped with several easy-to-update soil and chemical databases. Particular databases are built into the corresponding macro sheets, and permanent values of variables are hard-coded. Not all of the macro sheets contain a database. For a list of macro sheets containing databases, see the List of Macro Sheets.

Updating Permanent Databases

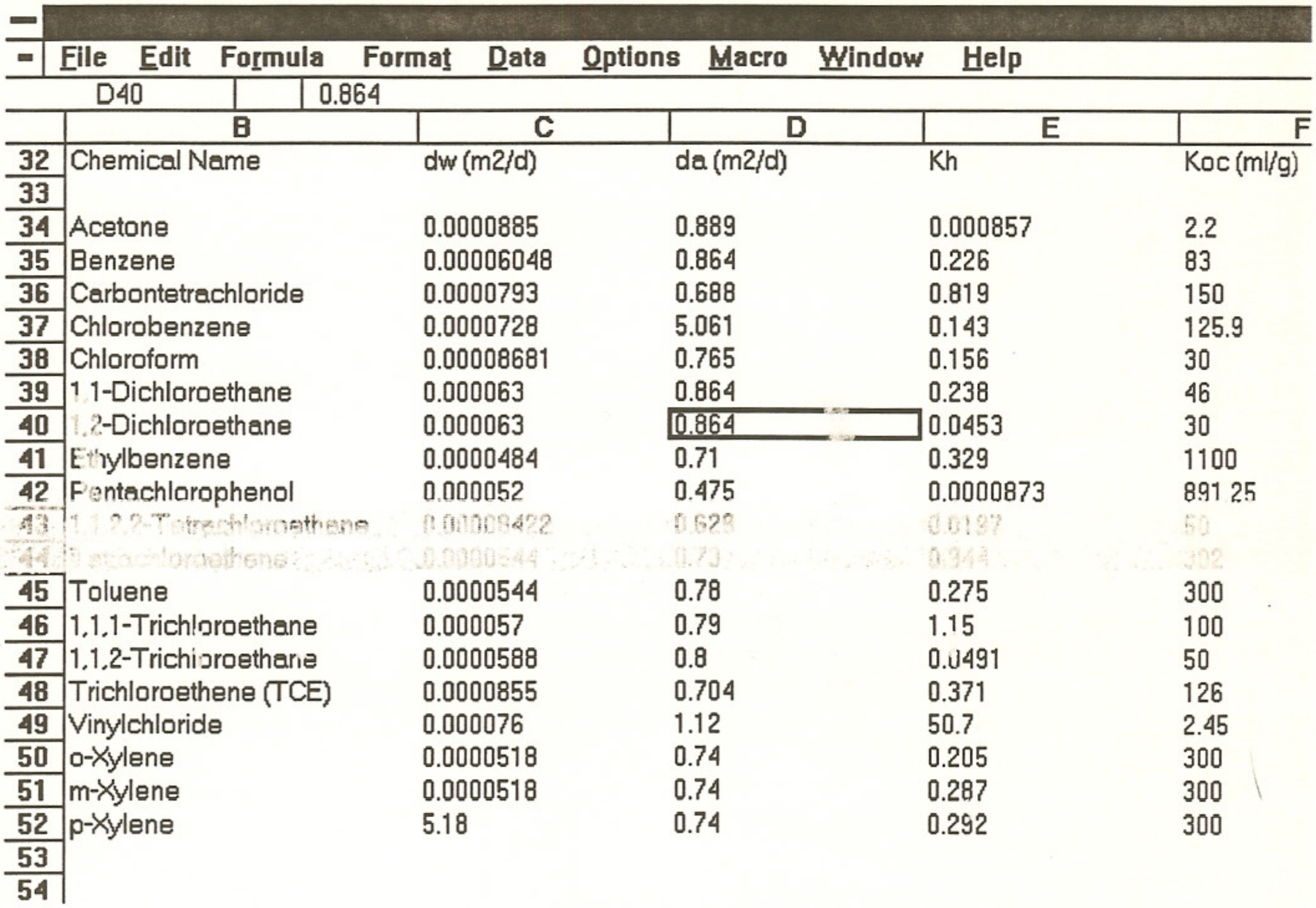
Updating Permanent Databases

Changing Permanent Values of Existing Variables

Several macro sheets used in this preprocessor contain permanent databases. The values of corresponding soil and chemical properties are hard-coded into the macro sheets. To change a permanent value of an existing database entry, you must first find the macro filename from the List of Macro Sheets used, then open the appropriate file in Microsoft Excel to make changes. Once the file is open, locate the light-gray shaded area within the file. The light-gray shaded area contains parameter values for the corresponding variables whose names are listed immediately above the shaded area. Next, locate the value to be changed within the shaded area and select the cell containing that value. Type in the new value, then press the "ENTER" key on the keyboard. Repeat the same procedure for other existing parameters to be changed. When done, select the first cell in the macro sheet (A1) and save the file by using File Save option in the main menu. You may now quit from Microsoft Excel.

Example

To illustrate this procedure, a typical macro sheet containing a database is shown below.

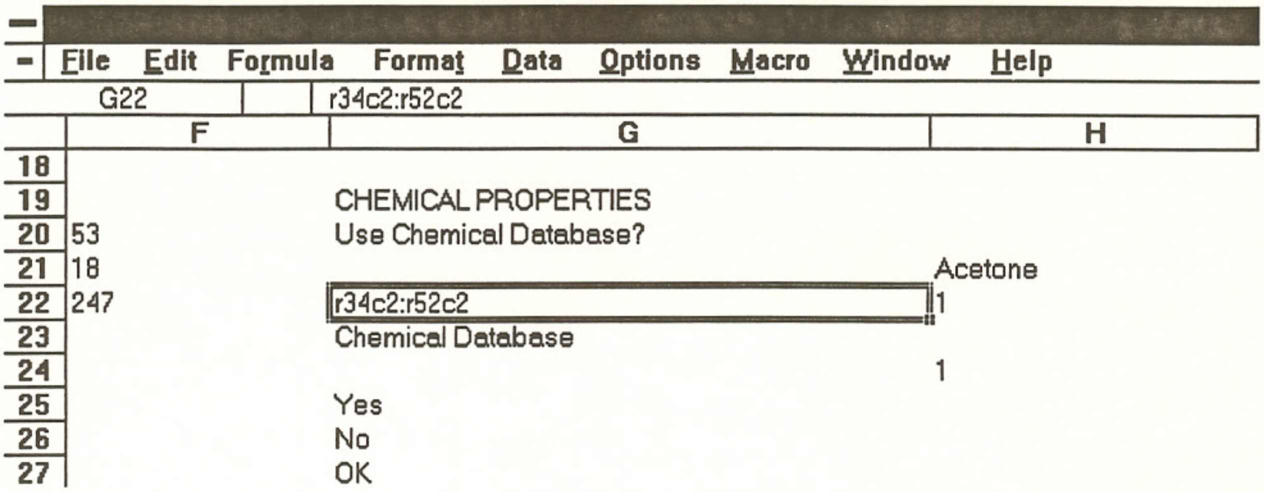


	B	C	D	E	F
32	Chemical Name	dw (m2/d)	da (m2/d)	Kh	Koc (ml/g)
33					
34	Acetone	0.0000885	0.889	0.000857	2.2
35	Benzene	0.00006048	0.864	0.226	83
36	Carbontetrachloride	0.0000793	0.688	0.819	150
37	Chlorobenzene	0.0000728	5.061	0.143	125.9
38	Chloroform	0.00008681	0.765	0.156	30
39	1,1-Dichloroethane	0.000063	0.864	0.238	46
40	1,2-Dichloroethane	0.000063	0.864	0.0453	30
41	Ethylbenzene	0.0000484	0.71	0.329	1100
42	Pentachlorophenol	0.000052	0.475	0.0000873	891.25
43	1,1,2,2-Tetrachloroethane	0.00008422	0.628	0.0137	50
44	Tetrachloroethene	0.0000544	0.73	0.944	302
45	Toluene	0.0000544	0.78	0.275	300
46	1,1,1-Trichloroethane	0.000057	0.79	1.15	100
47	1,1,2-Trichloroethane	0.0000588	0.8	0.0491	50
48	Trichloroethene (TCE)	0.0000855	0.704	0.371	126
49	Vinylchloride	0.000076	1.12	50.7	2.45
50	o-Xylene	0.0000518	0.74	0.205	300
51	m-Xylene	0.0000518	0.74	0.287	300
52	p-Xylene	5.18	0.74	0.292	300
53					
54					

