

MODEL FOR EVALUATION OF THE IMPACT OF CONTAMINATED SOIL ON GROUNDWATER

PHASE I

FINAL REPORT

Submitted to the New Jersey Department of Environmental Protection and
Energy

by

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Preface

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

This is the final report for Phase I of this project, and it contains the mathematical development, the underlying assumptions, a comprehensive description of model operation, method of solution, sensitivity analysis, and a literature survey for adsorption/desorption.

This report supersedes the draft final report submitted to NJDEP on 9/17/1990. Substantial changes have been made in the computation of evapotranspiration, the units used for the model input and output, and the sensitivity analysis.

The following personnel are involved in this project:

Principal Investigators:	Dr. George P. Korfiatis, Stevens
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Project Administrator:	Mr. William Librizzi, NJIT

The model was developed by Dr. Korfiatis and Dr. Talimcioglu at Stevens Institute of Technology. The literature survey for the adsorption/desorption coefficients

was performed by Dr. Uchrin and Mr. Williams at Rutgers.

Preface

This report contains the description of a one-dimensional continuous reactor model for heterogeneous, isothermal, and unsteady-state. The model is based on the NUTS, a development regulatory clean-up levels for contaminants in the model, and was based on an early input to groundwater.

This is the final report for Phase I of this project, and it contains the results of model development, the modeling results, a comprehensive description of model operation, method of solution, sensitivity analysis, and a literature survey for other models.

This report supersedes the draft final report submitted to NUTS on 01/15/1990. Substantial changes have been made in the composition of report structure, the order of the model input and output, and the sensitivity analysis. The following persons are involved in this project:

Principal Investigator:	Dr. George F. Uchirin, Rutgers
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Project Administrator:	Mr. William Uchirin, NUTS

The model was developed by Dr. Uchirin and Dr. Christopher J. Uchirin at Rutgers University. The literature survey for the other models was conducted by Dr. Uchirin.

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Chapter 1

Introduction

Both numerical and analytical models have been used to predict the transport and fate of contaminants in subsurface environment. Analytical models are restrictive since they usually apply only to simple systems under steady-state conditions. In addition, non-linearities of the problem are treated in a very approximate fashion, thus limiting the accuracy of prediction. Numerical models, on the other hand, are able to describe complex boundary conditions and fully transient processes at the expense of significantly higher computational effort.

The present work entails the development of a deterministic, one-dimensional numerical model for predicting the transport and fate of a single dissolved contaminant in the unsaturated soil zone. The model describes major controlling transport mechanisms, namely, advection, dispersion, adsorption/desorption, volatilization, and biodegradation. The mathematical formulation of each of these mechanisms is based on present state-of-the-art knowledge. Several simplifying assumptions are made in order to be able to describe the complex processes mathematically. Some of these assumptions have been extensively reported in the literature, and have been found to be reasonable within the context of accepted accuracy.

The model employs a trial and error procedure to determine what concentrations

of a single contaminant can be allowed to remain in the soil column based on an allowable concentration at the free surface aquifer below the source.

Chapter 2

Flow and Transport Mechanisms

2.1 Moisture Flow

Richards' equation [70] has been almost exclusively used to describe the movement of water in soils under partially saturated conditions. This equation is usually found in the literature either in the moisture content form or in the pressure head form. The one-dimensional moisture content form of Richards' equation is written without a source/sink term as follows:

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

in which

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 $[L^2/T]$

This equation is highly non-linear due to the fact that both hydraulic conductivity and soil diffusivity are functions of the moisture content. This equation, therefore, cannot be solved analytically.

The soil diffusivity coefficient, also called the capillary diffusivity coefficient, was defined by Klute [51] as:

$$D(\theta_w) = -K(\theta_w) \frac{d\psi}{d\theta_w} \quad (2.2)$$

where $\psi = \text{Suction head } [L]$.

The moisture flux is described by Darcy's law as follows:

$$q_w = K(\theta_w) - D(\theta_w) \frac{\partial \theta_w}{\partial z} \quad (2.3)$$

Alternatively, the pressure head form of the Richards' equation is given as follows:

$$C(\psi) \frac{\partial \psi}{\partial t} + \frac{\partial}{\partial z} K(\psi) + \frac{\partial}{\partial z} \left[K(\psi) \frac{\partial \psi}{\partial z} \right] = 0 \quad (2.4)$$

where

$$C(\psi) = \frac{d\theta_w}{d\psi} = \text{Specific water storativity}$$

Equation (2.4) also exhibits a strong non-linearity because C and K are functions of ψ .

The solution of Equation (2.1) or Equation (2.4) requires the knowledge of the soil moisture retention properties ($\theta_w - \psi$ relationship) and the hydraulic conductivity versus moisture content relationship. Several investigators have proposed parametric expressions describing these relationships. The most frequently used expressions are outlined below:

2.1.1 Soil Moisture Retention

The soil moisture retention properties exhibit strong hysteretic behavior [11]. The relation between the pressure head, ψ , and the moisture content, θ_w , is not unique. Therefore, ψ cannot be determined directly from the knowledge of θ_w without investigating the past wetting-drying history of the specific soil considered. Such hysteretic behavior can be modeled by using different parametric relationships for wetting and drying phases of the moisture transport. The hysteresis of the soil moisture retention is neglected in this study.

Several parametric relationships are addressed in the following sections.

Campbell (1974)/Clapp and Hornberger (1978)

Clapp and Hornberger [19] employed an exponential relation based on the equation proposed by Campbell [14] of the form:

$$\psi = \psi_s \left[\frac{\theta_w}{\theta_s} \right]^{-b} \quad (2.5)$$

where

ψ_s = Saturation suction head

θ_s = Saturation moisture content

b = Empirical constant (characteristic of the soil)

van Genuchten (1980)

van Genuchten [89] derived the following empirical relationship experimentally:

$$S_e = [1 + (\alpha\psi)^n]^{-m} \quad (2.6)$$

where

S_e = Reduced water content

α, n, m = Empirical parameters

The empirical parameter m is taken as $1 - (1/n)$.

S_e is also defined by Campbell [14] as:

$$S_e = \frac{\theta_w - \theta_f}{\theta_s - \theta_f} \quad (2.7)$$

where θ_f is the field capacity.

2.1.2 Hydraulic Conductivity

Although Klute [51] noted that K versus θ_w relationship is literally hysteresis free, both K and D are affected by the hysteresis of θ_w versus ψ relationship. The following sections outline K versus θ_w relationships proposed by several authors.

Campbell (1974)

Campbell [14] suggested the following expression for the hydraulic conductivity:

$$K(\theta_w) = K_s \left[\frac{\theta_w}{\theta_s} \right]^m \quad (2.8)$$

The exponent m is usually taken as $2b + 3$ where b is the exponent used in Equation (2.5).

Mualem (1978)

Mualem [58] generalized the equation proposed by Campbell [14] in which he allowed the empirical exponent, n , to vary with soil type. He showed theoretically that n can

take values lower than 3 for granular soils and larger than 3 for textured soils. These findings were verified experimentally. The proposed equation is written as follows:

$$K(\theta_w) = K_s \left[\frac{\theta_w - \theta_f}{\theta_s - \theta_f} \right]^n \quad (2.9)$$

where n is a coefficient of the soil type.

Ragab (1981)

Ragab et al. [67] proposed the following relationship:

$$K(\theta_w) = A\theta_w^b \quad (2.10)$$

where A, b are empirical constants.

Mualem (1976)/van Genuchten (1980)

Mualem [57] proposed the following model:

$$K(\theta_w) = K_s S_e^\gamma \left[\frac{f(S_e)}{f(1)} \right]^2 \quad (2.11)$$

in which

$$f(S_e) = \int_0^{S_e} \frac{1}{\psi(z)} dz \quad (2.12)$$

where γ is an empirical parameter, usually taken equal to $1/2$. van Genuchten [89] derived the following relationship by substituting Equation (2.6) into Equation (2.11):

$$K(\theta_w) = K_s S_e^\gamma \left[1 - \left(1 - S_e^{1/m} \right)^m \right]^2 \quad (2.13)$$

2.1.3 Soil Diffusivity

The soil diffusivity coefficient has also been addressed by several investigators. The following sections outline several equations adopted in this study.

Clapp and Hornberger (1978)

The following empirical equation can be derived by substituting Equation (2.5) into Equation (2.2):

$$D(\theta_w) = K(\theta_w)b \frac{\psi_s}{\theta_s} \left(\frac{\theta_w}{\theta_s} \right)^{-(b+1)} \quad (2.14)$$

It should be noted that the empirical coefficient b used in the above equation is the same coefficient used in Equation (2.5).

Gardner (1958)

Gardner et al. [32] suggested the following expression for the intermediate range of moisture contents:

$$D(\theta_w) = D_0 e^{\beta(\theta_w - \theta_0)} \quad (2.15)$$

where

$$D_0 = \text{Diffusivity corresponding to } \theta_w = \theta_0$$

$$\beta, \theta_0 = \text{Empirical constants}$$

van Genuchten (1980)

The following equation is derived from Equations (2.2), (2.6), and (2.7):

$$D(\theta_w) = \frac{K(\theta_w)}{\alpha(n-1)(\theta_s - \theta_f)(1 - S_e^{1/m})^m S_e^{1/m}} \quad (2.16)$$

Several numerical models have been developed to predict unsaturated moisture transport by solving either Equation (2.1) or Equation (2.4) by finite difference or finite element approximations [30, 72, 42, 53, 90, 91].

Hills et al. [39] compared the solutions of the water content and the pressure head based equations by using implicit finite differences. The advantages of solving the moisture content equation as opposed to the suction head based equation are as follows [39]:

- Relatively low mass balance errors are produced;
- The solution is relatively insensitive to dry initial conditions;
- Longer time steps can be accommodated in the simulation;
- The solution requires substantially less CPU time for initially dry conditions.

Disadvantages of the moisture content based algorithms include:

- The numerical scheme exhibits instabilities at moisture contents very close to saturation;
- Boundary conditions are difficult to define accurately.

For the purposes of the present project, it is believed that an algorithm based on the moisture equation is more desirable. This assessment is based on the fact that simulations over large time periods are required, and the ability to use relatively large time steps is crucial.

2.2 Solute Transport and Fate

2.2.1 Movement Mechanisms

The transport and the ultimate fate of pollutants in the vadose zone are governed by various mechanisms which depend on soil, chemical and biological properties, and other factors such as atmospheric conditions. Volatile organic compounds (VOCs) under unsaturated conditions ultimately partition into three distinct phases, namely solid, liquid (both aqueous and non-aqueous), and gaseous. Since mass is conserved, the total quantity of a single chemical within a unit volume is [45]:

$$C_T = \rho_b C_A + \theta_w C_L + \theta_a C_G + \theta_i C_I \quad (2.17)$$

where

C_T = Total concentration of a single chemical $[M/L^3]$

ρ_b = Soil bulk density $[M/L^3]$

C_A = Adsorbed chemical concentration $[M/M]$

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

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

θ_a = Volumetric air content $[L^3/L^3]$

C_G = Gaseous phase concentration $[M/L^3]$

θ_i = Volumetric immiscible phase content $[L^3/L^3]$

C_I = Immiscible phase concentration $[M/L^3]$

If the immiscible phase is not present in the system, the last term of Equation (2.17) is dropped. Thus, the total concentration can be expressed in three phases as follows:

$$C_T = \rho_b C_A + \theta_w C_L + \theta_a C_G \quad (2.18)$$

There are three major mechanisms responsible for the movement of the VOC solutes in the porous media:

Advection (Mass Flow)

Chemical mass is transported by virtue of liquid flow. The advective flux is described as follows:

$$J_A = q_w C_L \quad (2.19)$$

where

$$J_A = \text{Advective flux } [M/L^2T]$$

$$q_w = \text{Moisture flux } [L/T]$$

Hydrodynamic Dispersion

This is the combined effect of mechanical dispersion and molecular diffusion that causes spreading of the chemical in the soil, and it is described as the following:

$$J_{HD} = -\theta_w E \frac{\partial C_L}{\partial z} \quad (2.20)$$

where

$$J_{HD} = \text{Hydrodynamic dispersive flux } [M/L^2T]$$

$$E = \text{Hydrodynamic dispersion coefficient } [L^2/T]$$

The hydrodynamic dispersion coefficient can be written as [9]:

$$E = \epsilon_w + D_w \quad (2.21)$$

in which

$$\epsilon_w = \frac{|q_w|}{\theta_w} \alpha_w \quad (2.22)$$

$$D_w = d_w \tau_w \quad (2.23)$$

where

ϵ_w = Mechanical dispersion coefficient $[L^2/T]$

D_w = Molecular diffusion coefficient in soil water $[L^2/T]$

α_w = Dispersivity $[L]$

d_w = Bulk water diffusion coefficient of the chemical $[L^2/T]$

τ_w = Tortuosity factor in soil water

Using the Penman-type model, i.e. $\tau = \tau_a = \tau_w$ [63, 61], the tortuosity factor has been empirically derived by Millington and Quirk [55] as:

$$\tau_w = \frac{\theta_w^{10/3}}{n^2} \quad (2.24)$$

where n is the soil porosity, i.e. $n = \theta_a + \theta_w = \theta_s$

Vapor Diffusion

The movement of vapor through soils is assumed to exhibit Fickian behavior [45]. The diffusive flux is then described as follows:

$$J_{VD} = -D_a \frac{\partial C_G}{\partial z} \quad (2.25)$$

$$D_a = d_a \theta_a \tau_a \quad (2.26)$$

where

J_{VD} = Diffusive flux in vapor $[M/L^2T]$

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

d_a = Bulk air diffusion coefficient of the chemical $[L^2/T]$

τ_a = Tortuosity factor in soil air

The tortuosity factor, τ_a , is generally assumed to be of the form used for the water diffusion, and is described by the model proposed by Millington and Quirk [55] as follows:

$$\tau_a = \frac{\theta_a^{10/3}}{n^2} \quad (2.27)$$

The one-dimensional continuity equation for the total chemical mass can then be written for the three mechanisms presented above as the following [37]:

$$\frac{\partial C_T}{\partial t} + \frac{\partial}{\partial z}(J_A + J_{HD} + J_{VD}) = 0 \quad (2.28)$$

The above equation describes the transport of a single substance in the porous medium, accounting for the mass flow, hydrodynamic dispersion, and vapor diffusion.

2.2.2 Adsorption/Desorption

Adsorption refers to the bonding of the dissolved solute to the soil mineral surfaces or to the organic matter surfaces. Desorption is the reverse of this process. The effect of adsorption on the overall chemical transport phenomenon is to immobilize the moving chemical molecules in both gaseous and liquid phases temporarily. Soil sorption, a term interchangeably used for both adsorption and desorption processes, is a physicochemical process that involves the increase or the decrease of solutes at the soil-water interface.

Because of the extreme complexities of the soil solution and bonding mechanisms, engineering approximations such as the use of distribution coefficients have gained general acceptance in describing the adsorption capacity of a given chemical. A frequently made assumption is that the adsorption process is completely reversible. Virtually all organic chemicals studied exhibit hysteresis in adsorption-desorption relationships [84, 86].

The mass transfer from the liquid phase to the solid phase (adsorption) and the solid phase to the liquid phase (desorption) has been investigated extensively, and several models have been proposed in the literature. A detailed description of the kinetics of sorption is given by Uchrin [84], and much research has shown that the net adsorption component of sorption occurs rather quickly such that instantaneous local adsorption can be assumed [84]. This allows for the use of a linear adsorption isotherm, the slope of which is termed the solid/liquid partition coefficient. There may be, however, a pronounced resistance to desorption, which may occur at a slower rate. DiToro and Horzempa [27] were among the first to define two components to sorption: one readily reversible, and one resistant to desorption. Ahlert, et al. [6] showed the effect that this non-reversibility could have on transport processes.