The chemical properties are hard-coded into the macro file named CPAR.XLM. Line 40 of this macro sheet gives chemical properties of 1,2 Dichloroethane. Column B of the macro sheet within the shaded area contains the chemical names, Column C contains the diffusion coefficients in water in m2/d units, Column D contains the diffusion coefficients in air in m2/d units, Column E contains the dimensionless Henry's Constants, and Column F contains the normalized adsorption (distribution) coefficients of the chemical with respect to carbon content of the soil in ml/g units. As an example, if you would like to change the permanent value of the diffusion coefficient of 1,2 Dichloroethane in air, you must select cell D40, and type in the new value (say 0.9), then select the first cell in the macro sheet (A1). By using the File menu, you must save the macro sheet using the "Save" option. You may now quit from Microsoft Excel.

Inserting/Deleting Items

The shaded areas in the macro sheets, which are used to store permanent values of variables, are logically defined to <u>Dialog Boxes</u> by using the "R1C1" cell referencing system. As shown below, the example of CPAR.XLM contains the database logical definition in cell G22 as "r34c2:r52c2", indicating that the chemical names used as items in the pull-down list are written in Column 2 (B), starting from Row 34 to Row 52.



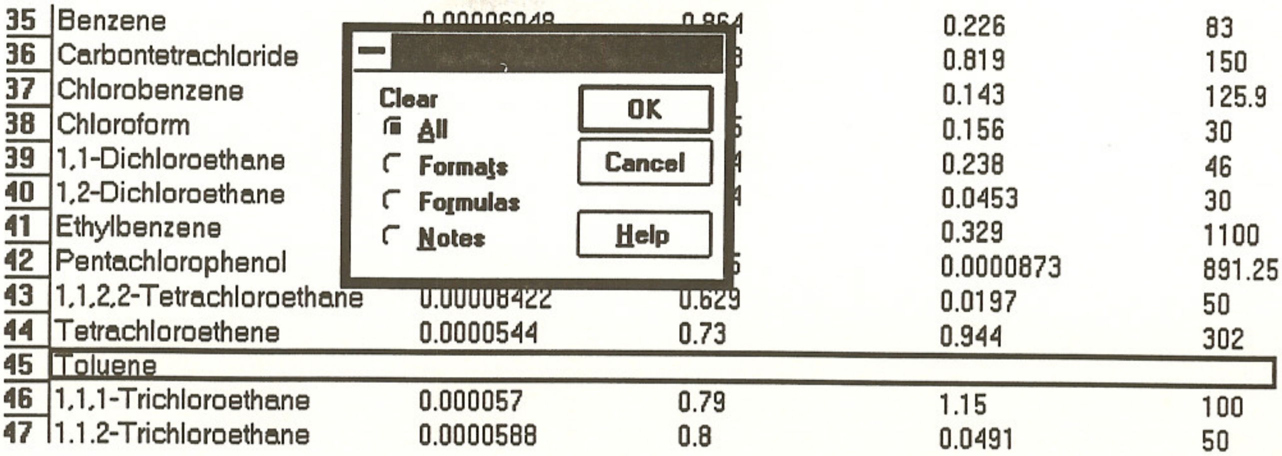
G22 r34c2:r52c2

	F	G	H
18			
19		CHEMICAL PROPERTIES	
20	53	Use Chemical Database?	
21	18		Acetone
22	247	r34c2:r52c2	1
23		Chemical Database	
24			1
25		Yes	
26		No	
27		OK	

If any of the chemicals is to be removed from the database permanently, the corresponding cells for that chemical must be selected in the shaded region, and the contents of these cells must be deleted by using Edit-Clear-All option. Then, the remaining data entries must be selected and moved up in the place of deleted entries by using Edit-Cut and Edit-Paste options. Lastly, the database logical definition must be changed to reflect the new parameter area. To illustrate this, consider the following example:

Example

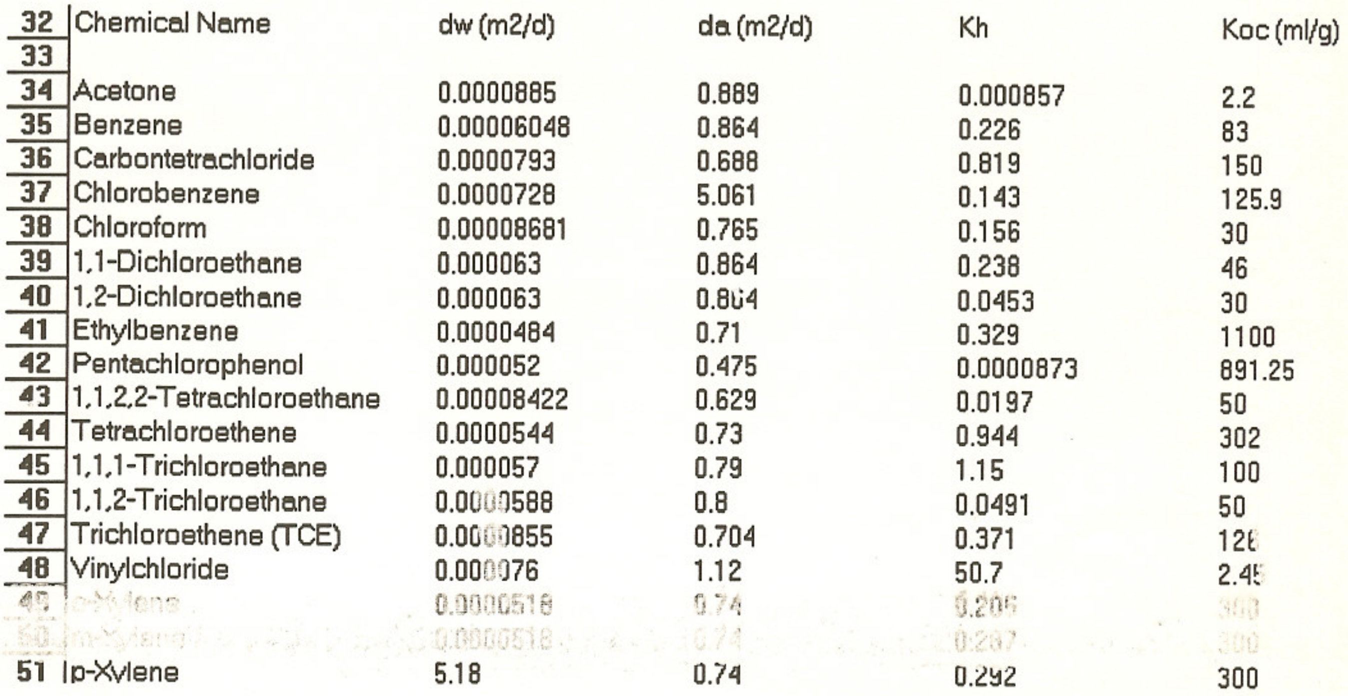
To delete the data entry in CPAR.XLM for Toluene, you must first locate the parameter values for Toluene in the shaded area of CPAR.XLM (Line 40, Columns B, C, D, E and F), then select the cells containing parameter values for Toluene. Next, you must "Clear" the cells by using the Edit menu as illustrated below.



Clear
● All
○ Formats
○ Formulas
○ Notes

35	Benzene	0.00006048	0.864	0.226	83
36	Carbontetrachloride			0.819	150
37	Chlorobenzene			0.143	125.9
38	Chloroform			0.156	30
39	1,1-Dichloroethane			0.238	46
40	1,2-Dichloroethane			0.0453	30
41	Ethylbenzene			0.329	1100
42	Pentachlorophenol			0.0000873	891.25
43	1,1,2,2-Tetrachloroethane	0.00008422	0.629	0.0197	50
44	Tetrachloroethene	0.0000544	0.73	0.944	302
45	Toluene				
46	1,1,1-Trichloroethane	0.000057	0.79	1.15	100
47	1,1,2-Trichloroethane	0.0000588	0.8	0.0491	50

Then, to move rest of the entries one line up, you must select lines 46 through 52, columns B, C, D, E and F and use the "Cut" option from the Edit menu. Next, you must select cell B45 and use the "Paste" option from the Edit menu. After this operation, the permanent data area will look like the following:



32	Chemical Name	dw (m2/d)	da (m2/d)	Kh	Koc (ml/g)
33					
34	Acetone	0.0000885	0.889	0.000857	2.2
35	Benzene	0.00006048	0.864	0.226	83
36	Carbontetrachloride	0.0000793	0.688	0.819	150
37	Chlorobenzene	0.0000728	5.061	0.143	125.9
38	Chloroform	0.00008681	0.765	0.156	30
39	1,1-Dichloroethane	0.000063	0.864	0.238	46
40	1,2-Dichloroethane	0.000063	0.864	0.0453	30
41	Ethylbenzene	0.0000484	0.71	0.329	1100
42	Pentachlorophenol	0.000052	0.475	0.0000873	891.25
43	1,1,2,2-Tetrachloroethane	0.00008422	0.629	0.0197	50
44	Tetrachloroethene	0.0000544	0.73	0.944	302
45	1,1,1-Trichloroethane	0.000057	0.79	1.15	100
46	1,1,2-Trichloroethane	0.0000588	0.8	0.0491	50
47	Trichloroethene (TCE)	0.0000855	0.704	0.371	126
48	Vinylchloride	0.000076	1.12	50.7	2.45
49	o-Xylene	0.0000518	0.74	0.205	300
50	m-Xylene	0.0000518	0.74	0.207	300
51	p-Xylene	5.18	0.74	0.292	300

Notice that the new data area is now from row 34 to row 51, not 52. Therefore, the database logical definition in cell G22 must be changed to reflect the new data area, and it should read "r34c2:r51c2". To complete database update, you must select the first cell (A1) and save the macro sheet by using the "Save" option from the File menu.

Inserting new items into the database file is accomplished by using a similar approach. The new item can be included at the end of the light-gray shaded area, provided that the cells for the new parameter values are shaded by using the "Patterns" option from the Format menu. Again, the database logical definition in "R1C1" format should be altered to reflect the new entry. If the entries in the pull-down list of the dialog box are to be sorted alphabetically, the user must select the entire data area first, then use the "Sort" option from the Data menu.

Button # 1: UNITS

This button is used to specify which units are implemented in model operation. IMPACT v3.0 is designed for daily time increments, therefore, the time units are always in days. However, the spatial units can be feet, meters, inches or centimeters. When Button 1 is implemented, a corresponding dialog box is called to prompt user to select appropriate units. The default for this button is pre-set to "Feet-Day" units. The following table shows the appropriate values written into the data region, depending on the option selected from the dialog box

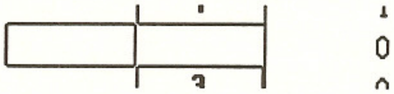
Feet-Day Units	1
Meter-Day Units	2
Inch-Day Units	3
Centimeter-Day Units	4

This is a test!

1   1

Button # 2: MODELS

This button is used to specify which submodel is used in model operation. IMPACT v3.0 is designed to be executed in two distinct modes: 1) Moisture Balance Model only; 2) Moisture Balance and Mass Transport. If the latter is selected, "0" will be written in the data region. However, if the first option is selected, certain lines in the worksheet which contain input related to mass transport will be hidden first and "1" will be written in the data region. This button does not have a default option.



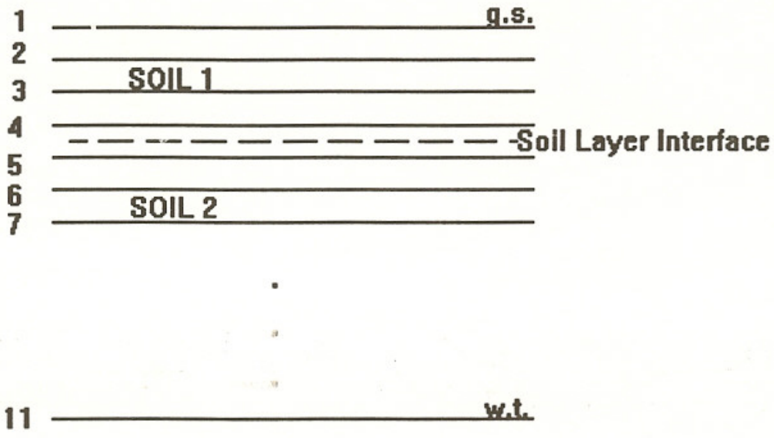
Buttons

Button # 3: SOIL TYPE

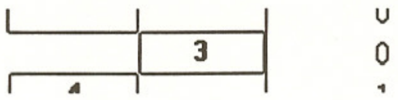
This button is used to specify whether the soil in the unsaturated zone is homogeneous or layer-heterogeneous. If the homogeneous soil option is selected, "0" will be written in the data region. This option is used as a default in the dialog box. However, if the layer-heterogeneous option is selected, first "1" will be written in the data region, and a secondary dialog box is called to prompt user to input how many layers of different soil exist in the unsaturated zone. The maximum soil layers allowable in IMPACT v3.0 is four; therefore, the dialog box does not accept a value greater than four. In addition, this dialog box restricts users to enter the number of soil layers less than two, since it would indicate the homogeneous option. Once the number of soil layers is given, an additional line containing the value will be added into the worksheet, and a third dialog box will be called. This dialog box prompts users to input node numbers immediately above the soil layer interfaces for each soil type. The node numbers are layer interfaces from the spatial discretization. It should be noted that the node numbers cannot be zeros and the soil layer interfaces are always selected on half-layer interfaces (between two full layer interfaces). The following example explains the numerical discretization for a two-layer system.

Example

Consider the following scenario: The unsaturated zone, which is 10 feet in depth, consists of two distinct soil layers. The first soil layer is located from the ground surface to a depth of 3.5 feet, and the rest of the region contains the second soil type. If the unsaturated zone is discretized by 1 foot intervals as shown in the figure given below, the first layer interface is the ground surface (z = 0 ft), the second layer interface is 1 foot deep from the ground surface (z = 1 ft), and similarly, the last layer interface is the groundwater water table (z = 10 ft). The node number immediately above the second soil type is therefore equal to 4 according to the discretization.



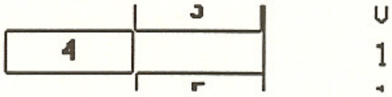
Once the node numbers are given, Button 3 will first insert an additional line containing these values into the worksheet and hides certain rows from the worksheet (Buttons 4, 5, 6 and 11). Furthermore, additional lines will also be inserted into the worksheet for soil parameter input (see Button 18).



Buttons

Button # 4: K-THETA RELATIONSHIP

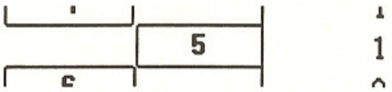
This button is used to specify which submodel is used in soil-moisture retention characteristics. There are four submodels built in IMPACT v3.0, namely, Campbell, Mualem, Ragab, and van Genuchten's. Only Campbell's relationship is implemented in this worksheet, however, the others are shown as options in the dialog box for future inclusion. The default option is therefore set to Campbell's relationship. When this option is selected, "1" is written in the data region. If any other option is selected, a warning message is displayed. If the soil type is layer-heterogeneous, this button is hidden since IMPACT v3.0 assumes the Campbell's relationship for heterogeneity.