Sorption of a pollutant can be considered as a pseudo-reversible reaction in which the pollutant can exist in either an adsorbed state, $A \cdot S$, or in solution, A [84]. This process is illustrated schematically in Figure (2.1). The letter S denotes available adsorption sites. Two components comprise the adsorption process. The first is a very rapid association from the bulk fluid to the solid surface. The second is a very slow diffusion into the solid matrix which frees locations on the bulk solid for more of the former to occur. The former process is readily reversible while the latter quite resistant. Thus, the adsorption process can be summarized as a sum of the two processes, such that:

$$\text{Total adsorption} = \text{initial adsorption} + \text{intraparticle diffusion}$$

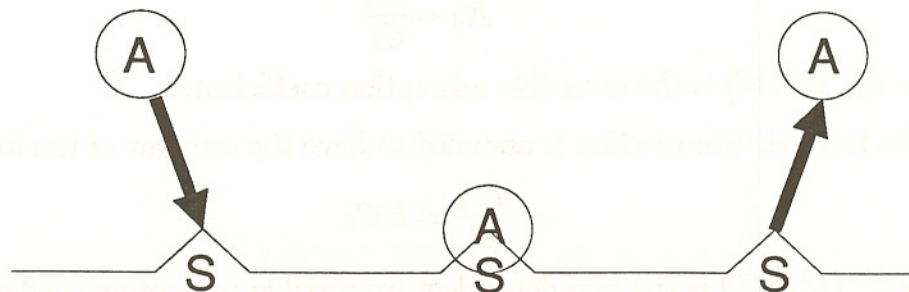
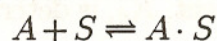


Figure 2.1: Sorption schematic (from Uchirin, 1986)

The initial adsorption reaction can be considered to have a mechanism:



The intraparticle diffusion is slow and rate limiting.

2.2.3 Chemical Partitioning

In order to estimate the transport and fate of VOCs in the air-soil-water system, it is necessary to describe the partitioning of the chemical in three phases. In the present study, the following equilibrium relationships are adopted to readily define the partitioning between different phases:

The partitioning between the liquid and the air phases is assumed to follow Henry's law:

$$H = \frac{C_L}{C_G} \quad (2.29)$$

where H is the Henry's constant, defined as the ratio of aqueous solubility to the saturated vapor concentration of the chemical at 20°C [9]. This definition is the inverse of that more generally used in the literature as $K_H = C_G/C_L$.

The partitioning between the liquid and the solid phases is also assumed to be linear. The initial adsorption reaction is fast and reversible; thus, it is characterized

by an equilibrium expression of the form:

$$K_d = \frac{C_A}{C_L} \quad (2.30)$$

where K_d [L^3/M] is the reversible adsorption coefficient.

The intraparticle reaction is assumed to have the rate law of the form:

$$\frac{dC_A}{dt} = k' C_L \quad (2.31)$$

where k' [L^3/MT] is the rate dependent irreversible adsorption coefficient.

Combining Equations (2.30) and (2.31) gives:

$$\frac{dC_A}{dt} = K_d \frac{dC_L}{dt} + k' C_L \quad (2.32)$$

The partitioning coefficient, K_d , is determined by batch tests. It can be expressed in terms of the organic carbon content, and is given by the relationship [49]:

$$K_d = K_{oc} \times OC \quad (2.33)$$

where K_{oc} [L^3/M] is the normalized coefficient of adsorption with respect to organic carbon content, or alternatively called as the fugacity coefficient, and OC is the organic carbon content of the soil.

Combining Equations (2.28) and (2.18), the mass continuity equation then becomes:

$$\frac{\partial(\rho_b C_A + \theta_w C_L + \theta_a C_G)}{\partial t} + \frac{\partial}{\partial z}(J_A + J_{HD} + J_{VD}) = 0 \quad (2.34)$$

Using the partitioning relationships and Equation (2.32), the above equation can be written in terms of the liquid phase concentration as follows:

$$K_d \rho_b \frac{\partial C_L}{\partial t} + k' \rho_b C_L + \frac{\partial(\theta_w C_L)}{\partial t} + \frac{1}{H} \frac{\partial(\theta_a C_L)}{\partial t} + \frac{\partial(q_w C_L)}{\partial z} = \frac{\partial}{\partial z} \left[\theta_w E \frac{\partial C_L}{\partial z} \right] + \frac{\partial}{\partial z} \left[\frac{D_a}{H} \frac{\partial C_L}{\partial z} \right] \quad (2.35)$$

Rearranging terms and adding a sink term to describe the mass losses due to biotransformation reveals:

$$\frac{\partial(\theta_w C_L)}{\partial t} + K_d \rho_b \frac{\partial C_L}{\partial t} + k' \rho_b C_L + \frac{1}{H} \frac{\partial(\theta_a C_L)}{\partial t} + \frac{\partial(q_w C_L)}{\partial z} = \frac{\partial}{\partial z} \left[\left(\theta_w E + \frac{D_a}{H} \right) \frac{\partial C_L}{\partial z} \right] - \theta_w R \quad (2.36)$$

where R is the sink term representing mass losses due to the biotransformation process. This equation is the governing equilibrium mass transport equation which accounts for all the movement mechanisms mentioned earlier.

The following section addresses the biotransformation process in the porous media.

2.2.4 Biotransformation

The term biotransformation is a general term describing the effect of living organisms on the fate of organic compounds. Biodegradation is a more specific term generally used to refer a biological transformation of an organic compound into more simple products by biochemical reactions.

The transformation of some VOCs due to biological activity within the porous media is considered to be an important factor to the ultimate fate of contaminants. Several rate expressions have been used to describe biotransformation. Most of the biodegradation models have focused on degradation in the aquatic systems, not in soils [88]. However, it is commonly assumed that similarities exist between the two systems. The rate expressions proposed by Monod [56] have been widely used, and they account for both microbial growth and substrate utilization. The rate of microbial change, R_x , is described as follows [26]:

$$R_x = \frac{\mu_m X C_L}{K_m + C_L} - k_e X \quad (2.37)$$

where

R_x = Rate of microbial growth per unit volume $[M/L^3T]$

μ_m = Microorganism's maximum specific growth rate $[1/T]$

K_m = Substrate concentration at 1/2 of μ_m $[M/L^3]$

X = Microorganism concentration $[M/L^3]$

k_e = Endogenous decay coefficient of microorganisms $[1/T]$

The substrate utilization rate is described as [26]:

$$R_s = \frac{k X C_L}{K_m + C_L} \quad (2.38)$$

where k $[1/T]$ is the maximum rate of substrate utilization per unit mass of microorganisms, and is defined as the following:

$$k = \frac{\mu_m}{Y} \quad (2.39)$$

in which Y is the biomass yield coefficient.

At dynamic population equilibrium condition, the microbial concentration becomes constant with respect to time, thus the Monod expression becomes:

$$R_s = \frac{k_x C_L}{K_m + C_L} \quad (2.40)$$

where $k_x = kX = \text{constant}$.

At high substrate concentrations ($C_L \gg K_m$), R_s becomes a constant:

$$R_s = k_x = k_0 \quad (2.41)$$

At low substrate concentrations ($C_L \ll K_m$), R_s becomes a first order expression:

$$R_s = \frac{k_x C_L}{K_m} = k_1 C_L \quad (2.42)$$

This formulation assumes that microorganisms utilize substrate from the liquid phase only. Nonbiological transformations are not included in the present model.

Jury et al. [46] studied the first order biodegradation equilibrium, and derived the following relationship that describes the first order coefficient:

$$k_1 = \frac{\ln(2)}{\tau} \quad (2.43)$$

where τ [days] is the effective half-life of the organic chemical. The values of τ have been given for selected compounds by Jury et al. [46].

Chapter 3

Climatic Processes

3.1 General

Climatic processes account for the full cycle of precipitation, evapotranspiration, and runoff events. The net infiltration through the soil surface is due to the combination of these events. The primary driving force of flow through the vadose zone, therefore, is a function of the climatic processes.

The following sections address the aforementioned meteorological and hydrological processes in detail. The model presented in this study has an option to incorporate the real hydrological data from a database of rainfall and temperature values observed in Newark, New Jersey. The evapotranspiration rates are computed by using one of the two methods proposed by Penman [63, 64] and Thornthwaite [81], respectively. The runoff event is implemented in the model via the empirical method proposed by the Soil Conservation Service [74]. Finally, the net infiltration through the ground surface is computed by the water balance method developed by Thornthwaite and Mather [82].

Table 3.1: Mean monthly precipitation rates observed in Newark, New Jersey during 1959-1989 (inches)

Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
3.34	3.09	3.86	3.77	3.86	2.99	4.45	3.80	3.64	2.93	3.94	3.52

3.2 Precipitation

The model requires the input of rainfall values in order to compute the net infiltration. There are two options provided in this study to implement the precipitation input: 1) User supplied precipitation rates which are given either for individual time steps or as a constant; 2) Actual daily precipitation rates. For the latter, the rainfall values, observed in Newark, New Jersey for the last thirty years, are obtained on an hourly basis from the National Climatic Data Center in Asheville, North Carolina. Assuming one-day storm events, this data were evaluated statistically to obtain average daily rainfall rates. Table (3.1) tabulates the results of this analysis. The average yearly total rainfall was found to be 43.2 inches. Figure (3.1) is a graphical representation of Table (3.1). Figure (3.2) shows the annual precipitation rates over the thirty year-period, starting from January 1959 to December 1988.

3.3 Surface Temperatures

Real-time surface temperatures are also incorporated in the model in a similar fashion. The results of the statistical analysis are shown graphically in Figure (3.3). Table (3.2) tabulates these results with standard deviations. These values are utilized in the calculation of evapotranspiration values.

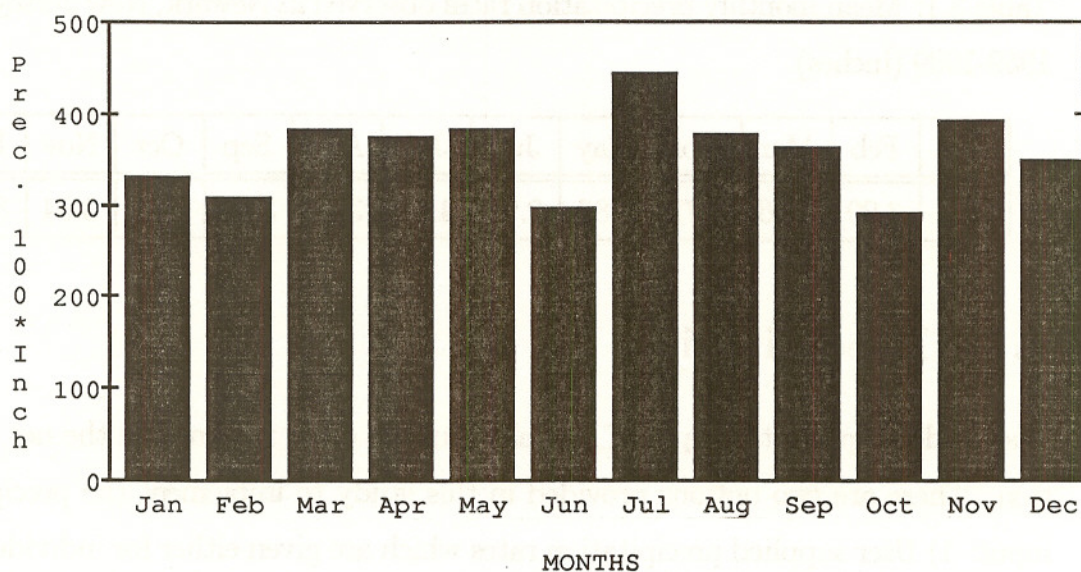


Figure 3.1: Mean monthly precipitation rates observed in Newark, New Jersey during 1959-1989

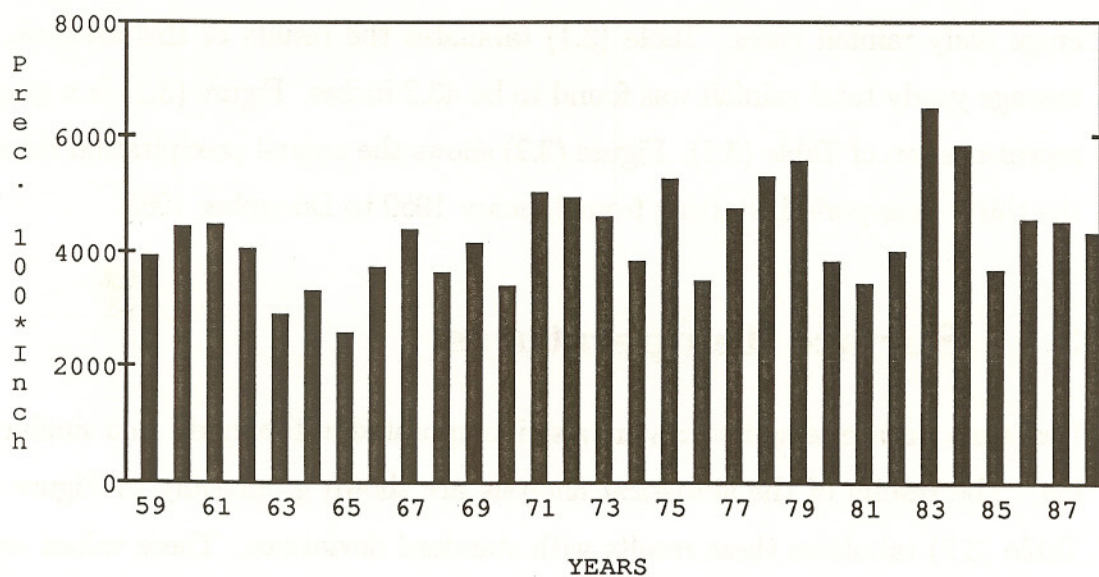


Figure 3.2: Annual total precipitation rates observed in Newark, New Jersey during 1959-1989

Table 3.2: Mean monthly temperature values observed in Newark, New Jersey during 1959-1989

Months	Temperatures ($^{\circ}F$)	Standard Deviations ($^{\circ}F$)
Jan	30.2	4.3
Feb	32.8	3.7
Mar	41.7	3.2
Apr	52.3	2.4
May	62.9	2.9
Jun	71.9	1.9
Jul	77.1	1.8
Aug	75.9	1.8
Sep	68.3	2.5
Oct	57.0	2.9
Nov	46.9	2.7
Dec	35.8	3.8

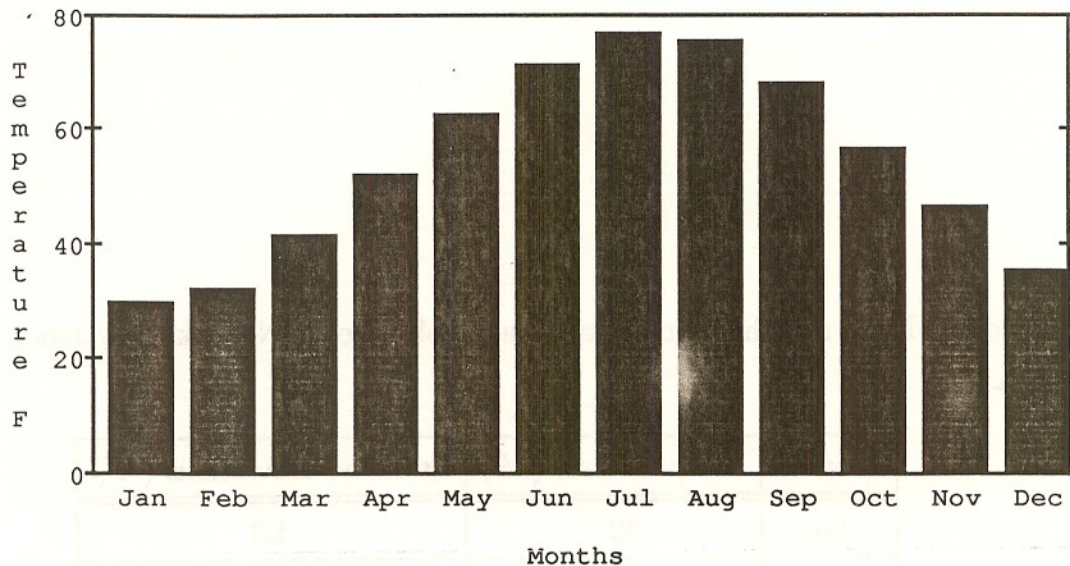


Figure 3.3: Mean monthly temperature values observed in Newark, New Jersey during 1959-1989

3.4 Evapotranspiration

The term evapotranspiration is commonly used to describe two processes, namely evaporation and transpiration. Evaporation refers to the change of water from the liquid phase to the gaseous phase. Evaporation may occur from open water surfaces or from soil surfaces. Transpiration occurs directly from plant leaves. The term potential evapotranspiration refers to the rate of evapotranspiration from a given surface with vegetation cover which occurs when the water supply to the surface is unlimited. Therefore, when limiting conditions in water supply exist, the actual evapotranspiration value is always less than the potential evapotranspiration.