Buttons

Button # 5: D-THETA RELATIONSHIP

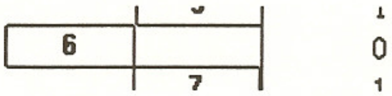
This button is used to specify which submodel is used in moisture content versus soil diffusivity relationship. There are two submodels implemented in IMPACT v3.0, namely, Clapp and Hornberger, and Gardner's. The latter is not implemented in this preprocessor, however, it is shown in the dialog box for future inclusion. The default option is set to Clapp and Hornberger's relationship. If this is selected, "1" is written in the data region. If any other option is selected, a warning message is displayed. Like Button 4, if the soil type is layer-heterogeneous, this button is hidden from the worksheet.



Buttons

Button # 6: INITIAL MOISTURE CONTENT

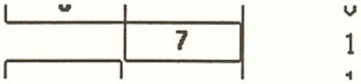
This button is used to specify whether or not the initial moisture content of the soil is constant with respect to depth. If the initial volumetric moisture content is constant with respect to depth, "0" will be written in the data region. This option is the default in the dialog box. However, if it is variable with respect to depth, "1" will be written. Like Buttons 4 and 5, if the soil type is layer-heterogeneous, this button is hidden from the worksheet, since IMPACT v3.0 assumes that the initial moisture content is constant for each layer.



Buttons

Button # 7: PRECIPITATION

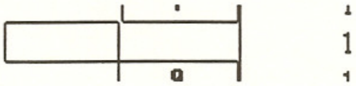
This button is used to specify if precipitation rate is constant or variable with respect to time or the actual daily precipitation values from rainfall database are to be used. The first option, precipitation is variable with respec to time, is not implemented in this preprocessor. Therefore, if selected, a warning message is displayed. Whe the precipitation is constant with respect to time (second option), "1" is written in the data region. The third option specifies that the actual rainfall data will be used from the database. If this option is selected, "2" is written in the data region. This is the default option.



Buttons

Button # 8: EVAPOTRANSPIRATION

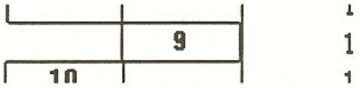
Like Button 7, this button is used to specify whether the evapotranspiration input is constant or variable with respect to time or to be calculated by using either Penman's or Thornthwaite's method. The first option, variabl with respect to time, is not implemented in this preprocessor. If chosen, the dialog box displays a warning message. If the evapotranspiration is constant with respect to time (second option), "2" will be written in the data region, and depending on the value of Button 7, certain lines will be hidden from the worksheet. If the evapotranspiration is computed by using the actual temperatures from the database (third option), "1" will be written in the data region, and again, certain lines will be hidden from the worksheet. This option is used as th default.



Buttons

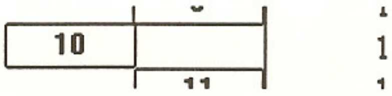
Button # 9: PRINT MOISTURE PROFILE

This button is used to specify whether or not the computed volumetric moisture content values are printed in the main output file. If the first option is selected, "0" will be written in the data region and the moisture profiles will be printed out by the model. If the second option is selected, however, "1" will be written in the data regio and the profiles will not be printed. The latter is the default for this button.



Button # 10: PRINT MOISTURE FLUXES

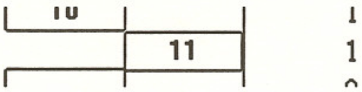
Like Button 9, this button is used to specify whether or not the moisture fluxes (velocities) are printed in the main output file. If the first option is selected, "0" will be written in the data region and the moisture fluxes will be printed out by the model. If the second is selected, however, "1" will be written in the data region, and the fluxes will not be printed. The latter is the default for this button.



Buttons

Button # 11: BOTTOM B.C. FOR FLOW

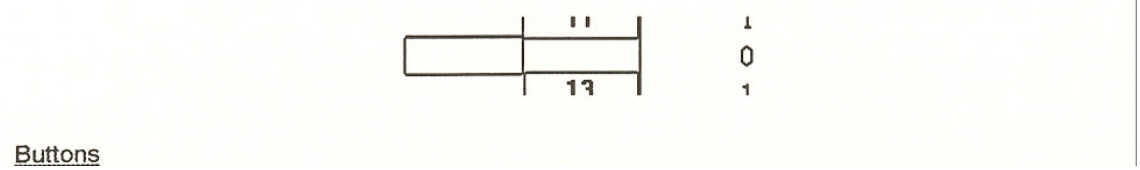
This button is used to specify the type of boundary condition to be used in the moisture balance model for the lower boundary of the solution domain (groundwater table). There are two distinct types of boundary conditions implemented into the model. The first option specifies a saturation condition (moisture content at the groundwater table is always at saturation value), which is a boundary condition of the first kind. The second option specifies a gravity flow condition (no-flux condition at the groundwater table), which is a boundary condition of the second kind. The latter is the default option. If the first option is chosen, "0" will be written in the data region. If the second option is chosen, "1" will be written in the data region. It should be noted that thi button will be hidden if the soil type (Button 3) is layer-heterogeneous, since the model assumes a gravity flow condition for heterogeneous soils.



Buttons

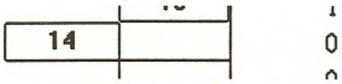
Button # 12: TYPE OF CONTAMINANT

This button is used to specify whether or not the biodegradation process is taken into account by the model. The first option runs IMPACT v3.0 in biodegradation mode, whereas the second option neglects biodegradation in th mass transport mechanisms. If the first option is selected, "0" will be written in the data region, however, if the second option is selected, "1" will be written and Buttons 16 and 32 will be hidden from the worksheet. The default is set to be the "no biodegradation" case.



Button # 14: INITIAL CONCENTRATION PROFILE

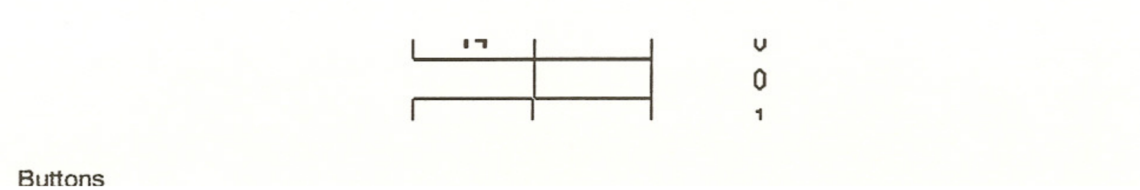
This button is used to specify whether or not the initial total soil concentration profile with respect to depth of the unsaturated zone is constant. If the first option is selected, "0" will be written in the data region. If the second option (variable concentration distribution) is selected, "1" will be written in the data region. This is the default option.



Buttons

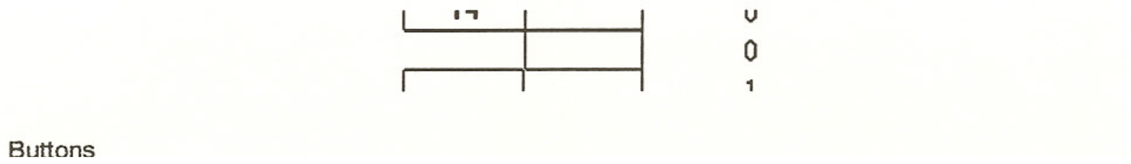
Button # 15: DILUTE MODEL

This button is used to specify whether or not the DILUTE (saturated zone transport) model is used in model operation. If the DILUTE model is executed (first option), "0" will be written in the data region. This is the default option in the preprocessor. If the dilute model is skipped in model operation (second option), "1" will
written in the data region and Buttons 38 through 43 will be hidden from the worksheet.