In this study, two methods are considered in predicting the potential evapotranspiration from soil surfaces. Penman [63, 64] derived an equation for predicting evaporation from open water surfaces. He then experimentally adjusted this equation to predict evapotranspiration from soil surfaces. Penman's theory combines

two mechanisms which are instrumental to the evapotranspiration process: the mass transfer and the energy balance. The mass transfer theory considers the turbulent vapor transport by diffusion processes, whereas the energy balance theory considers the heat energy delivered by solar radiation.

The second method implemented in the present study is addressed by Thornthwaite [81]. Thornthwaite derived a semi-empirical equation to describe the potential evapotranspiration from soil surfaces. This equation received wide acceptance because it is fairly accurate and simple to use. Thornthwaite's equation was found to be applicable to the present study because of the fact that he conducted his experiments in New Jersey using actual climatic data.

3.4.1 Penman's Equation

The theory proposed by Penman [63] is incorporated in the model in two stages, namely, the constant rate stage and the falling rate stage. The constant rate stage is the period during which evaporation is controlled by external meteorological conditions. The falling rate stage, however, is the period during which evaporation is limited by available water content in the soil.

Constant Rate Evaporation

Penman's equation is written as follows:

$$E_0 = \frac{\Delta H_0 + \gamma E_a}{\Delta + \gamma} \quad (3.1)$$

where

$$E_0 = \text{Potential evaporation [mm H}_2\text{O/day]}$$

$$H_0 = \text{Net solar radiation [mm H}_2\text{O/day]}$$

γ = Psychrometric constant [mm Hg/°F]

E_a = Evaporation by forced convection [mm H₂O/day]

Δ = Slope of the temperature versus vapor pressure
curve at mean temperature [mm Hg/°F]

The general form of E_a is as follows:

$$E_a = f(u)(e_a - e_d)$$

where

$f(u)$ = Wind velocity function

e_a = Saturation vapor pressure @ mean temperature

e_d = Mean vapor pressure @ dew - point temperature

Penman suggested the following relationship for E_a [64]:

$$E_a = 0.35(e_a - e_d)(1 + 0.0098w) \quad (3.2)$$

where

w = Mean wind velocity @ 2m above ground surface [miles/day]

E_a is in [mm H₂O/day], e_a and e_d are in [mm Hg] units in the above equation.

The net solar radiation, H_0 , is calculated from the empirical relation:

$$H_0 = R(1 - \lambda)(0.18 + 0.55S) - \sigma T_a^4(0.56 - 0.092e_d^{0.5})(0.1 + 0.9S) \quad (3.3)$$

where

R = Mean monthly solar radiation evaporated per day [mm H₂O/day]

λ = Albedo constant

σ = Boltzmann constant

T_a = Mean air temperature [K°]

S = $\frac{\text{Actual duration of sunshine}}{\text{Maximum duration of sunshine}}$

It must be noted that in order for Equation (3.1) to be dimensionally correct, Δ and γ must have units of $mm\ Hg$ per degree $^\circ F$ so that E_0 will be in $mm\ H_2O$ per day. Values for R and Δ are given by Chow [18]. The slope of the temperature versus saturation vapor pressure can be calculated from the following formula:

$$\Delta = 422.22 \left(\frac{5205}{T^2} \right) e^{(13.95 - \frac{5205}{T})} \quad (3.4)$$

where T is the mean daily temperature [K°] and Δ is in $mm\ H_2O$ per degree $^\circ F$.

The values of e_a and e_d can be calculated by the empirical relationship proposed by Bosen [12]:

$$e_k = 33.8639 \left[(0.00738T_k + 0.8072)^8 - 0.000019|1.8T_k + 48| + 0.001316 \right] \quad (3.5)$$

where

$$e_k = \begin{cases} e_a \text{ [millibars]} & \text{for } T_k = \text{Mean daily temperature } [^\circ C] \\ e_d \text{ [millibars]} & \text{for } T_k = \text{Dew point temperature } [^\circ C] \end{cases} \quad (3.6)$$

If the soil is bare of vegetation, E_0 is equal to the soil evaporation, E_{so} . If the soil has vegetation, E_{so} is commonly computed on the basis of the leaf area index (LAI) [71, 65]. LAI is defined as the ratio of the area of leaves to the area of the soil surface. It is often measured on a relative scale of 0 to 3, where 0 indicates no vegetation, and 3 indicates a full cover of vegetation. The potential soil evaporation, E_{so} , can be computed from the following relation:

$$E_{so} = E_0 e^{-0.4(LAI)} \quad \text{for } 0 \leq LAI \leq 3 \quad (3.7)$$

Perrier and Gibson [65] suggested the following for the plant transpiration, E_p :

$$E_p = \frac{E_0(LAI)}{3} \quad \text{for } 0 \leq LAI \leq 3 \quad (3.8)$$

The total evapotranspiration, E_t , can then be computed as the following:

$$E_t = E_{so} + E_p \quad (3.9)$$

Falling Rate Evaporation

During the falling rate stage, evaporation is controlled by the properties and the moisture characteristics of the soil. Falling rate evaporation can be predicted by solving the unsaturated flow equation. Neglecting the gravity term, Equation (2.1) then becomes:

$$\frac{\partial \theta_w}{\partial t} = \frac{\partial}{\partial z} \left[D(\theta_w) \frac{\partial \theta_w}{\partial z} \right] \quad (3.10)$$

The above equation was solved analytically by Crank [23] for a semi-infinite column of soil with constant diffusivity. This solution gives the moisture flux, q_w , at the boundary as follows:

$$q_w = (\theta_{w_i} - \theta_{w_0}) \left(\frac{D}{\pi t} \right)^{1/2} \quad (3.11)$$

where

θ_{w_i} = Initial moisture content

θ_{w_0} = Moisture content at the boundary

The cumulative evaporation is obtained by integrating Equation (3.11) with respect to time:

$$E_0 = 2(\theta_{w_i} - \theta_{w_0}) \left(\frac{Dt}{\pi} \right)^{1/2} \quad (3.12)$$

Since the diffusivity, D , is a function of the moisture content, an average value of D should be used in the above equation. Crank [23] suggested the following weighted-mean diffusivity, $\bar{D}$:

$$\bar{D} = \frac{1.85}{(\theta_{w_i} - \theta_{w_0})^{1.85}} \int_{\theta_{w_0}}^{\theta_{w_i}} D(\theta_w) (\theta_{w_i} - \theta_{w_0})^{0.85} d\theta_w \quad (3.13)$$

The transition from the constant rate to falling rate evaporation is sharp [38]. Since this transition point is not known *a priori*, the evaporative capacity of the soil to release water must both be computed and compared for each time interval. For decreasing surface moisture content, the lesser of the two capacities will control.

3.4.2 Thornthwaite's Equation

The general form of Thornthwaite's equation is written as the following [81]:

$$E_t = CT^a \quad (3.14)$$

where

E_t = Monthly potential evapotranspiration [cm]

C = Empirical coefficient

a = $67.5 \times 10^{-8}(I)^3 - 77.1 \times 10^{-6}(I)^2 + 0.0179(I) + 0.492$ [$^{\circ}C$]

I = Annual heat index = $\sum_{m=1}^{12} \left(\frac{T}{5} \right)^{1.51}$ [$^{\circ}C$]

T = Monthly mean temperature [$^{\circ}C$]

Table 3.3: Values of the adjustment factor, b , used in Thornthwaite's equation (from Gray, 1973)

Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
0.84	0.83	1.03	1.11	1.24	1.25	1.27	1.18	1.04	0.96	0.83	0.81

The coefficient C depends on the percentage of sunshine in a given period. Under the assumption of 12 hours of sunshine per day and 30 days per month, C was found to be $1.62(10/I)^a$. Thornthwaite's equation was adjusted with another coefficient, b , for the fact that duration of sunshine is not always 12 hours a day and actual durations of the months are used. The potential evapotranspiration can then be expressed as follows [33]:

$$E_t = 1.62b \left(\frac{10T}{I} \right)^a \quad (3.15)$$

Table (3.3) gives the values of the adjustment factor, b , for the 40° latitude (New Jersey's approximate location).

As mentioned earlier, the average values of the monthly temperatures for the last 30 years were computed using the monthly minimum and maximum temperature values observed in Newark, New Jersey. The results tabulated in Table (3.2) are substituted into Equation (3.15) when Thornthwaite option is selected during the program execution.

3.5 Runoff

The model estimates runoff using the Soil Conservation Service (SCS) method [74, 13], and subtracts the runoff values from the precipitation values. The following

section outlines the SCS method:

3.5.1 Soil Conservation Service Method

The SCS method is an empirical approach for obtaining runoff over finite areas for single storm events. It should be noted that this method was developed and calibrated in English units. Figure (3.4) graphically shows the infiltration rates with respect to time. The surface runoff, R_s , is obtained using the following empirical relationship:

$$R_s = \frac{(P - I_a)^2}{P - I_a + S} \quad (3.16)$$

for

$$P \geq I_a \text{ and } S \geq I_a + F$$

where I_a is an initial retention volume, F is the total infiltration, and S is the potential maximum surface retention. The initial abstraction is commonly taken as $I_a = 0.2S$. The runoff then becomes:

$$R_s = \frac{(P - 0.2S)^2}{P + 0.8S} \quad (3.17)$$

where

$$\begin{aligned} R_s &= \text{Runoff [inches]} \\ P &= \text{Precipitation [inches]} \\ S &= \frac{1000}{CN} - 10 \text{ [inches]} \end{aligned} \quad (3.18)$$

The CN in the above equation is called the curve number, a parameter dependent on soil type and moisture conditions. A list of CN numbers can be found in Bras

Table 3.4: Runoff Curve Numbers I (from Soil Conservation Service, 1985)

Land Use or Cover	Treatment or Practice	Hydrologic Condition	Soil Group			
			A	B	C	D
Fallow	Straight Row	—	77	86	91	94
Row Crops	Straight Row	Poor	72	81	88	91
	Straight Row	Good	67	78	85	89
	Contoured	Poor	70	79	84	88
	Contoured	Good	65	75	82	86
	Terraced	Poor	66	74	80	82
	Terraced	Good	62	71	78	81
Small Grain	Straight Row	Poor	65	76	84	88
	Straight Row	Good	63	75	83	87
	Contoured	Poor	63	74	82	85
	Contoured	Good	61	73	81	84
	Terraced	Poor	61	72	79	82
	Terraced	Good	59	70	78	81
Closed Seed	Straight Row	Poor	66	77	85	89
	Straight Row	Good	58	72	81	85
	Contoured	Poor	64	75	83	85
	Contoured	Good	55	69	78	83
	Terraced	Poor	63	73	80	83
	Terraced	Good	51	67	76	80

Table 3.5: Runoff Curve Numbers II (from Soil Conservation Service, 1985)

Land Use or Cover	Treatment or Practice	Hydrologic Condition	Soil Group			
			A	B	C	D
Pasture or Range	Contoured	Poor	68	79	86	89
		Fair	49	69	79	84
		Good	39	61	74	80
		Poor	47	67	81	88
		Fair	25	59	75	83
		Good	6	35	70	79
Meadow		Good	30	58	71	78
Woods		Poor	45	66	77	83
		Fair	36	60	73	79
		Good	25	55	70	77
Farmsteads		—	59	74	82	86
Dirt Road		—	72	82	87	89
Hard Surface Road		—	74	84	90	92

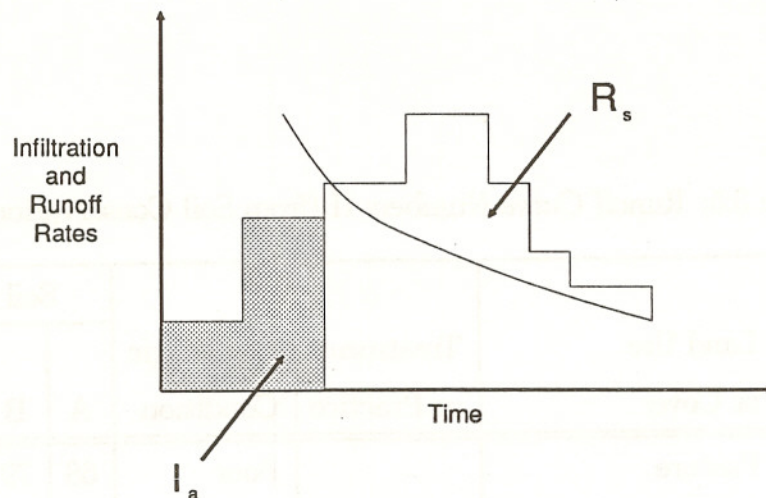


Figure 3.4: Implied behavior of infiltration and runoff by the SCS method (from Bras, 1990)

[13]. Tables (3.4) and (3.5) give the values of CN values for categories of soil-cover complexes [74]. The soils in the SCS method are classified by Viessman et al. [93] as follows:

- A (Low runoff potential) Soils having high infiltration rates even thoroughly wetted and consisting chiefly of deep well to excessively drained sands or gravels. They have a high rate of water transmission.
- B Soils having moderate infiltration rates if thoroughly wetted and consisting chiefly of moderately deep to deep, moderately well to well-drained soils with moderately fine to moderately coarse textures. They have a moderate rate of water transmission.
- C Soils having slow infiltration rates if thoroughly wetted and consisting chiefly of soils with a layer that impedes the downward movement of water, or soils with moderately fine to fine texture. They have a slow rate of water transmission.

- D** (High runoff potential) Soils having very slow infiltration rates if thoroughly wetted and consisting chiefly of clay soils with a high swelling potential, soils with a permanent high water table, soils with a claypan or clay layer at or near the surface, and shallow soils over nearly impervious material. They have a very slow rate of water transmission.

In this model, the precipitations over a 24 hour period are assumed as single storm events.

3.6 Net Infiltration

The net infiltration through the soil surface into the vadose zone is a combination of the aforementioned processes. The rate of the net infiltration, I , can be computed via the conservation of mass as follows:

$$I = P - E_t - R_s \quad (3.19)$$

As mentioned earlier, the evapotranspiration value computed by the method proposed by Thornthwaite [81] corresponds to the potential evapotranspiration. This is the maximum evapotranspiration value that can occur for unlimited water supply. In reality, however, water supply is limited. Therefore, there is a need to adjust the potential evapotranspiration values during dry seasons. In the present study, a water balancing model is adopted to compute the actual evapotranspiration values. The following section addresses this model in detail.

3.6.1 Water Balance Method

The water balance method [62] allows the estimation of the rate of the net infiltration. This method assumes a one-dimensional flow and conservation of mass. In general,

the mass conservation of water through the soil cover where vegetation thrives is written as follows:

$$P + SR + IR = I + R_s \quad (3.20)$$

where P is the precipitation, SR is the input water from the surrounding runoff, IR is the input water from irrigation, I is the infiltration, and R_s is the surface runoff.

The percolation of water through the soil cover is defined as follows:

$$PER = I - E_t^* - dS_T \quad (3.21)$$

where E_t^* is the actual evapotranspiration and dS_T is the change in moisture storage in the soil cover, i.e. root zone.

If the moisture content in the soil cover is kept below the field capacity, leachate will not occur from the precipitation, provided that there is no other source. Figure (3.5) shows the water-holding characteristics of various soils with the U.S. Department of Agriculture (USDA) classification. The shaded area in the figure represents the available water utilized by plants within the root zone. Even though there is no leachate within this zone for the moisture values below field capacity and above wilting point, some of the water will be lost due to the plant transpiration.

Thornthwaite and Mather [82] tabulated the moisture storage values, S_T , within the soil cover after the potential evapotranspiration has occurred. A partial table from this study is given in Table (3.6). The potentially available soil moisture can be computed as follows:

$$PS_T = (\theta_f - \theta_{wilt})d_r \quad (3.22)$$

where

PS_T = Potentially available soil moisture storage [L]

θ_f = Field capacity [L/L]

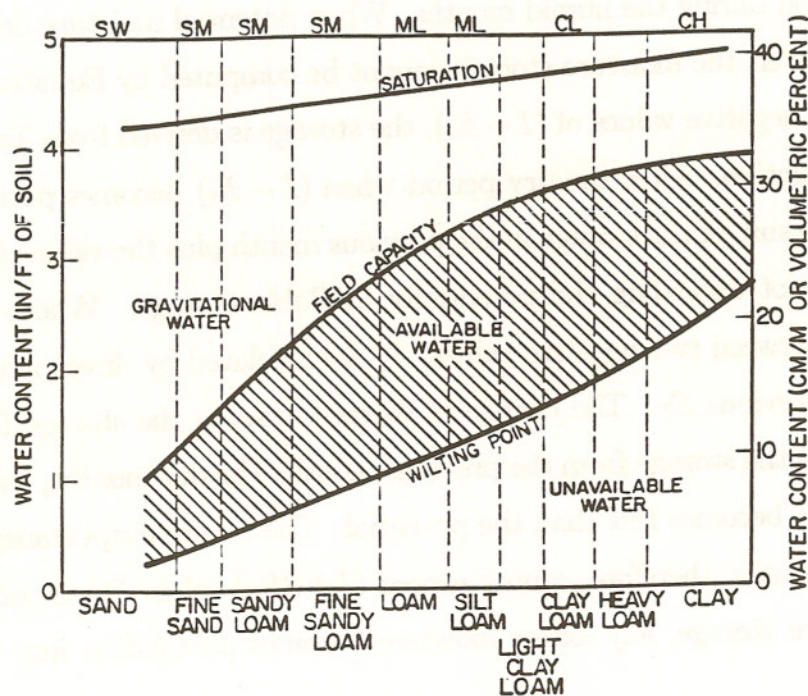


Figure 3.5: Water-holding characteristics of various soils with USDA classification (from Oweis and Khera, 1990)

$$\theta_{wilt} = \text{Wilting point } [L/L]$$

$$d_r = \text{Depth of root zone } [L]$$

When the annual value of $(I - E_t)$ is positive, the area is known as a humid area. For humid areas, the moisture storage in the soil cover is calculated by the equation given above. The actual evapotranspiration is also taken equal to the potential evapotranspiration during the humid months. When potential moisture deficiencies are present, however, the moisture storage cannot be computed by Equation (3.22). For months with negative values of $(I - E_t)$, the storage is derived from Table (3.6) via linear interpolation. After the dry period when $(I - E_t)$ becomes positive, the storage, S_T , is the sum of the storage in the previous month plus the value of $(I - E_t)$ for that month, not exceeding the potentially available storage. Where positive $(I - E_t)$ occurs between two negative values, S_T is calculated by direct addition of $(I - E_t)$ to the previous S_T . The change of storage, dS_T , is the storage from the current month less the storage from the previous month. For dry months, the actual evapotranspiration becomes less than the potential. The actual evapotranspiration values for these months, therefore, cannot exceed $(I + dS_T)$ value. For months with maximum moisture storage, any excess moisture becomes percolation into the soil column.

Table 3.6: Soil moisture retention after potential evapotranspiration has occurred (from Oweis and Khera, 1990)

[illegible]

Chapter 4

Mathematical Model Formulation

This chapter presents the mathematical formulations of the transport processes discussed earlier. First, the model assumptions are outlined, then the governing moisture flow equation is formulated with the appropriate boundary and initial conditions. Finally, the mass transport equation which was derived in Chapter 2 is presented in a similar manner.

4.1 Assumptions

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

1. Soil is 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. There is no loss or gain due to system sinks or sources other than those specifically discussed in previous chapters;

5. Hysteretic behavior in the moisture retention properties is not considered;
6. Hysteretic behavior of the adsorption/desorption processes is neglected;
7. The groundwater table does not fluctuate substantially in comparison with the thickness of the unsaturated zone;
8. The groundwater table is assumed to be free of any contamination at the onset of simulation;
9. The air is at the atmospheric pressure and stationary within the soil;
10. Interactions between various chemical constituents and competitive effects are not considered;
11. Biotransformation takes place in the liquid phase only;
12. Oxygen is not a limiting factor for biological growth within the vadose zone;
13. Partitioning of the contaminant mass from one phase to another is assumed to be linear;
14. In the computation of the surface runoff, the cumulative 24-hour rainfall is assumed as a single storm event.

4.2 Moisture Flow

The mathematical model formulation is based on the transport mechanisms and the fate processes described in Chapter 2. Equation (2.1) is solved to provide estimates of volumetric moisture contents and fluxes in one dimension which is taken vertically downward from the soil surface. The governing equation is written in the following form:

$$\frac{\partial \theta_w}{\partial t} + \frac{\partial K(\theta_w)}{\partial z} - \frac{\partial}{\partial z} \left[D(\theta_w) \frac{\partial \theta_w}{\partial z} \right] = 0 \quad (4.1)$$

where

$$\theta_w = \text{Volumetric moisture content } [L^3/L^3]$$

$$t = \text{Time coordinate } [T]$$

$$z = \text{Space coordinate taken positive downward } [L]$$

$$K(\theta_w) = \text{Hydraulic conductivity } [L/T]$$

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

The moisture flux equation is given as:

$$q_w = K(\theta_w) - D(\theta_w) \frac{\partial \theta_w}{\partial z} \quad (4.2)$$

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

4.2.1 Initial Condition

$$\theta_w(z) = \theta_{w_i}(z) \quad @ \quad t = 0 \quad (4.3)$$

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

4.2.2 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 [52].

1. Flux boundary condition during infiltration events:

$$I = K(\theta_w) - D(\theta_w) \frac{\partial \theta_w}{\partial z} \quad (4.4)$$

and

$$\frac{\partial \theta_w}{\partial z} \leq 0 \quad @ \quad z = 0 \quad \text{for } 0 \leq t \leq t_p \quad (4.5)$$

$$I = P - R_s - E_t^* \quad (\text{net infiltration rate}) \quad [L/T]$$

$$P = \text{Precipitation rate} \quad [L/T]$$

$$E_t^* = \text{Actual evapotranspiration rate from the surface} \quad [L/T]$$

$$R_s = \text{Surface runoff rate} \quad [L/T]$$

$$t_p = \text{Time required for the surface to become saturated} \quad [T]$$

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:

$$\theta_w = \theta_s \quad (4.6)$$

and

$$\frac{\partial \theta_w}{\partial z} = 0 \quad @ \quad z = 0 \quad \text{for } t_p < t \leq t_e \quad (4.7)$$

where

$$K_s = \text{Saturated hydraulic conductivity} \quad [L/T]$$

$$\theta_s = \text{Saturated moisture content} \quad [L^3/L^3]$$

$$t_e = \text{Time when net precipitation becomes less than } K_s \quad [T]$$

b) If $I < K_s$, the flux boundary condition described in Equation (4.4) 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:

$$K(\theta_w) - D(\theta_w) \frac{\partial \theta_w}{\partial z} = -E_t^* \quad @ \quad z = 0 \quad \text{for } t'_e \leq t \leq t_n \quad (4.8)$$

where

t'_e = Time of moisture flux cessation at the surface [T]

t_n = Time to initiation of a new moisture flux event or
time required to reach the air - 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:

$$\theta_w = \theta_{ad} \quad (4.9)$$

and

$$\frac{\partial \theta_w}{\partial z} = 0 \quad @ \quad z = 0 \quad \text{for } t_n < t \leq t_c \quad (4.10)$$

where

θ_{ad} = Air - dry moisture content [L^3/L^3]

t_c = 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 mentioned earlier in Chapter 3.

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.

$$\frac{\partial \theta_w}{\partial z} = 0 \quad @ \quad z = z_L \quad for \quad t > 0 \quad (4.11)$$

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.

$$\theta_w = \theta_s \quad @ \quad z = z_L \quad for \quad t > 0 \quad (4.12)$$

4.3 Contaminant Transport

The equilibrium advection-dispersion equation for the transport of contaminants in partially saturated soils was derived in Chapter 2 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 . Based on the

relationships presented in Section 2.2, the governing mass transport equation is written as:

$$\frac{\partial(\theta_w C_L)}{\partial t} + K_d \rho_b \frac{\partial C_L}{\partial t} + k' \rho_b C_L + \frac{1}{H} \frac{\partial(\theta_a C_L)}{\partial t} + \frac{\partial(q_w C_L)}{\partial z} = \frac{\partial}{\partial z} \left[\left(\theta_w E + \frac{D_a}{H} \right) \frac{\partial C_L}{\partial z} \right] - \theta_w R \quad (4.13)$$

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 $[M/L^3T]$

If Monod kinetics are assumed, the R term in Equation (4.13) is substituted by the R_s of Equation (2.38). In this case, however, a mass balance equation for the microorganisms must be written as follows [26]:

$$\frac{\partial(\theta_w X)}{\partial t} + \frac{\partial(q_w X)}{\partial z} = \frac{\partial}{\partial z} \left[\theta_w \epsilon_w \frac{\partial X}{\partial z} \right] + \frac{\mu_m X C_L \theta_w}{K_m + C_L} - k_e X \theta_w \quad (4.14)$$

where

X = Microorganism concentration $[M/L^3]$

ϵ_w = Mechanical dispersion coefficient [L^2/T]

μ_m = Microorganism's maximum specific growth rate [$1/T$]

K_m = Substrate concentration at $1/2$ of μ_m [M/L^3]

k_e = Endogenous decay coefficient of microorganisms [$1/T$]

This equation assumes that the microorganism transport is controlled by advection and mechanical dispersion. The dispersive term is neglected in the equation given above since it is assumed that advection dominates the transport of microorganisms [26].

Equations (4.13) and (4.14) 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, however, the microbial concentration becomes constant with respect to time. Therefore, Equation (4.13) is decoupled by using Equations (2.41) or (2.42) for substrate limiting conditions. For nonbiodegradable transport, Equation (4.13) is solved without the R term.

Equation (4.13) is similar to that reported by Baehr [9].

4.3.1 Initial Condition

The initial condition is implemented in the form:

$$C_L(z, 0) = C_{Li} \quad @ \quad t = 0 \quad (4.15)$$

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

4.3.2 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:

$$\frac{\partial C_L(0, t)}{\partial z} = 0 \quad @ \quad z = 0 \quad (4.16)$$

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:

$$\frac{\partial C_L}{\partial z} = \text{constant} \quad (4.17)$$

therefore

$$\frac{\partial^2 C_L}{\partial z^2} = 0 \quad @ \quad z = z_L \quad \text{for } t > 0 \quad (4.18)$$

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.

Chapter 5

Method of Solution

This chapter outlines the solution methods used in the present study for the moisture and the mass transport equations. The governing equations are discretized by using central differences. Resulting discretized equations are presented in the following sections.

5.1 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 (5.1) represents the (z, t) plane with the space coordinates for $i = 1, 2, \dots, n$, and the time coordinates for $k = 1, 2, \dots, m$. The grid is considered to be fixed, and is represented by Δz and Δt for space and time increments, respectively.

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

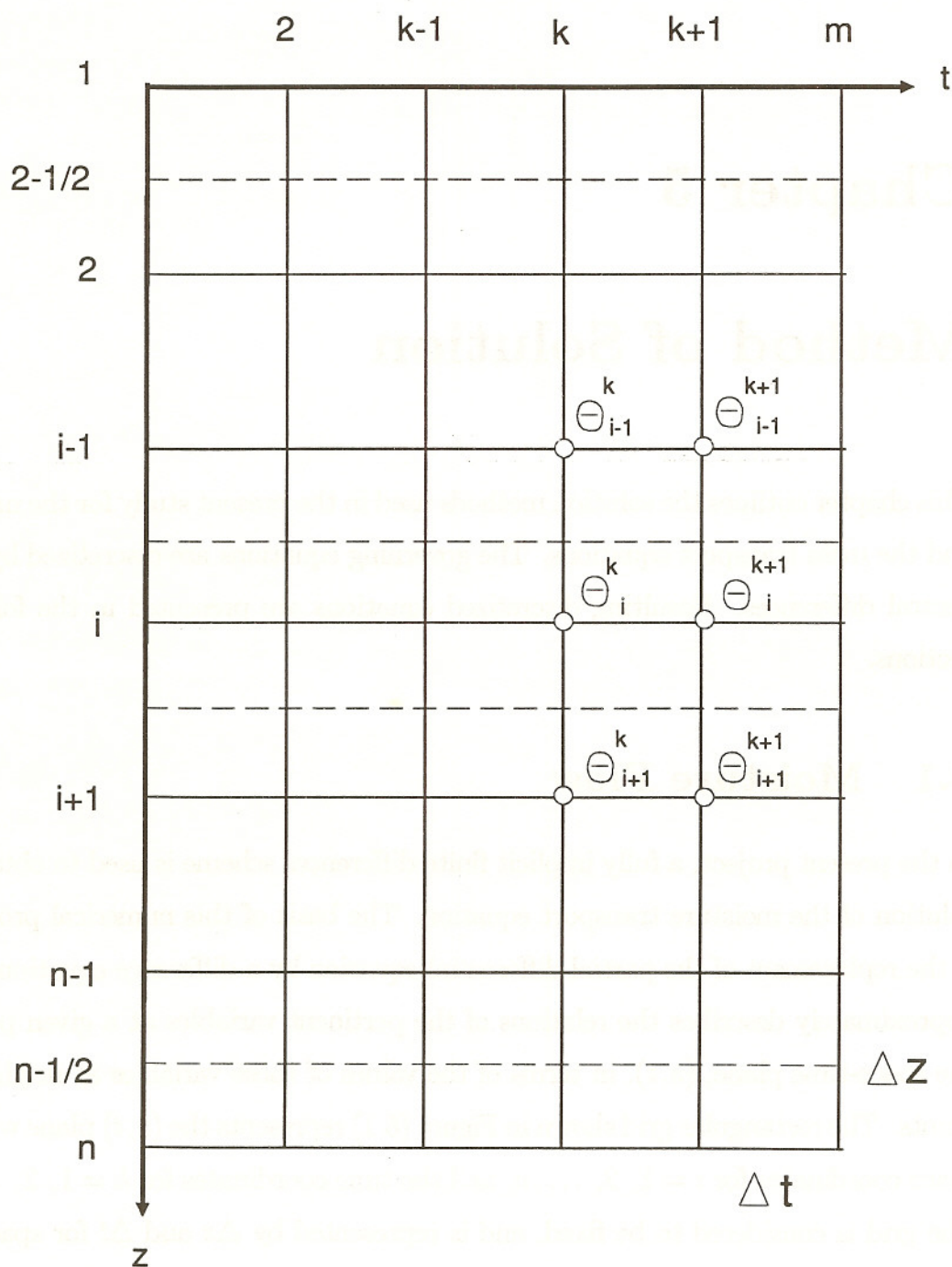


Figure 5.1: Time-space discretization for fully implicit finite differences

$$\frac{\partial \theta_w}{\partial t} + \frac{\partial K(\theta_w)}{\partial z} - \frac{\partial}{\partial z} \left[D(\theta_w) \frac{\partial \theta_w}{\partial z} \right] = 0 \quad (5.1)$$

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

$$\begin{aligned} \left[-\frac{1}{\Delta z} D_{i-1/2}^{k+1} \right] \theta_{i-1}^{k+1} + \left[\frac{1}{\Delta z} D_{i+1/2}^{k+1} + \frac{1}{\Delta z} D_{i-1/2}^{k+1} + \frac{\Delta z}{\Delta t} \right] \theta_i^{k+1} + \\ \left[-\frac{1}{\Delta z} D_{i+1/2}^{k+1} \right] \theta_{i+1}^{k+1} = \frac{\Delta z}{\Delta t} \theta_i^k - K_{i+1/2}^{k+1} + K_{i-1/2}^{k+1} \end{aligned} \quad (5.2)$$

The terms D and K appearing in Equation (5.2) need to be evaluated at the interfaces $i-1/2$ and $i+1/2$ of the i^{th} layer. This is accomplished by taking harmonic means through the interfaces of neighboring layers. Namely:

$$K_{i-1/2}^{k+1} = \frac{K_{i-1}^{k+1} D_i^{k+1} + K_i^{k+1} D_{i-1}^{k+1}}{D_{i-1}^{k+1} + D_i^{k+1}} \quad (5.3)$$

$$D_{i-1/2}^{k+1} = 2 \frac{D_{i-1}^{k+1} D_i^{k+1}}{D_{i-1}^{k+1} + D_i^{k+1}} \quad (5.4)$$

and

$$K_{i+1/2}^{k+1} = \frac{K_i^{k+1} D_{i+1}^{k+1} + K_{i+1}^{k+1} D_i^{k+1}}{D_i^{k+1} + D_{i+1}^{k+1}} \quad (5.5)$$

$$D_{i+1/2}^{k+1} = 2 \frac{D_i^{k+1} D_{i+1}^{k+1}}{D_i^{k+1} + D_{i+1}^{k+1}} \quad (5.6)$$

5.1.1 Boundary Conditions

The discretized equations given above are for the intermediate layers, i.e. $i = 2, \dots, n-1$. 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:

$$\left[\frac{1}{\Delta z} D_{1+1/2}^{k+1} + \frac{\Delta z}{2\Delta t} \right] \theta_1^{k+1} + \left[-\frac{1}{\Delta z} D_{1+1/2}^{k+1} \right] \theta_2^{k+1} = \frac{\Delta z}{2\Delta t} \theta_1^k - K_{1+1/2}^{k+1} + I^{k+1} \quad (5.7)$$

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:

$$\left[\frac{\Delta z}{\Delta t} + \frac{1}{\Delta z} D_{2+1/2}^{k+1} \right] \theta_2^{k+1} + \left[-\frac{1}{\Delta z} D_{2+1/2}^{k+1} \right] \theta_3^{k+1} = \frac{\Delta z}{\Delta t} \theta_2^k - K_{2+1/2}^{k+1} + K_p^{k+1} \quad (5.8)$$

where

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

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

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:

$$\left[\frac{1}{\Delta z} D_{1+1/2}^{k+1} + \frac{\Delta z}{2\Delta t} \right] \theta_1^{k+1} + \left[-\frac{1}{\Delta z} D_{1+1/2}^{k+1} \right] \theta_2^{k+1} = \frac{\Delta z}{2\Delta t} \theta_1^k - K_{1+1/2}^{k+1} - E_t^{k+1} \quad (5.9)$$

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,

$$\left(D \frac{\Delta \theta}{\Delta z} \right)_n^{k+1} = 0 \quad @ \quad z = z_L \quad (5.10)$$

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

$$\left[-\frac{1}{\Delta z} D_{n-1/2}^{k+1} \right] \theta_{n-1}^{k+1} + \left[\frac{1}{\Delta z} D_{n-1/2}^{k+1} + \frac{\Delta z}{2\Delta t} \right] \theta_n^{k+1} = \frac{\Delta z}{2\Delta t} \theta_n^k - K_n^{k+1} + K_{n-1/2}^{k+1} \quad (5.11)$$

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.