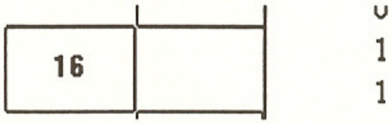
Button # 15: DILUTE MODEL

This button is used to specify whether or not the DILUTE (saturated zone transport) model is used in model operation. If the DILUTE model is executed (first option), "0" will be written in the data region. This is the default option in the preprocessor. If the dilute model is skipped in model operation (second option), "1" will b written in the data region and Buttons 38 through 43 will be hidden from the worksheet.



Button # 16: TYPE OF DEGRADATION

This button is used to specify the type of degradation mechanism to be used in model operation. IMPACT v3.0 is designed to handle biodegradation in two modes: 1) Monod Kinetics; 2) Dynamic Population Equilibrium Conditions. Button 16 is only visible if the type of contaminant is set to "Biodegradable" by Button 12. The first option, Monod Kinetics, is not implemented in this preprocessor; therefore, if selected, a warning message is displayed. However, if the second option (equilibrium conditions) is selected, "1" will be written in the data region and a secondary dialog box is displayed to prompt user to choose whether the degradation mechanism is zero or first order. The first option in this dialog box indicates a zero order mechanism, and if selected, "0" will be written in the data region. The second option which is the default indicates a first order mechanism and "1" will be written in the data region.

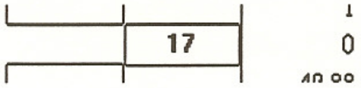


Buttons

Button # 17: CONCENTRATION REDUCTION

IMPACT v3.0 model is equipped with an iteration scheme to compute soil clean-up levels within the contaminant source located in unsaturated zone based on the maximum concentration observed either at the groundwater table or at any receptor location (compliance point) within the underlying aquifer. If the DILUTE model is executed in model operation (see Button 15), the optimization scheme will be performed for any receptor location(s) within the aquifer. However, if the DILUTE model is not executed, the optimization will be based on the maximum concentration observed at the groundwater table. The reduction scheme is implemented in IMPACT v3.0 as either reducing the initial concentration values in the source, keeping the thickness of the contaminated layer constant, or reducing the thickness, keeping the concentration values constant. The first represents the situation attained by any of the soil remediation techniques, the second represents the situation of soil excavation and replacement by clean soil.

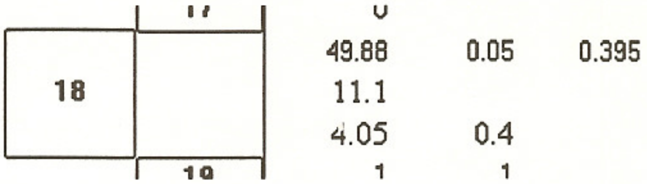
This button is used to specify whether or not the concentration reduction scheme is implemented. If the concentration reduction scheme is not implemented (first option), "0" will be written in the data region. If the second option is selected, however, "1" will be written in the data region and a secondary dialog box will be displayed to prompt user to select the type of reduction scheme. The first option which is the default specifies the initial concentration reduction scheme, and if selected, "0" will be written in the data region. The second option represents the contaminated layer thickness reduction, and if selected, "1" will be written in the data region. Then, a third dialog box will be displayed to prompt user to enter the allowable groundwater concentration in parts per billion. When this value is entered, it will be recorded in the data region.



Button # 18: SOIL PARAMETERS

This button is used to enter certain soil-specific parameters used in IMPACT v3.0. The first row in the worksheet corresponding to Button 18 gives values of saturated hydraulic conductivity, field capacity, saturated volumetric moisture content, and air-dry volumetric moisture content, respectively. The second row gives the empirical power, **m** , used in Clapp and Hornberger's hydraulic conductivity versus moisture content relationship (see technical documentation of IMPACT), and similarly, the third row gives the empirical power, **b** , used in Campbell's suction pressure (head) versus moisture content relationship (retention properties) and the saturated suction head values, respectively. It should be noted that all moisture content values and the empirical coefficients are dimensionless, the hydraulic conductivity is in velocity units (L/T) and the saturated suction head is in length units (L).

When Button 18 is executed, a dialog box is displayed to prompt the user to enter soil specific parameters for the first soil layer and for other soil layers for layer-heterogeneous soils. There is a database of soil types built-in to the dialog box, which contains values of the aforementioned variables for four types of soils, namely sand, sandy loam, silty clay loam, and silty clay. If the database option is selected (first option in the dialog box), the user may select the name of the soil type from the pull-down menu to automatically enter the built-in values for all variables. The dimensioned variables are automatically converted to appropriate dimensions according to the option used in Button 1. If the database option is not used, the user must enter values for each of the variables in the second dialog box, supplying values in appropriate dimensions.

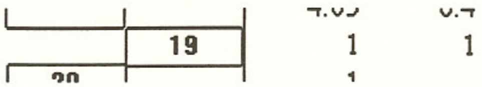


49.88	0.05	0.395
11.1		
4.05	0.4	
1	1	

Buttons

Button # 19: DISCRETIZATION PARAMETERS 1

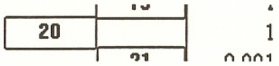
This button is used to enter the main spatial and temporal increments used in the geometric discretization of th problem. The first value refers to spatial increment in the discretized domain and is given in the appropriate units set by Button 1. The second value refers to the time increment used in the time-marching scheme, and is always given in days. It should be noted that if the climatic databases are used for actual rainfall and temperature values, there is a restriction in the value of the time increment that it cannot be more than 5 days o less than 1 day, and fractions of a day are not allowed. If the databases are not utilized, however, there is no restriction on the time increment.



Buttons

Button # 20: PRINTOUT FREQUENCY

This button is used to enter printout frequency for output purposes. The printout frequency is an integer multiple of the time increment used in the time-marching scheme. The results are printed in the main output file with respect to this frequency. In addition, if the DILUTE model is used (see Button 15), this value is used to determine how fine or course the input concentration profile at the groundwater table is taken into account, thus, affecting the accuracy of the saturated zone results. The printout frequency cannot be equal to or smaller than zero, therefore, it is restricted in the dialog box.



Buttons

Appendix B

Chemical Properties Used in Databases

CHEMICAL PROPERTIES OF SELECTED COMPOUNDS

CHEMICAL	CASRN	WATER SOLUBILITY (mg/L)	Koc (mL/g)	Henry's Constant (atm m3/mol)	Dimension-less Henry's Constant	Half lives in Soil, Days	First order constant 1/days	Half lives in Groundwater, Days	First order constant 1/day	Water Diffusion Coefficients 10^5 m^2/day	Air Diffusion Coefficients m^2/day	Water Diffusion Coefficients 10^5 m^2/day	Air Diffusion Coefficients m^2/day
	h	a		a	m	b		b		l	l		
					(T=20 C)								
Acetone	67-64-1	1000000h	2.20c	2.06E-05	8.57E-04	7	0.099021	14	0.049511	8.85k		9.442711734	0.889042578
Acrylonitrile	107-13-1	79000	0.85c	8.83E-05	3.67E-03	23	0.030137	46	0.015068			9.414412513	#VALUE!
Benzene	71-43-2	1780	100d	5.43E-03	2.26E-01	16	0.043322	16	0.043322	6.048	0.864	8.251289501	0.690200363
Bromodichloromethane	75-27-4	4500h	61.66h	2.12E-04	8.82E-03		#DIV/0!		#DIV/0!			#DIV/0!	#DIV/0!
Bromoform	75-25-2	3033	218.77h	6.12E-04	2.55E-02	180	0.003851	365	0.001899			#DIV/0!	#DIV/0!
Bromomethane	74-83-9	18040	7	5.26E-03	2.19E-01	28	0.024755		#DIV/0!			#DIV/0!	#DIV/0!
2-Butanone (MEK)	78-93-3	268000	4.5c	2.74E-05	1.14E-03	7	0.099021		#DIV/0!			#DIV/0!	#DIV/0!
Carbon tetrachloride	56-23-5	1160	150f	1.97E-02	8.19E-01	360	0.001925	360	0.001925	80.63k		7.929760072	0.687581675
Chlorobenzene	108-90-7	500	125.9h	3.45E-03	1.43E-01	150	0.004621	300	0.00231	7.28k		7.399528137	5.061393866
Chloroform	67-66-3	7900	30e	3.75E-03	1.56E-01	180	0.003851	1800	0.000385			8.681252767	0.76506365
Chloromethane	74-87-3	5350	6.00g	9.38E-03	3.90E-01	28	0.024755		#DIV/0!			#DIV/0!	#DIV/0!
Dibromochloromethane	128-48-1	4000h	83.2h	9.90E-04	4.12E-02	180	0.003851	180	0.003851			#DIV/0!	#DIV/0!
1,2-Dichlorobenzene	95-50-1	145	400e	1.88E-03	7.82E-02	180	0.003851	360	0.001925			#DIV/0!	#DIV/0!
1,3-Dichlorobenzene	541-73-1	123	400e	3.55E-03	1.48E-01	180	0.003851	360	0.001925			#DIV/0!	#DIV/0!
1,4-Dichlorobenzene	106-46-7	80	650e	1.64E-03	6.82E-02	180	0.003851	360	0.001925			#DIV/0!	#DIV/0!
1,1-Dichloroethane	75-34-3	5100	46g	5.72E-03	2.38E-01	154	0.004501	154	0.004501	6.3	0.864	8.748178764	0.768437244
1,2-Dichloroethane	107-06-2	8700	30e	1.09E-03	4.53E-02	180	0.003851	360	0.001925	6.3	0.864	9.014722224	0.768437244
1,1-Dichloroethene	75-35-4	400	200e	1.54E-03	6.41E-02	180	0.003851	132	0.005251			#DIV/0!	#DIV/0!
1,2-Dichloroethene (trans)	156-60-5	6300	59c	6.60E-03	2.75E-01	180	0.003851		#DIV/0!			#DIV/0!	0.786349301
1,2-Dichloroethene (cis)	156-59-2	3500	49c	7.51E-03	3.12E-01	180	0.003851		#DIV/0!			#DIV/0!	0.786349301
1,3-Dichloropropane	542-75-6	2800		1.80E-01	7.49E+00	11.3	0.06134	11.3	0.06134			#DIV/0!	#DIV/0!
Ethylbenzene	100-41-4	167	1100c	7.90E-03	3.29E-01	10	0.069315	228	0.00304	4.84	0.71	6.549121582	0.580442638
Hexachloroethane	67-72-1	8	2188h	2.50E-03	1.04E-01	180	0.003851	365	0.001899			#DIV/0!	#DIV/0!
Lindane	58-89-9	7.5	1072h	3.25E-06	1.35E-04		#DIV/0!		#DIV/0!			#DIV/0!	#DIV/0!
4-Methyl-2-pentanone (MIBK	108-10-1	17000h	22g	5.14E-05	2.14E-03	7	0.099021	14	0.049511			#DIV/0!	#DIV/0!
Methylene chloride	75-09-2	19400	25f	2.57E-03	1.07E-01	28	0.024755		#DIV/0!	7.43	1.04	#DIV/0!	#DIV/0!
Pentachlorophenol	87-86-5	14l	891.25h	2.10E-06	8.73E-05	178	0.003894	1533	0.000452	5.2l	0.475l	5.175478421	0.474601813
1,1,1,2-Tetrachloroethane	630-20-6	1100	100e	2.79E-03	1.16E-01	66	0.010502	66	0.010502			#DIV/0!	#DIV/0!
1,1,2,2-Tetrachloroethane	79-34-5	3000	50e	4.74E-04	1.97E-02	45	0.015403	45	0.015403			8.422023934	0.628746971
Tetrachloroethene	127-18-4	160	302d	2.27E-02	9.44E-01	360	0.001925	720	0.000963	5.44	0.73	7.69176104	0.638790269
Toluene	108-88-3	522	200d	6.61E-03	2.75E-01	22	0.031507	28	0.024755	5.44	0.78	7.281175162	0.628414335
1,1,1-Trichloroethane	71-55-6	720	100d	2.76E-02	1.15E+00	273	0.002539	546	0.00127	5.7	0.79	#DIV/0!	0.686979918
1,1,2-Trichloroethane	79-00-5	4420	50e	1.18E-03	4.91E-02	365	0.001899	730	0.00095	5.88	0.8	#DIV/0!	0.686979918
Trichloroethene (TCE)	79-01-6	1100	100d	8.92E-03	3.71E-01	360	0.001925	1620	0.000428	8.55k	0.7035l	8.31195965	0.699949872
Vinyl chloride	75-01-4	1100h	2.45h	1.22E+00	5.07E+01	180	0.003851	2850	0.000243	7.6	1.12	10.79218935	0.926603988
o-Xylene	95-47-6	186	300.0f	4.93E-03	2.05E-01	28	0.024755	360	0.001925	5.18	0.74	6.604782757	0.580501085
m-Xylene	108-38-3	162	300.0f	6.91E-03	2.87E-01	28	0.024755	56	0.012378	5.18	0.74	6.527195183	0.535633879
p-Xylene	106-42-3	179	300.0f	7.01E-03	2.92E-01	28	0.024755	56	0.012378	5.18	0.74	6.494659415	0.53557995

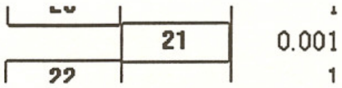
c EPA, 1986
d Korfiatis and Talimcioglu, 1991
e Calculated from water solubility and equation in Roy and Griffen, 1985
f Roy and Griffen, 1985
g Jury et. al. 1990
h Knox, Sabatani, and Canter, 1993
i Mohiuddin, 1993
j Brandon et. al., 1992
k Thibodeaux, 1979
l Reid and Sherwood, 1977
m Calculated