5.1.2 Solution of Finite Difference Equations

Equation (5.2) 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:

$$A\vec{\theta} = \vec{B} \quad (5.12)$$

where

A = Coefficient matrix of the system

$\vec{\theta}$ = Moisture vector

$\vec{B}$ = Column vector

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 (5.12) becomes:

$$\begin{bmatrix} d_1 & c_1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ a_2 & d_2 & c_2 & 0 & \cdots & 0 & 0 & 0 \\ 0 & a_3 & d_3 & c_3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & a_{n-1} & d_{n-1} & c_{n-1} \\ 0 & 0 & 0 & 0 & \cdots & 0 & a_n & d_n \end{bmatrix} \begin{Bmatrix} \theta_1^{k+1} \\ \theta_2^{k+1} \\ \theta_3^{k+1} \\ \vdots \\ \theta_{n-1}^{k+1} \\ \theta_n^{k+1} \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_{n-1} \\ b_n \end{Bmatrix} \quad (5.13)$$

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

The second row of the coefficient matrix, $\mathbf{A}$, can be written of the form:

$$d'_2 \theta_2^{k+1} + c_2 \theta_3^{k+1} = b'_2 \quad (5.14)$$

where

$$d'_2 = d_2 - \frac{a_2}{d_1} c_1 \quad (5.15)$$

$$b'_2 = b_2 - \frac{a_2}{d_1} b_1 \quad (5.16)$$

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

$$d'_{n-1} \theta_{n-1}^{k+1} + c_{n-1} \theta_n^{k+1} = b'_{n-1} \quad (5.17)$$

where

$$d'_{n-1} = d_{n-1} - \frac{a_{n-1}}{d'_{n-2}} c_{n-2} \quad (5.18)$$

$$b'_{n-1} = b_{n-1} - \frac{a_{n-1}}{d'_{n-2}} b'_{n-2} \quad (5.19)$$

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

$$\theta_l^{k+1} = \frac{b'_l - c_l \theta_{l+1}^{k+1}}{d'_l} \quad (5.20)$$

where

$$b'_l = b_l - \frac{a_l}{d'_{l-1}} b'_{l-1} \quad (5.21)$$

$$d'_l = d_l - \frac{a_l}{d'_{l-1}} c_{l-1} \quad (5.22)$$

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

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

$$\theta_n^{k+1} = \frac{b'_n}{d'_n} \quad (5.23)$$

5.1.3 Moisture Flux Computation

Once the volumetric moisture contents are computed, the moisture flux for the i^{th} layer is obtained as follows [52]:

$$q_i^{k+1} = K_i^{k+1} - D_i^{k+1} \left(\frac{\Delta \theta}{\Delta z} \right)_i^{k+1} \quad (5.24)$$

Korfiatis [52] 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 (5.2).

The moisture flux can then be written as a function of depth, z , of the form:

$$\begin{aligned} q_i^{k+1} = K_i^{k+1} - D_i^{k+1} \left\{ 2 \left[\frac{\theta_{i-1}^{k+1}}{(z_{i-1} - z_i)(z_{i-1} - z_{i+1})} + \right. \right. \\ \left. \frac{\theta_i^{k+1}}{(z_i - z_{i-1})(z_i - z_{i+1})} + \frac{\theta_{i+1}^{k+1}}{(z_{i+1} - z_{i-1})(z_{i+1} - z_i)} \right] z_i + \\ \frac{\theta_{i-1}^{k+1}}{z_{i-1} - z_i} + \frac{\theta_i^{k+1}}{z_i - z_{i-1}} - \left[\frac{\theta_{i-1}^{k+1}}{(z_{i-1} - z_i)(z_{i-1} - z_{i+1})} + \right. \\ \left. \frac{\theta_i^{k+1}}{(z_i - z_{i-1})(z_i - z_{i+1})} + \frac{\theta_{i+1}^{k+1}}{(z_{i+1} - z_{i-1})(z_{i+1} - z_i)} \right] (z_i + z_{i-1}) \left. \right\} \quad (5.25) \end{aligned}$$

5.2 Contaminant Transport

The governing contaminant transport equation in terms of the liquid phase concentrations was derived in Chapter 2 as the following:

$$\frac{\partial(\theta_w C_L)}{\partial t} + K_d \rho_b \frac{\partial C_L}{\partial t} + k' \rho_b C_L + \frac{1}{H} \frac{\partial(\theta_a C_L)}{\partial t} + \frac{\partial(q_w C_L)}{\partial z} =$$

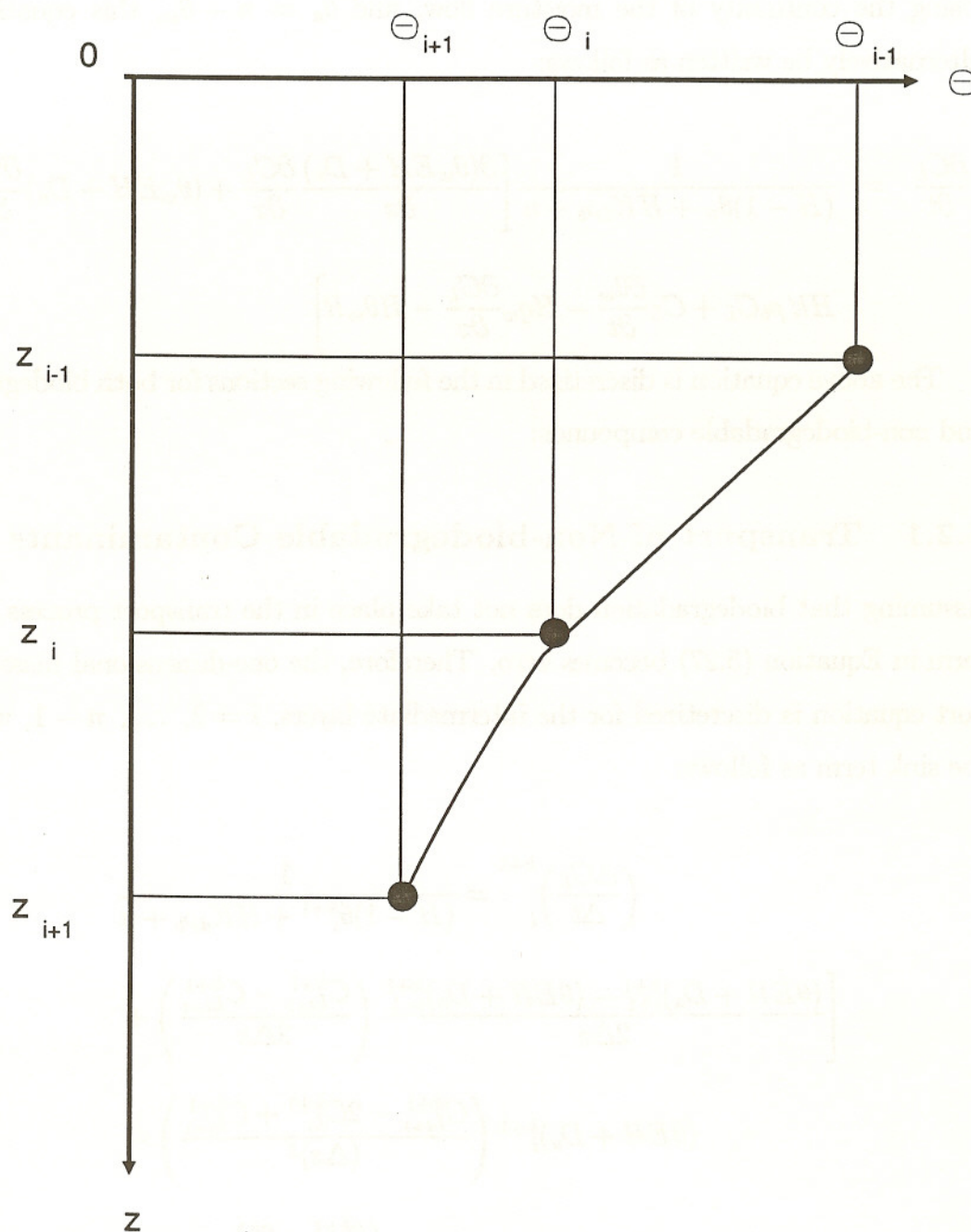


Figure 5.2: Three-point moisture profile for the computation of moisture flux (from Korfiatis, 1984)

$$\frac{\partial}{\partial z} \left[\left(\theta_w E + \frac{D_a}{H} \right) \frac{\partial C_L}{\partial z} \right] - \theta_w R \quad (5.26)$$

Using the continuity of the moisture flow, and $\theta_a = n - \theta_w$, this equation can alternatively be written as follows:

$$\begin{aligned} \frac{\partial C_L}{\partial t} = & \frac{1}{(H-1)\theta_w + HK_d\rho_b + n} \left[\frac{\partial(\theta_w EH + D_a)}{\partial z} \frac{\partial C_L}{\partial z} + (\theta_w EH + D_a) \frac{\partial^2 C_L}{\partial z^2} - \right. \\ & \left. HK'\rho_b C_L + C_L \frac{\partial \theta_w}{\partial t} - Hq_w \frac{\partial C_L}{\partial z} - H\theta_w R \right] \end{aligned} \quad (5.27)$$

The above equation is discretized in the following sections for both biodegradable and non-biodegradable compounds:

5.2.1 Transport of Non-biodegradable Contaminants

Assuming that biodegradation does not take place in the transport process, the R term in Equation (5.27) becomes zero. Therefore, the one-dimensional mass transport equation is discretized for the intermediate layers, $i = 2, \dots, n-1$, without the sink term as follows:

$$\begin{aligned} \left(\frac{\Delta C_L}{\Delta t} \right)_i^{k+1} = & \frac{1}{(H-1)\theta_i^{k+1} + HK_d\rho_b + n} \\ & \left[\frac{(\theta EH + D_a)_{i+1}^{k+1} - (\theta EH + D_a)_{i-1}^{k+1}}{2\Delta z} \left(\frac{C_{Li+1}^{k+1} - C_{Li-1}^{k+1}}{2\Delta z} \right) + \right. \\ & (\theta EH + D_a)_i^{k+1} \left(\frac{C_{Li+1}^{k+1} - 2C_{Li}^{k+1} + C_{Li-1}^{k+1}}{(\Delta z)^2} \right) - \\ & \left. HK'\rho_b C_{Li}^{k+1} + \left(\frac{\theta_i^{k+1} - \theta_i^k}{\Delta t} \right) C_{Li}^{k+1} - \right] \end{aligned}$$

$$Hq_i^{k+1} \left(\frac{C_{L_{i+1}}^{k+1} - C_{L_{i-1}}^{k+1}}{2\Delta z} \right) \quad (5.28)$$

Boundary Conditions

1. Top Boundary Condition

Equation (5.27) is discretized for the first layer using the boundary condition

$\frac{\partial C_L}{\partial z} = 0$ @ $z = 0$ as follows:

$$\left(\frac{\Delta C_L}{\Delta t} \right)_1^{k+1} = \frac{1}{(H-1)\theta_1^{k+1} + HK_d\rho_b + n} \left[-Hk'\rho_b C_{L_1}^{k+1} + \left(\frac{\theta_1^{k+1} - \theta_1^k}{\Delta t} \right) \left(\frac{C_{L_1}^{k+1} + C_{L_2}^{k+1}}{2} \right) \right] \quad (5.29)$$

The concentration C_{L_1} at the top boundary was described as an average concentration of the first two layers. This approximation was adopted to circumvent a numerical difficulty arisen when attempted to describe the uppermost layer. However, this approximation is consistent with the numerical scheme used for discretization, namely, the central differences. When the second top boundary condition ($C_L = 0$) is used, there is no need to discretize the equation since $\frac{\partial C_L}{\partial t}$ becomes zero.

2. Bottom Boundary Condition

Similarly, the mass transport equation for the n^{th} layer is discretized for the boundary condition $\frac{\partial C_L}{\partial z} = f$ @ $z = z_L$ in the following manner:

$$\left(\frac{\Delta C_L}{\Delta t} \right)_n^{k+1} = \frac{1}{(H-1)\theta_n^{k+1} + HK_d\rho_b + n}$$

$$\left[\frac{(\theta EH + D_a)_{n-1}^{k+1} - (\theta EH + D_a)_n^{k+1}}{\Delta z} \left(\frac{C_{L_n}^{k+1} - C_{L_{n-1}}^{k+1}}{\Delta z} \right) - \right. \\ \left. Hk' \rho_b C_{L_n}^{k+1} + \left(\frac{\theta_n^{k+1} - \theta_n^k}{\Delta t} \right) C_{L_n}^{k+1} - Hq_n^{k+1} \left(\frac{C_{L_n}^{k+1} - C_{L_{n-1}}^{k+1}}{\Delta z} \right) \right] \quad (5.30)$$

5.2.2 Transport of Biodegradable Contaminants

Monod Kinetics

If Monod kinetics are assumed, Equations (4.13) and (4.14) should be solved simultaneously. The R term in Equation (4.13) will be replaced by the R_s term given in Equation (2.38). Hence, the discretized form of the mass transport equation becomes:

$$\left(\frac{\Delta C_L}{\Delta t} \right)_i^{k+1} = \frac{1}{(H-1)\theta_i^{k+1} + HK_d \rho_b + n} \\ \left[\frac{(\theta EH + D_a)_{i+1}^{k+1} - (\theta EH + D_a)_{i-1}^{k+1}}{2\Delta z} \left(\frac{C_{L_{i+1}}^{k+1} - C_{L_{i-1}}^{k+1}}{2\Delta z} \right) + \right. \\ \left. (\theta EH + D_a)_i^{k+1} \left(\frac{C_{L_{i+1}}^{k+1} - 2C_{L_i}^{k+1} + C_{L_{i-1}}^{k+1}}{(\Delta z)^2} \right) - Hk' \rho_b C_{L_i}^{k+1} + \right. \\ \left. \left(\frac{\theta_i^{k+1} - \theta_i^k}{\Delta t} \right) C_{L_i}^{k+1} - Hq_i^{k+1} \left(\frac{C_{L_{i+1}}^{k+1} - C_{L_{i-1}}^{k+1}}{2\Delta z} \right) - \right. \\ \left. \frac{Hk\theta_i^{k+1} X_i^{k+1} C_{L_i}^{k+1}}{K_m + C_{L_i}^{k+1}} \right] \quad (5.31)$$