CALCULATION OF DIFFUSION COEFFICIENTS

	MW	Vc	Tc	Pc	Zc	Va	$\sum \vartheta_a$	Dw	Da
	g/mole	cm^3/mole	K	bar		cm^3/mole		m^2/day	m^2/day
Acetone	58.08	209	508.1	47	0.232	76.976501	66.86	9.44E-05	0.889043
Acrylonitrile	53.064	210	536	45.6	0.21	77.362533	C3H3N	9.41E-05	#VALUE!
Benzene	78.114	259	562.2	48.9	0.271	96.379132	110.88	8.25E-05	0.6902
Bromodichloromethane						0		#DIV/0!	#DIV/0!
Bromoform						0		#DIV/0!	#DIV/0!
Bromomethane						0		#DIV/0!	#DIV/0!
2-Butanone (MEK)						0		#DIV/0!	#DIV/0!
Carbon tetrachloride	153.823	275.9	556.4	45.6	0.272	102.97994	94.5	7.93E-05	0.687582
Chlorobenzene	112.559	308	632.4	45.2	0.265	115.57024		7.4E-05	5.061394
Chloroform	119.378	238.9	536.4	53.7	0.293	88.555468	76.98	8.68E-05	0.765064
Chloromethane						0		#DIV/0!	#DIV/0!
Dibromochloromethane						0		#DIV/0!	#DIV/0!
1,2-Dichlorobenzene						0		#DIV/0!	#DIV/0!
1,3-Dichlorobenzene						0		#DIV/0!	#DIV/0!
1,4-Dichlorobenzene						0		#DIV/0!	#DIV/0!
1,1-Dichloroethane	98.96	236	523	50.7	0.275	87.429227	79.92	8.75E-05	0.768437
1,2-Dichloroethane	98.96	225	566	53.7	0.259	83.163381	79.92	9.01E-05	0.768437
1,1-Dichloroethene						0		#DIV/0!	#DIV/0!
1,2-Dichloroethene (trans)	96.944		513	48.1		0	75.96	#DIV/0!	0.786349
1,2-Dichloroethene (cis)	96.944		537	56		0	75.96	#DIV/0!	0.786349
1,3-Dichloropropane						0		#DIV/0!	#DIV/0!
Ethylbenzene	106.168	374	617.2	36	0.262	141.64926	151.8	6.55E-05	0.580443
Hexachloroethane						0		#DIV/0!	#DIV/0!
Lindane						0		#DIV/0!	#DIV/0!
4-Methyl-2-pentanone (MIBK)						0		#DIV/0!	#DIV/0!
Methylene chloride						0		#DIV/0!	#DIV/0!
Pentachlorophenol	266.3	543.82	814.4	32.92		209.70167	203.96	5.18E-05	0.474602
1,1,1,2-Tetrachloroethane						0		#DIV/0!	#DIV/0!
1,1,2,2-Tetrachloroethane	167.85	250.7	661.2	58.4	0.266	93.144797	114.96	8.42E-05	0.628747
[illegible]	165.83	289.6	620.2	47.6	0.25	[illegible]	[illegible]	[illegible]	[illegible]
Toluene	92.141	[illegible]	591.8	41	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
1,1,1-Trichloroethane	133.405		545	43		0	97.44	#DIV/0!	0.68698
1,1,2-Trichloroethane	133.405		606	51.4		0	97.44	#DIV/0!	0.68698
Trichloroethene (TCE)	131.389	256	572	50.5	0.265	95.209513	93.48	8.31E-05	0.69995
Vinyl chloride	62.499	169	425	51.5	0.265	61.612684	58.44	0.000108	0.926604
o-Xylene	106.068	369	630.3	37.3	0.262	139.66529	151.8	6.6E-05	0.580501
m-Xylene	106.068	376	617.1	35.4	0.259	142.4432	181.8	6.53E-05	0.535634
p-Xylene	106.168	379	616.2	35.1	0.26	143.6345	181.8	6.49E-05	0.53558

Button # 21: CONVERGENCE CRITERION

This button is used to enter the convergence criterion which is utilized implicitly by the model for the accuracy of the results. It is set to 0.001 by default . This optimum value was found to yield accurate results by sensitivity analysis. However, the user has the option to change the value. It should be noted that lower the value, higher the accuracy will be, but the model will take a much longer time to execute.



Buttons

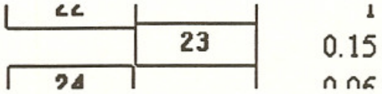
Button # 22: DISCRETIZATION PARAMETERS 2

This button is used to enter the number of nodes (layer interfaces) in the spatial discretization scheme and the number of time increments in the time-marching scheme (to set total simulation time), respectively. The number of layer interfaces or nodes are always one plus the total number of layers with a thickness set by the spatial increment (see Button 19). For instance, if the total depth of unsaturated zone is 10 feet, and this zone is discretized by 2 feet intervals, the number of nodes will be 6 since the first node (layer interface) is the ground surface at 0 foot. It should be noted that the number of layer interfaces are restricted to be less or equal to 400 by the model, similarly, the number of time increments are restricted to be less or equal to 2,234. If the values are not given in these ranges, the dialog box will not accept them.

Buttons

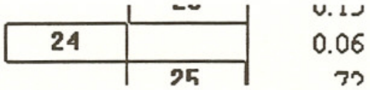
Button # 23: MOISTURE CONTENT

This button is used to enter initial volumetric moisture contents of the soil. If the initial moisture content i constant with respect to depth (see Button 6), only the moisture content for the first node will be given. However, if the initial moisture content is variable with respect to depth, the values must be supplied for a nodes.



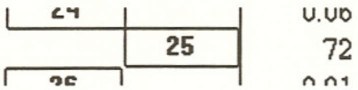
Button # 24: PRECIPITATION

This button is used to enter the constant value of the precipitation rate (in length per day units) if the precipitation is assumed to be constant with respect to time (see Button 7). If the climatic database is utilized this button is hidden from the worksheet.



Button # 25: SCS SOIL CURVE NUMBER

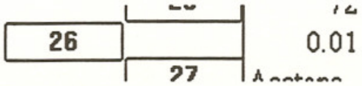
This button is used to enter the soil curve number (CN) of the Soil Conservation Service Method for computing surface runoff values. For more information about SCS method, see the technical documentation of IMPACT v3.0. The dialog box corresponding to Button 25 has a soil database for default CN values. There are four types of soils implemented in the database, namely, sand, sandy loam, silty clay loam, and silty clay. The user has the option to choose values from the database or enter the CN value for the corresponding soil (first soil layer in case of layer-heterogeneous formation). This button is hidden from the worksheet if the precipitation is constant with respect to time (see Button 7).



Buttons

Button # 26: EVAPOTRANSPIRATION

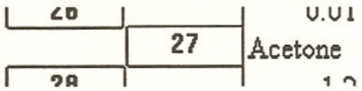
Like Button 24, this button is used to enter the constant value of evapotranspiration (in length per day units) if i
is constant with respect to time (see Button 8). If the climatic database is utilized, this button is hidden from th
worksheet.



Buttons

Button # 27: CONSTITUENT NAME

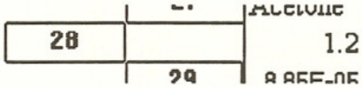
This button is used to enter the name of the compound existing in the contaminated layer. This is a text information used for identification purposes in the main output file. When this button is executed, the user has the option to enter the name of the compound directly or to select the name from the database of compounds which are built-into the dialog box. There are 19 compounds currently available in the database. When the database option is chosen, the user may select the name from the pull-down list to enter it into the worksheet. This button is hidden from the worksheet if the mass transport model is not implemented in model operation (se Button 2).



Buttons

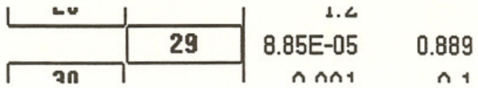
Button # 28: INITIAL TOTAL CONCENTRATION

This button is used to enter initial total soil concentration in mg/kg. If the initial concentration is constant with respect to depth (see Button 14), only one concentration value will be required for the model. The constant concentration value will be entered for the first layer interface (node) if no-mass-flux condition is used as a top boundary condition (see Button 13), otherwise it will be entered for the second node. If the concentration distribution is variable with respect to depth, values will be required for all nodes.



Button # 29: CHEMICAL PROPERTIES

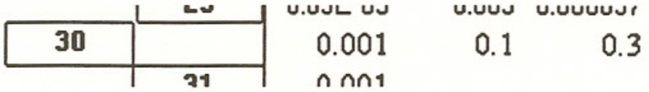
This button is used to enter chemical specific properties of the organic constituent used in the simulation. The dialog box associated with this button has the option to use built-in chemical database values for the selected compound. If the database option is selected, the user selects the name of the compound from the pull-down lis and presses the "OK" key. Subsequently, the following properties of the chemical are automatically written int the data region: diffusion coefficient of the chemical in water (in m2/d units), the diffusion coefficient of the chemical in air (in m2/d units), the dimensionless Henry's constant, and the normalized distribution (partitioning coefficient of the chemical with respect to carbon content of the soil (in ml/g units). If the database option is no utilized, a secondary dialog box prompts user to enter the aforementioned parameters in appropriate units.



29 8.85E-05 0.889

Button # 30: CHEMICAL PARAMETERS

This button is used to enter certain chemical specific parameters of the soil(s) utilized in model operation. The following parameters are prompted by the dialog box associated with this button: a first order decay coefficient representing irreversible adsorption in soils (in ml/g/d units), organic carbon content of the soil (in percentage), dispersivity of the soil (in appropriate length units), and soil bulk density (in g/cc). If the soil is layer-heterogeneous (see Button 3), this button will insert additional lines into the worksheet and the values of the parameters for each soil type must be entered respectively.