Similarly, the microbial growth equation (Equation 4.14), neglecting dispersion, is discretized as follows:

$$\left(\frac{\Delta X}{\Delta t}\right)_i^{k+1} = -\frac{q_i^{k+1}}{\theta_i^{k+1}} \left(\frac{X_{i+1}^{k+1} - X_{i-1}^{k+1}}{2\Delta z}\right) + \frac{\mu_m X_i^{k+1} C_{L_i}^{k+1}}{K_m + C_{L_i}^{k+1}} - k_e X_i^{k+1} \quad (5.32)$$

for $i = 2, 3, \dots, n-1$

and for the bottom layer:

$$\left(\frac{\Delta X}{\Delta t}\right)_n^{k+1} = -\frac{q_n^{k+1}}{\theta_n^{k+1}} \left(\frac{X_n^{k+1} - X_{n-1}^{k+1}}{\Delta z}\right) + \frac{\mu_m X_n^{k+1} C_{L_n}^{k+1}}{K_m + C_{L_n}^{k+1}} - k_e X_n^{k+1} \quad (5.33)$$

Substrate Limiting Conditions

At high substrate concentrations, R_s becomes a constant, therefore the discretization will take the following form:

$$\begin{aligned} \left(\frac{\Delta C_L}{\Delta t}\right)_i^{k+1} &= \frac{1}{(H-1)\theta_i^{k+1} + HK_d\rho_b + n} \\ &\left[\frac{(\theta EH + D_a)_{i+1}^{k+1} - (\theta EH + D_a)_{i-1}^{k+1}}{2\Delta z} \left(\frac{C_{L_{i+1}}^{k+1} - C_{L_{i-1}}^{k+1}}{2\Delta z}\right) + \right. \\ &(\theta EH + D_a)_i^{k+1} \left(\frac{C_{L_{i+1}}^{k+1} - 2C_{L_i}^{k+1} + C_{L_{i-1}}^{k+1}}{(\Delta z)^2}\right) - Hk'\rho_b C_{L_i}^{k+1} + \\ &\left. \left(\frac{\theta_i^{k+1} - \theta_i^k}{\Delta t}\right) C_{L_i}^{k+1} - Hq_i^{k+1} \left(\frac{C_{L_{i+1}}^{k+1} - C_{L_{i-1}}^{k+1}}{2\Delta z}\right) - Hk_0\theta_i^{k+1} \right] \end{aligned} \quad (5.34)$$

At low substrate concentrations, R_s becomes a first order expression:

$$\left(\frac{\Delta C_L}{\Delta t}\right)_i^{k+1} = \frac{1}{(H-1)\theta_i^{k+1} + HK_d\rho_b + n}$$

$$\begin{aligned}
& \left[\frac{(\theta EH + D_a)_{i+1}^{k+1} - (\theta EH + D_a)_{i-1}^{k+1}}{2\Delta z} \left(\frac{C_{L_{i+1}}^{k+1} - C_{L_{i-1}}^{k+1}}{2\Delta z} \right) + \right. \\
& (\theta EH + D_a)_i^{k+1} \left(\frac{C_{L_{i+1}}^{k+1} - 2C_{L_i}^{k+1} + C_{L_{i-1}}^{k+1}}{(\Delta z)^2} \right) - Hk' \rho_b C_{L_i}^{k+1} + \\
& \left. \left(\frac{\theta_i^{k+1} - \theta_i^k}{\Delta t} \right) C_{L_i}^{k+1} - Hq_i^{k+1} \left(\frac{C_{L_{i+1}}^{k+1} - C_{L_{i-1}}^{k+1}}{2\Delta z} \right) - Hk_1 \theta_i^{k+1} C_{L_i}^{k+1} \right] \quad (5.35)
\end{aligned}$$

Boundary Conditions

1. Top Boundary Condition

Similarly, for the top boundary condition, $\frac{\partial C_L}{\partial z} = 0$ @ $z = 0$, the governing equation becomes:

$$\begin{aligned}
& \left(\frac{\Delta C_L}{\Delta t} \right)_1^{k+1} = \frac{1}{(H-1)\theta_1^{k+1} + HK_d \rho_b + n} \\
& \left[-Hk' \rho_b C_{L_1}^{k+1} + \left(\frac{\theta_1^{k+1} - \theta_1^k}{\Delta t} \right) \left(\frac{C_{L_1}^{k+1} + C_{L_2}^{k+1}}{2} \right) - H\theta_1^{k+1} R_m^{k+1} \right] \quad (5.36)
\end{aligned}$$

where R_m^{k+1} is equal to the R_s of Equation (2.38) when Monod kinetics are used, or, alternatively, is equal to Equations (2.41) or (2.42) if substrate limiting conditions are considered.

2. Bottom Boundary Condition

For the n^{th} layer, the governing equation becomes:

$$\left(\frac{\Delta C_L}{\Delta t} \right)_n^{k+1} = \frac{1}{(H-1)\theta_n^{k+1} + HK_d \rho_b + n}$$

$$\begin{aligned}
& \left[\frac{(\theta EH + D_a)_n^{k+1} - (\theta EH + D_a)_{n-1}^{k+1}}{\Delta z} \left(\frac{C_{L_n}^{k+1} - C_{L_{n-1}}^{k+1}}{\Delta z} \right) - \right. \\
& \quad Hk' \rho_b C_{L_n}^{k+1} + \left(\frac{\theta_n^{k+1} - \theta_n^k}{\Delta t} \right) C_{L_n}^{k+1} - \\
& \quad \left. Hq_n^{k+1} \left(\frac{C_{L_n}^{k+1} - C_{L_{n-1}}^{k+1}}{\Delta z} \right) - H\theta_n^{k+1} R_m^{k+1} \right] \quad (5.37)
\end{aligned}$$

The discretized equations given in the previous sections form a set of ordinary differential equations. If the Monod kinetics option is selected, for n lines, $2n$ equations are generated. For limiting conditions, only n set of equations are to be solved. The solution method is described in the next section.

5.2.3 Hamming's Modified Predictor-Corrector Method

The discretized equations given above are solved by Hamming's modified predictor-corrector method similar to the scheme presented by Demetracopoulos et al. [26]. This method is also called the method of lines. This section outlines the procedure used in the present study [26, 15]:

Introducing new variables y_j for $j = 1, 2, \dots, q$ with $q = 2n$, and $x = t$ such that:

$$y_j = \begin{cases} C_{L_j} & \text{for } j = 1, 2, \dots, (q/2) \\ X_{j-q/2} & \text{for } j = (q/2 + 1), \dots, q \end{cases} \quad (5.38)$$

Equations of $\frac{\partial C_L}{\partial t}$ and $\frac{\partial X}{\partial t}$ can now be written in the general form:

$$\frac{dy_j}{dx} = f_j(x, y_1, y_2, \dots, y_q) \quad \text{for } j = 1, 2, \dots, q \quad (5.39)$$

Let $y_{j,i}$ be the final modification of the estimated solution for the j^{th} dependent variable, y_j , at x_i , and let $f_{j,i}$ be the estimate of f_j at x_i , i.e.

$$y_{j,i} = y_j(x_i) \quad (5.40)$$

$$f_{j,i} = f_j(x_i, y_{1,i}, y_{2,i}, \dots, y_{n,i}) \quad (5.41)$$

The Hamming's method is used for the solution Equation (5.39). Starting values for $y_{j,i}, y_{j,i-1}, y_{j,i-2}, y_{j,i-3}, f_{j,i}, f_{j,i-1}, f_{j,i-2}$ must be known. Initial conditions of the governing equations will supply the values of $y_{j,i}$. The fourth order Runge-Kutta method [15] is used to estimate the values of $y_{j,i-1}, y_{j,i-2}, y_{j,i-3}$. The derivatives $f_{j,i}, f_{j,i-1}, f_{j,i-2}$ are computed from Equation (5.39).

In terms of the new nomenclature, the procedure is outlined as follows:

1. The predicted solutions $y_{j,i+1,0}$, where the third index indicates the number of iterations, are computed for $j = 1, 2, \dots, q$ using:

$$y_{j,i+1,0} = y_{j,i-3} + \frac{4}{3}h(2f_{j,i} - f_{j,i-1} + 2f_{j,i-2}) \quad (5.42)$$

where h is the increment of the independent variable x , namely, Δt .

2. The predicted solutions are modified by local truncation errors, $e_{j,i}$, as follows:

$$y_{j,i+1,0}^* = y_{j,i+1,0} + \frac{112}{9}e_{j,i} \quad (5.43)$$

where

$$e_{j,i} = \frac{9}{121}(y_{j,i,1} - y_{j,i,0}) \quad (5.44)$$

3. The j^{th} corrector equation is applied for each dependent variable as follows:

$$y_{j,i+1,1} = \frac{1}{8} [9y_{j,i} - y_{j,i-2} + 3h(f_{j,i+1,0}^* + 2f_{j,i} - f_{j,i-1})] \quad (5.45)$$

where

$$f_{j,i+1,0}^* = f_j(x_{i+1}, y_{1,i+1,0}^*, y_{2,i+1,0}^*, \dots, y_{q,i+1,0}^*) \quad (5.46)$$

4. The local truncation error, $e_{j,i+1}$, is estimated by the following:

$$e_{j,i+1} = \frac{9}{121}(y_{j,i+1,1} - y_{j,i+1,0}) \quad (5.47)$$

5. The final value of $y_{j,i+1}$ is then computed from:

$$y_{j,i+1} = y_{j,i+1,1} - e_{j,i+1} \quad (5.48)$$

6. The derivatives, $f_{j,i+1}$, are then computed from Equation (5.39) as follows:

$$f_{j,i+1} = f_j(x_{i+1}, y_{1,i+1}, y_{2,i+1}, \dots, y_{n,i+1}) \quad (5.49)$$

This process is repeated for the next increment of the independent variable. In the outlined procedure above, the corrector equations are applied just once for each variable. However, in the present study, they are applied more than once for more accurate results. A detailed discussion of the procedure and an algorithm can be found in Carnahan et al. [15].

Chapter 6

Sensitivity Analysis

The sensitivity of the model output has been examined by varying key input parameters. Although most of the key input parameters have been examined, the user will still be required to perform several runs to ensure adequate understanding of the model operation and the sensitivity to a variety of input variables and boundary conditions. This is necessary due to the complexity of the model, the high degree of nonlinearities of the equations involved, and the variety of the options provided in the model.

The following section addresses the sensitivity runs performed for homogeneous soils. The last section in this chapter entails the verification of the numerical solution of the mass transport equation with an analytical solution that is derived for steady-state flow conditions.

6.1 Sensitivity Runs

The sensitivity runs have been performed by simulating the hypothetical scenario shown in Figure (6.1). This scenario involves a 30 feet thick unsaturated soil layer with the upper and lower 10 feet free of contamination, and the middle 10 feet

Table 6.1: 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_{wi}	0.15	0.20	0.30	0.35
CN	72	82	87	89
θ_{wilt}	0.02	0.07	0.10	0.15

contaminated by a single chemical constituent.

Simulations have been performed for four different soils and three different chemical compounds. The soils were chosen in the range of sand to silty clay. The hydrologic properties of these soils are shown in Table (6.1) as given by Clapp and Hornberger [19].

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

- Initial total concentration $C_T = 1 \text{ mg/kg}$
- Time discretization increment $\Delta t = 1 \text{ day}$
- Space discretization increment $\Delta z = 1 \text{ ft}$

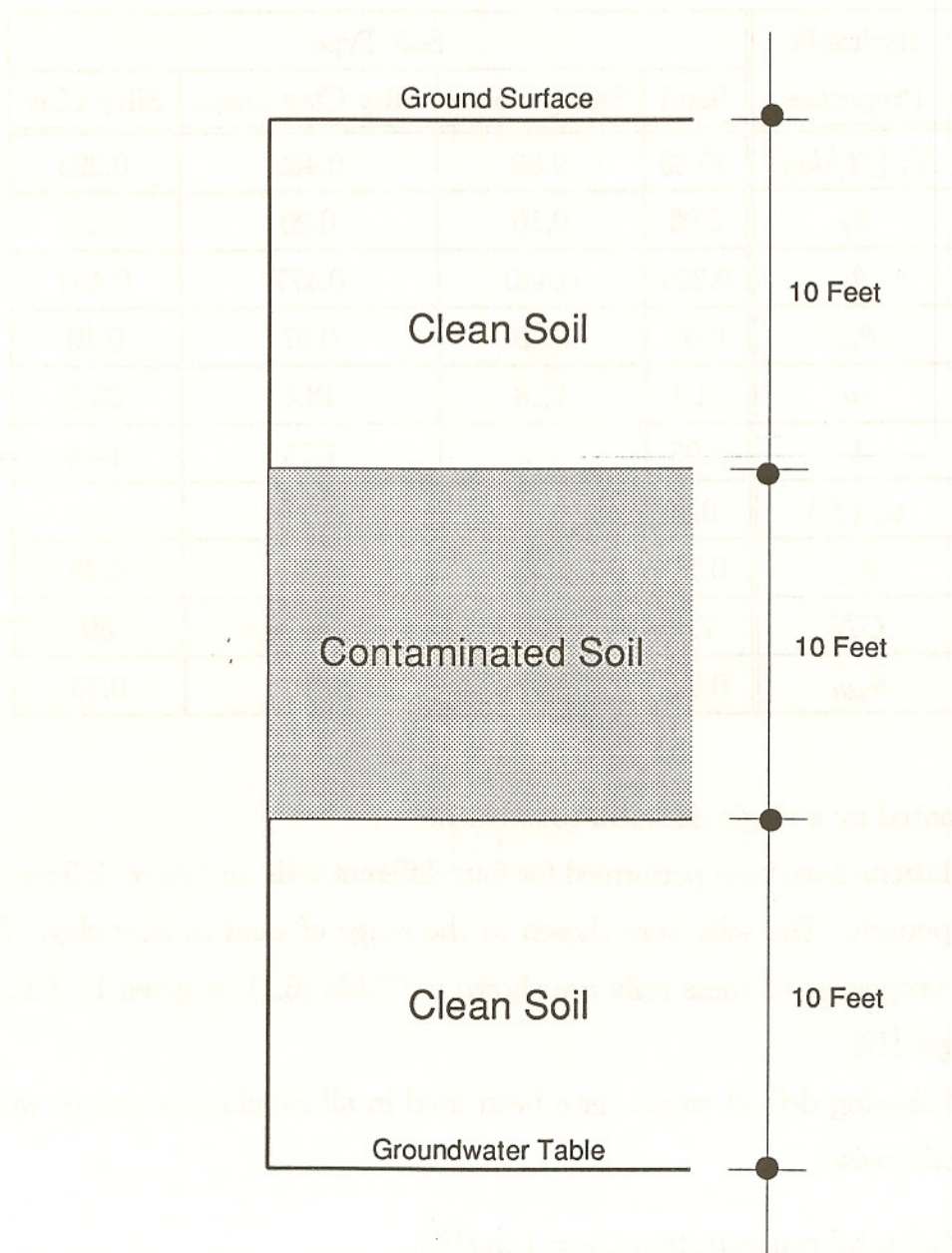


Figure 6.1: Contamination scenario used in sensitivity analysis

Table 6.2: 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

- Soil bulk density $\rho_b = 1.65 \text{ gr/cm}^3$
- Dispersivity $\alpha = 0.2 \text{ ft}$
- Root zone depth $d_r = 3 \text{ ft}$
- 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 (6.2).

Effect of Space and Time Discretization Increments Δz and Δt

The effect of the space and time discretization steps was examined for a sand layer contaminated with benzene. The simulations were performed for 2,000 days. Figure (6.2) is a plot of the moisture flux versus time for space increments ranging from 1 foot to 5 feet. It has been observed that the size of the space discretization increment has very little effect on the predicted moisture flux at the groundwater table. Close examination of the moisture profiles has also revealed that this effect

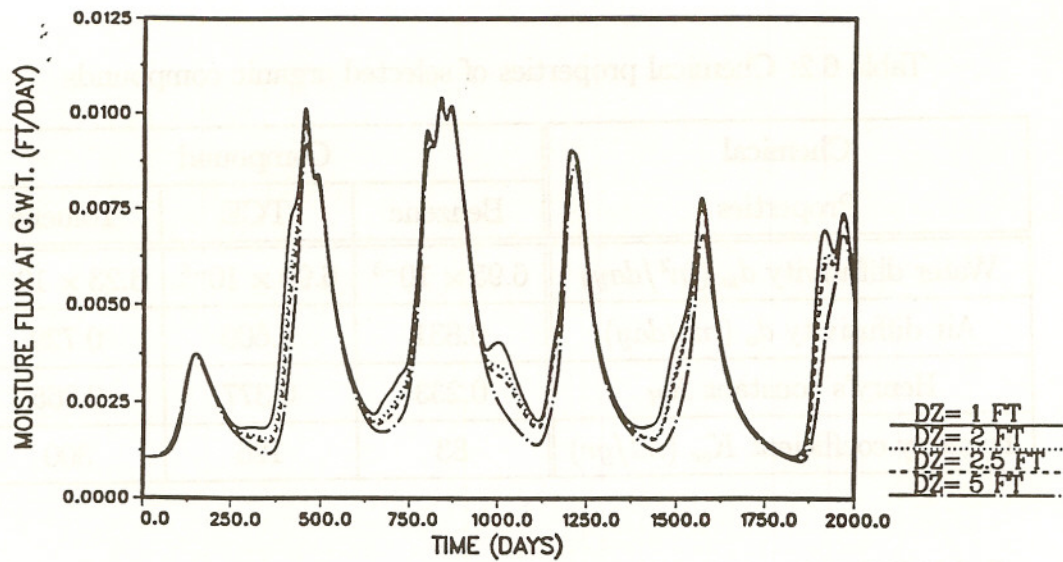


Figure 6.2: Effect of Δz on moisture fluxes at g.w.t. for sand

is negligible. When the liquid concentration predictions are compared, however, the effect of Δz is substantial as shown in Figure (6.3). This indicates that the solution of the mass transport equation is sensitive to the size of Δz . It is recommended that the smallest possible value of Δz be used to obtain more accurate results. Although this recommendation may be used as a rule of thumb, the choice of Δz is dependent and limited by the size of Δt .

Figures (6.4) and (6.5) indicate that the effect of the time increment on both moisture fluxes and liquid phase concentrations at the groundwater table is negligible. These runs were performed for sand contaminated with benzene, using a $\Delta z=5$ feet.

It is well known that the finite difference solution of the equations in this model is stable for an optimum value of the ratio $\Delta t/\Delta z$. This value is not known *a priori* and must be determined by sensitivity analysis for each simulation scenario. The ratio $\Delta t/\Delta z$ is known as a type of Courant number, which must have a value $\Delta t/\Delta z < r$ where r is an appropriate value for stable solutions. This condition is known as the

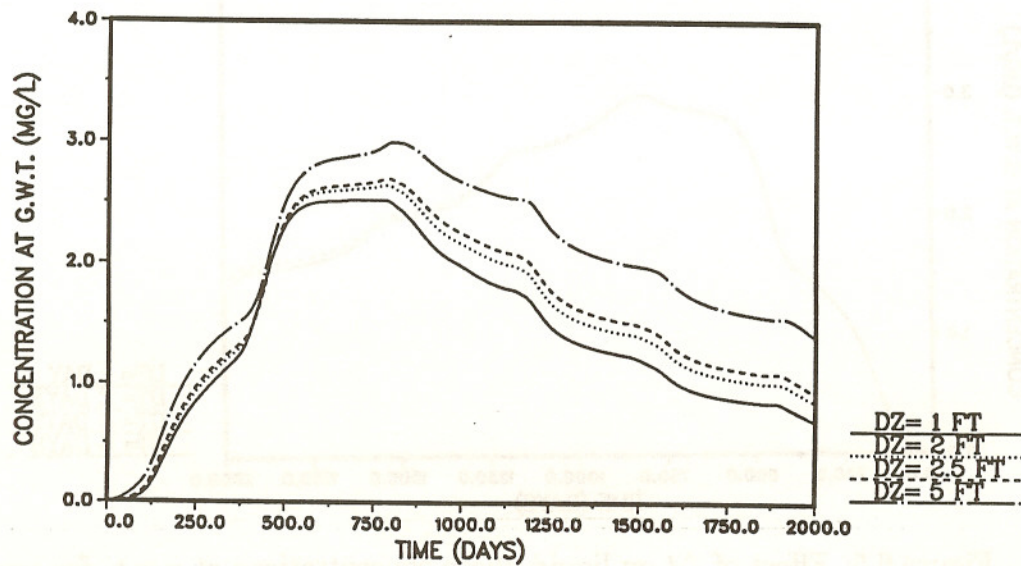


Figure 6.3: Effect of Δz on liquid phase concentrations at g.w.t. for sand

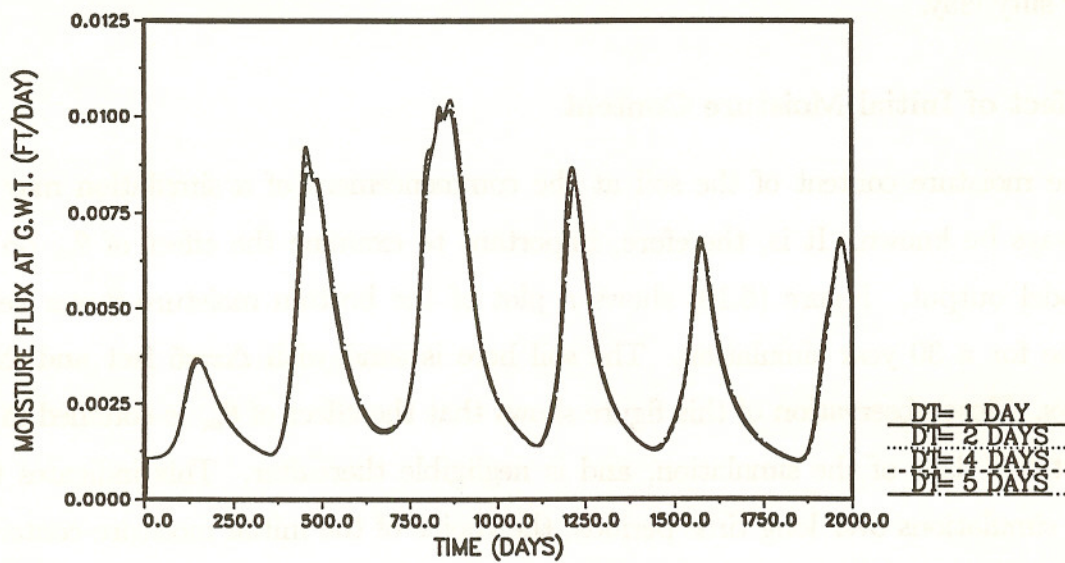


Figure 6.4: Effect of Δt on moisture fluxes at g.w.t. for sand

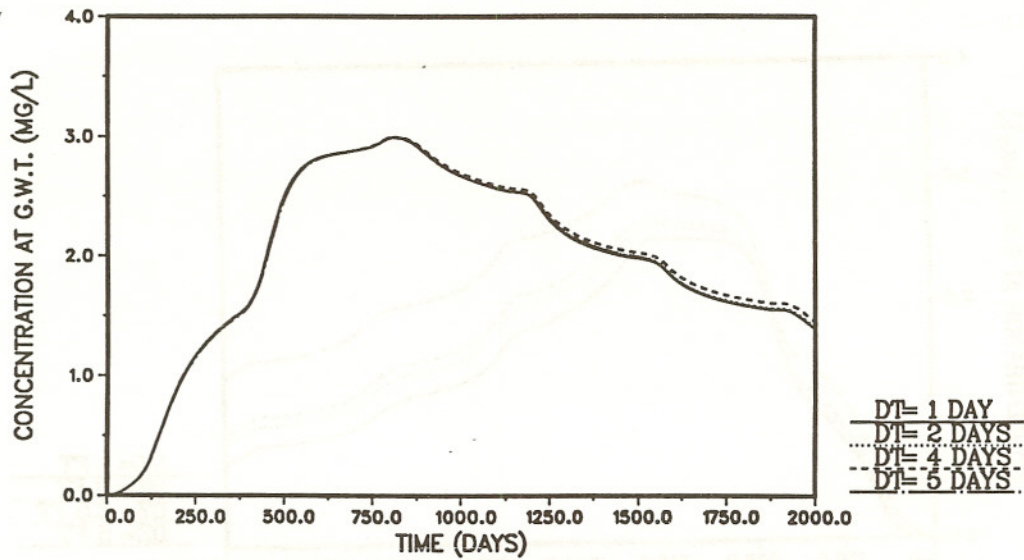


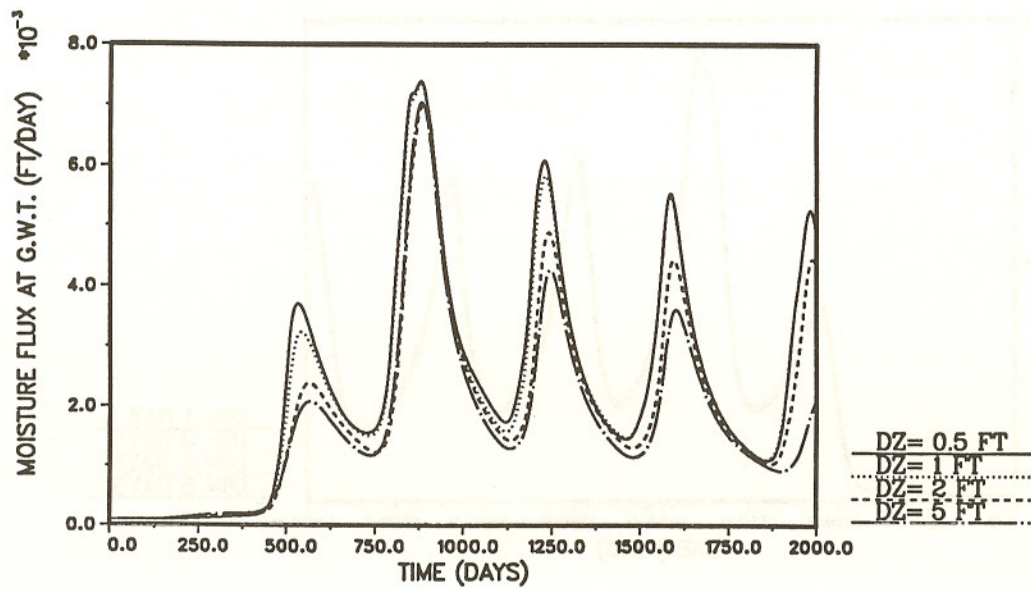
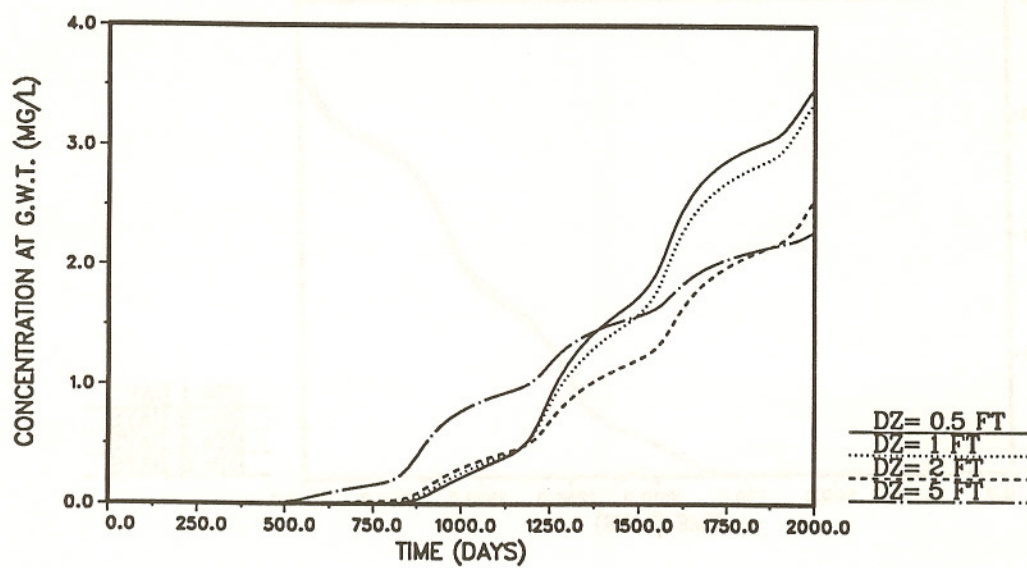
Figure 6.5: Effect of Δt on liquid phase concentrations at g.w.t. for sand

Courant-Friedrichs-Lewy (CFL) condition [1].

Figures (6.6) and (6.7) show the effect of Δz for a silty clay layer contaminated with benzene. Figures (6.8) and (6.9) show the similar observation of the Δt effect for silty clay.

Effect of Initial Moisture Content

The moisture content of the soil at the commencement of a simulation may not always be known. It is, therefore, important to examine the effect of θ_{wi} on the model output. Figure (6.10) shows a plot of the bottom moisture fluxes versus time for a 30 year simulation. The soil here is sand with $\Delta z = 5$ feet and $\Delta t = 5$ days. Close observation of this figure shows that the effect of θ_{wi} is confined in the first 500 days of the simulation, and is negligible thereafter. This indicates that for simulations over long time periods, the choice of the initial moisture content is not important. Instabilities in the solution of the moisture transport equation may occur if the chosen θ_{wi} value is close to the saturated moisture content or to the

Figure 6.6: Effect of Δz on moisture fluxes at g.w.t. for silty clayFigure 6.7: Effect of Δz on liquid phase concentrations at g.w.t. for silty clay