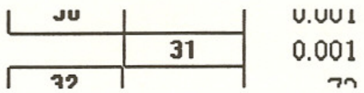


0.001 0.1 0.3

Buttons

Button # 31: BIODEGRADATION COEFFICIENT

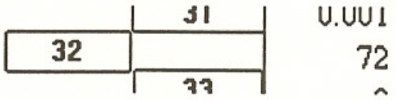
This button is used to enter equilibrium biodegradation coefficients of the chemical used in simulations. If the chemical is considered non-biodegradable (see Button 12), this button is hidden from the worksheet. If zero-order degradation mechanism is selected via Button 16, a dialog box is displayed to prompt user to enter the value of the biodegradation coefficient in mg/liter/day units. However, if the first order degradation mechanism is selected, the user is given an option to use the chemical database for degradation coefficients. If the database option is not utilized, a dialog box is displayed to manually enter the value in 1/day units.



Buttons

Button # 32: SCS CURVE NUMBER

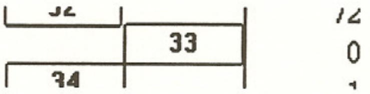
This button is used to enter the soil curve number (CN) of the Soil Conservation Service Method for computing surface runoff values. For more information about SCS method, see the technical documentation of IMPACT v3.0. The dialog box corresponding to Button 32 has a soil database for default CN values. There are four types of soils implemented in the database, namely, sand, sandy loam, silty clay loam, and silty clay. The user has the option to choose values from the database or enter the CN value for the corresponding soil (first soil layer in case of layer-heterogeneous formation). This button is hidden from the worksheet if the precipitation is computed using database (see Button 7).



Buttons

Button # 33: E.T. COMPUTATION

This button is used to specify which submodel is used to compute evapotranspiration values. If evapotranspiration is considered to be a constant for all time steps (see Button 8), this button is hidden from the worksheet. There are two options displayed in the dialog box associated with Button 33. The first, which is th default, specifies the Thornthwaite's method, the second specifies the Penman's method which is not implemented in this worksheet. If the Thornthwaite's method is selected, "0" will be written in the worksheet, however, if the Penman's method is selected, a warning message is displayed.



Buttons

Button # 34: SIMULATION START DATE

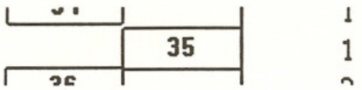
This button is used to specify the simulation start date as the day, month and year. This button is hidden from the worksheet if the precipitation is computed using database (see Button 7) or the evapotranspiration is constan with respect to time (see Button 8). The dialog box associated with Button 34 prompts the user to enter the simulation start date as the day, month and year, and the values are subsequently recorded in the data region.

0
1 1 1993

Buttons

Button # 35: TEMPERATURES

This button is used to specify whether or not the observed mean monthly temperatures are used in the evapotranspiration computations. If the evapotranspiration value is considered a constant with respect to time (see Button 8), this button is hidden from the worksheet. There are two options implemented in the dialog box associated with Button 35. The first option specifies that temperatures are manually entered by the user for each of the twelve months, and if selected, "0" will be written in the data region and twelve additional lines will be inserted into the worksheet for mean monthly temperatures. The default option associated with Button 35 specifies that the database values are utilized for mean monthly temperatures, and if selected, "1" will be written in the data region.



Buttons

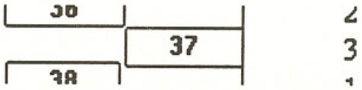
Button # 36: WILTING POINT

This button is used to specify the wilting point of the soil existing in the root zone as a percentage. It is hidde from the worksheet if the evapotranspiration value is considered a constant with respect to time (see Button 8

Buttons

Button # 37: ROOT ZONE DEPTH

This button is used to specify the root zone depth in appropriate length units for the water balance computation It is hidden from the worksheet if the evapotranspiration value is considered a constant with respect to time (se Button 8).



Buttons

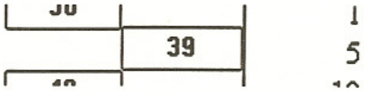
Button # 38: DISCRETIZATION PARAMETERS 3

Buttons 38 through 43 refer to input variables for the DILUTE (saturated zone) model. If the DILUTE model is not implemented in the model operation (see Button 15), these buttons will be hidden from the worksheet. Button 38 specifies the discretization parameters such as number of x locations (vertical scale), number of y locations (horizontal scale) and number of time instants to be simulated in the saturated zone application. Number of vertical and horizontal coordinates are restricted to be maximum 20 each, therefore only 400 distinct locations can be used in the computation of contaminant transport within the underlying aquifer. The number of simulation times is restricted to be 100 per model operation. Button 38 inserts additional lines into the worksheet depending upon the values of the aforementioned discretization parameters.

Buttons

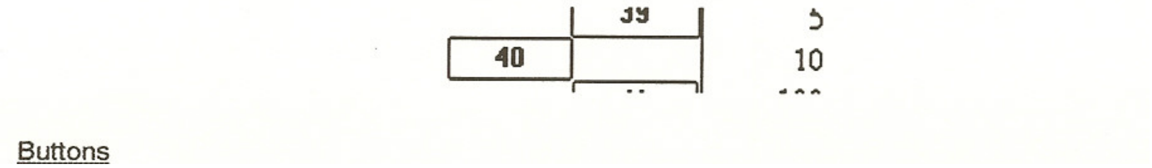
Button # 39: VERTICAL COORDINATES

This button is used to prompt the user to manually enter the vertical locations simulated in the DILUTE model. The number of vertical locations are determined via Button 3.



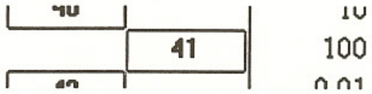
Button # 40: HORIZONTAL COORDINATES

This button is used to prompt the user to manually enter the horizontal locations simulated in the DILUT model. The number of horizontal locations are determined via Button 3.



Button # 41: SIMULATION TIMES

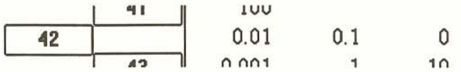
This button is used to prompt the user to manually enter the simulation times used in the DILUTE model. Th
number of simulation times are determined via Button 3.



Buttons

Button # 42: AQUIFER PROPERTIES

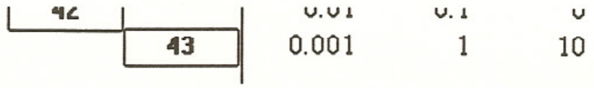
This button is used to enter aquifer specific parameters for the DILUTE model. The dialog box associated with this button prompts the user to manually enter the following properties: vertical (transverse) hydrodynamic dispersion coefficient, horizontal (longitudinal) hydrodynamic dispersion coefficient, vertical aquifer velocity, horizontal aquifer velocity, and half-length of the strip source which is assumed to be on top of the groundwater table. All values have to be entered by the user in appropriate units. For more information about the aforementioned variables see the technical manual of IMPACT v3.0.



Buttons

Button # 43: CHEMICAL PROPERTIES

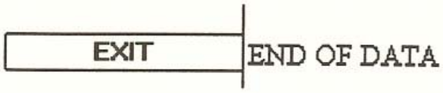
This button is used to enter chemical specific parameters for the DILUTE model. The dialog box associated witl this button prompts the user to manually enter the following properties: a first order equilibrium decay coefficient, retardation coefficient and the thickness of the aquifer. All values have to be entered by the user in appropriate units.



Buttons

EXIT

The last button in the worksheet is the EXIT button. The user must always use this button to exit or quit from the worksheet. When executed, the EXIT button displays a dialog box which contains two options. The first option is to create an input data file for the IMPACT model and exit from Microsoft Excel, the second option is to quit from the worksheet without creating an input file. If the first option is selected, a secondary dialog box is displayed for the user to manually enter a valid file name to be created. The input file is always created in the default directory where IMPACT v3.0 Preprocessor files reside.



Buttons