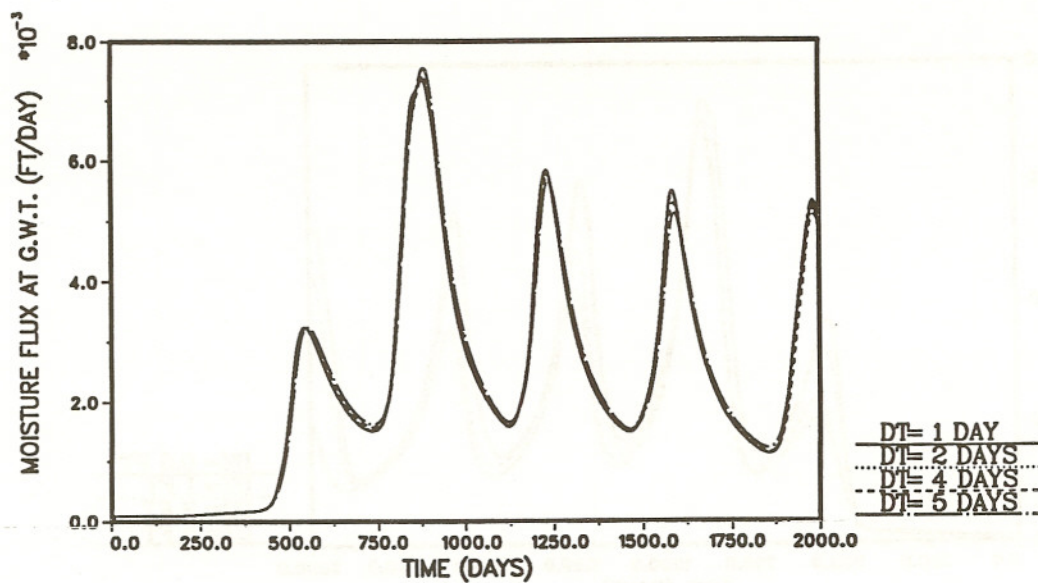


Figure 6.8: Effect of Δt on moisture fluxes at g.w.t. for silty clay

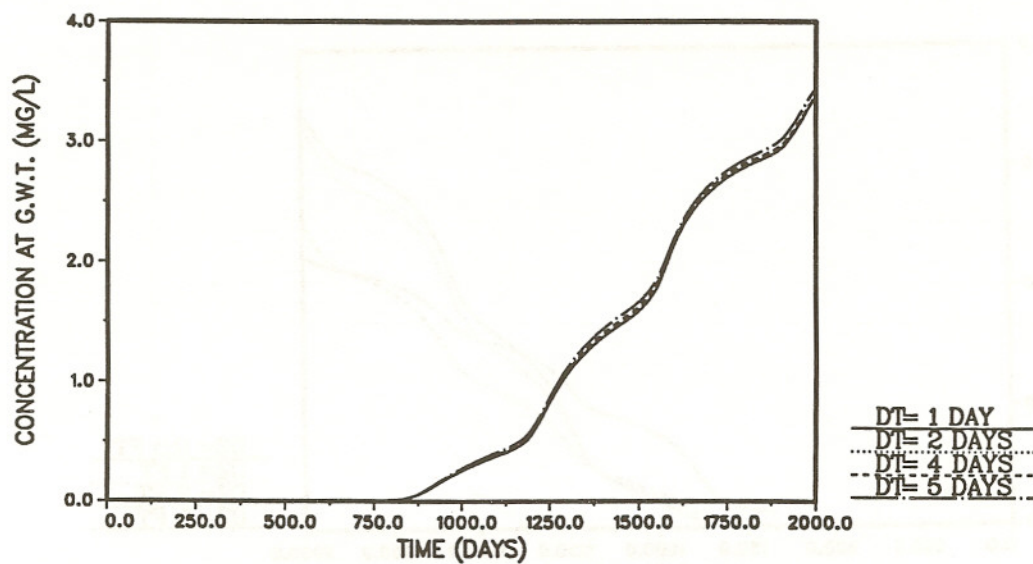


Figure 6.9: Effect of Δt on liquid phase concentrations at g.w.t. for silty clay

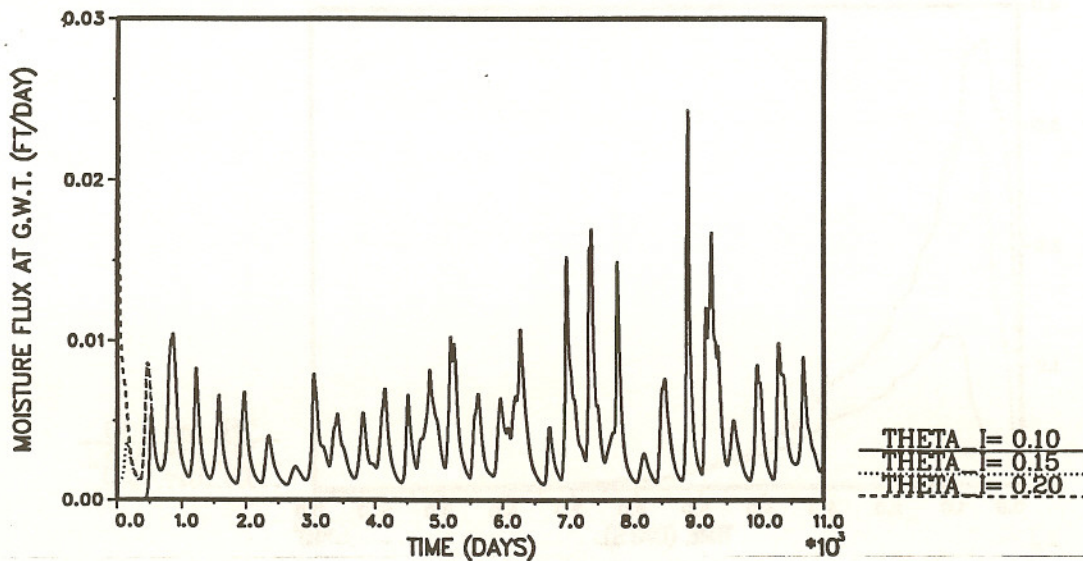


Figure 6.10: Effect of θ_{wi} on moisture fluxes at g.w.t. for sand

air-dry moisture content due to the sharp moisture gradients that are formed in the soil surface. Attention must also be given to the fact that the choice of initial moisture content will influence the liquid phase concentration for a given initial total concentration. This becomes clear when observing Equation (2.17) which shows that the total and the liquid phase concentrations are related via the moisture content of the soil. Figure (6.11) is a good example of the liquid phase partitioning due to the variations in the initial moisture content.

Comparison of Thornthwaite's and Penman's Methods

The mean monthly evapotranspiration value can be computed by the model via the two methods proposed by Thornthwaite and Penman, respectively. A 30 feet thick sand layer contaminated with benzene has been analyzed using both theories. Actual mean monthly temperatures were used for both simulations. Table (6.3) tabulates the relevant data used in the Penman's equation. It should be noted that most of this data are not readily available, therefore, they are estimated for the particular

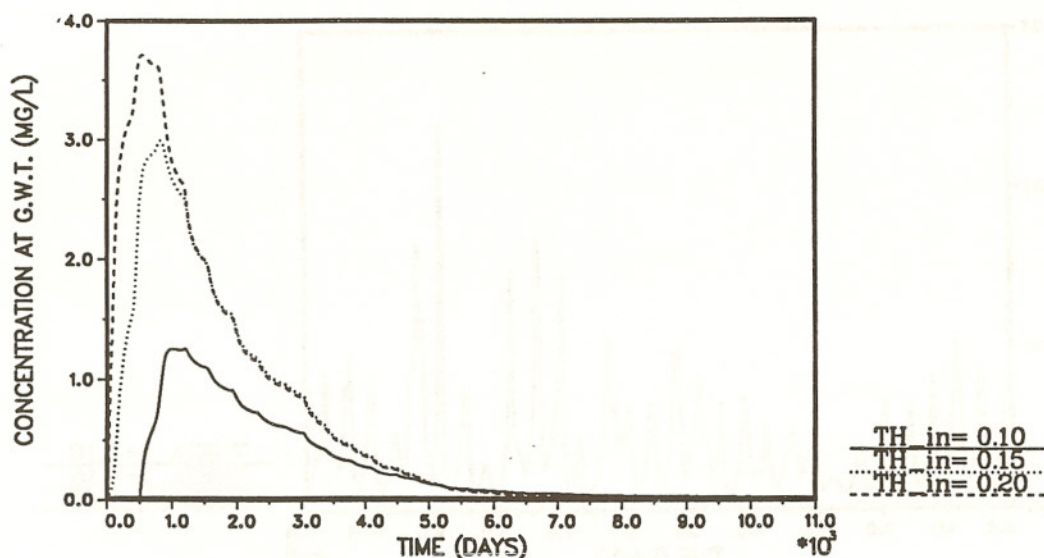


Figure 6.11: Effect of θ_{wi} on liquid phase concentrations at g.w.t. for sand

simulation presented herein. The simulations were performed with $\Delta z = 2$ feet and $\Delta t = 5$ days for a total of 10,000 days. Figure (6.12) shows the moisture fluxes at the groundwater table computed using both methods. A small difference in the magnitude of the fluxes is observed in the simulations. However, this cannot result in any significant conclusion since some of the data used in the Penman's equation were arbitrarily chosen. Figure (6.13) shows the liquid phase benzene concentration history at the groundwater table.

Effect of Bottom Boundary Condition of the Flow Equation

The model is equipped to handle two types of boundary conditions at the groundwater table for the solution of the moisture flow. First, the moisture content at the bottom of the domain is set to remain at the saturated moisture content for all time steps. When this happens, the moisture content distribution throughout the unsaturated zone becomes highly curvilinear, thus, increasing the instabilities of the model. A silty clay loam layer contaminated with benzene has been investigated

Table 6.3: Climatic data used in Penman's method

Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Mean Monthly Solar Radiation ($mm H_2O$)											
2.5	3.7	5.7	7.3	8.2	8.8	8.1	7.1	6.1	4.6	3.1	2.3
Mean Monthly Dew-point Temperature ($^{\circ}F$)											
18.1	16.4	27.1	37.7	50.3	66.9	71.1	67.6	51.2	34.2	23.5	17.2
Mean Monthly Wind Speed (mph)											
8.0	11.0	9.0	8.0	7.0	5.0	5.0	8.0	7.0	11.0	9.0	11.0
Mean Monthly Sunshine (%)											
60	64	71	74	77	80	81	73	69	63	59	62
Mean Monthly Leaf Area Index											
0	0.5	1.1	2.0	2.3	2.5	3.0	3.0	2.8	2.3	1.8	0.5

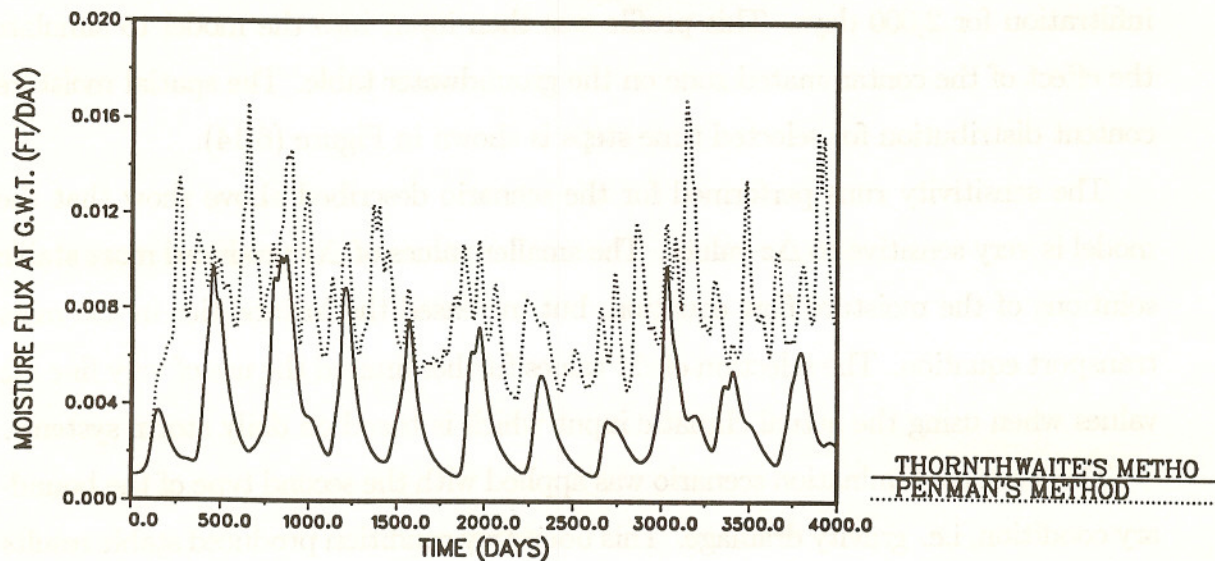


Figure 6.12: Effect of evapotranspiration computation method on moisture fluxes at g.w.t. for sand

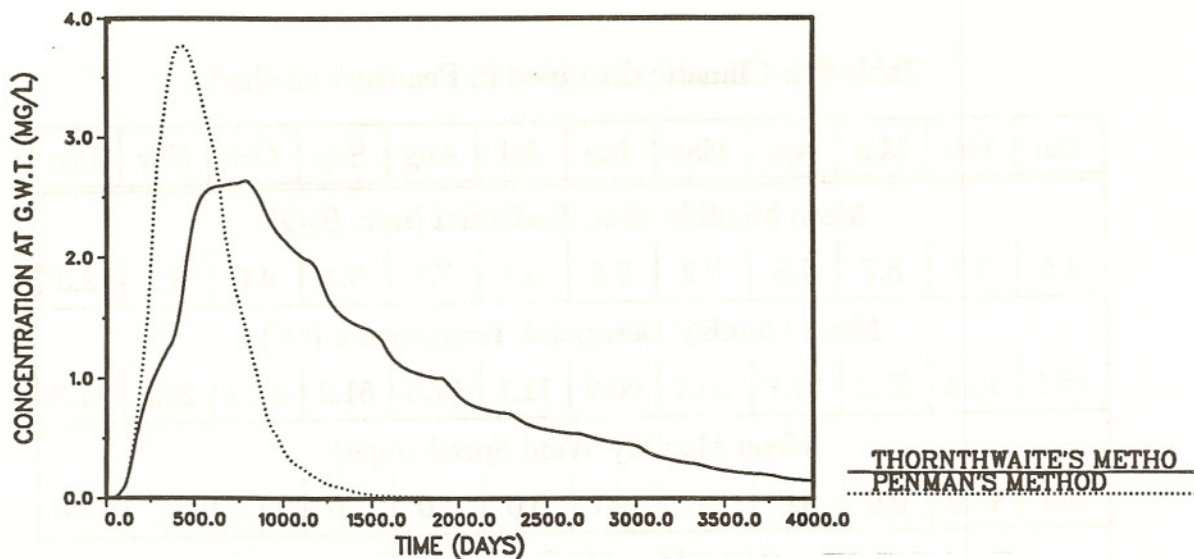


Figure 6.13: Effect of evapotranspiration computation method on liquid phase concentrations at g.w.t. for sand

with $\Delta t = 2$ days for 10,000 days. The initial moisture content profile, which represents the dry condition of the soil, was obtained by running the model without any infiltration for 2,000 days. This profile was then input into the model to simulate the effect of the contaminated zone on the groundwater table. The spatial moisture content distribution for selected time steps is shown in Figure (6.14).

The sensitivity runs performed for the scenario described above show that the model is very sensitive to Δz values. The smaller values of Δz produced more stable solutions of the moisture flow equation, but increased the instabilities in the mass transport equation. The selection of Δt values further limited the use of very fine Δz values when using the actual climatic input which is based on daily storm systems.

The same contamination scenario was applied with the second type of the boundary condition, i.e. gravity drainage. This boundary condition produced stable results in the solution of the moisture flow equation with comparatively greater values of Δz . Figure (6.15) shows the typical moisture distribution through the unsaturated

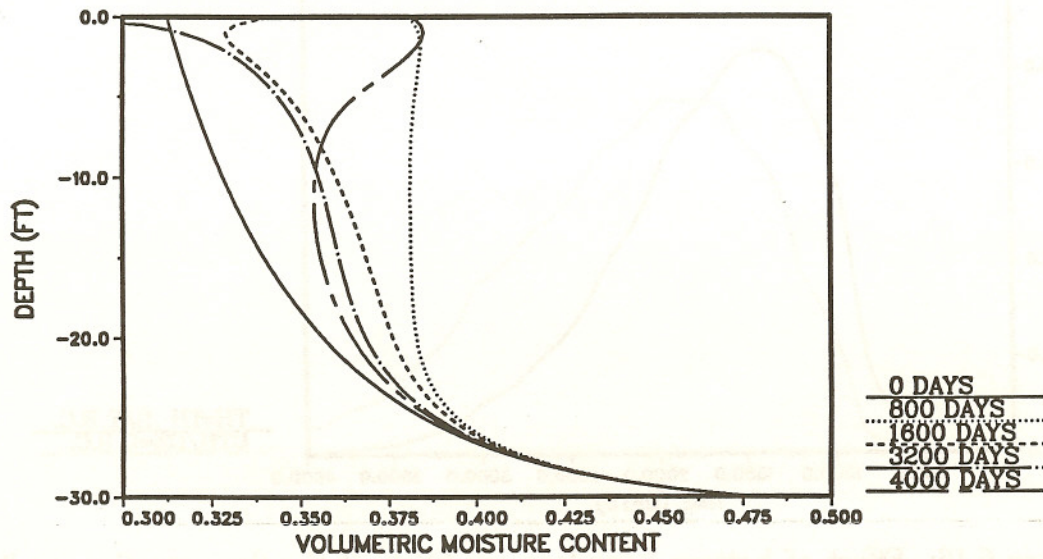


Figure 6.14: Moisture content distribution in the unsaturated zone with $\theta = \theta_{sat}$ boundary condition for silty clay loam

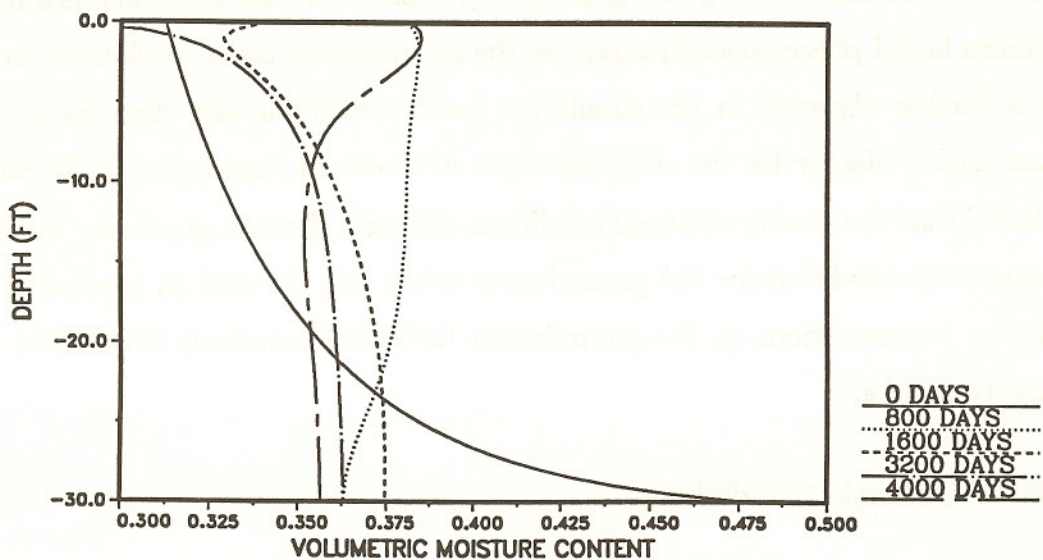


Figure 6.15: Moisture content distribution in the unsaturated zone with $\partial\theta/\partial z = 0$ boundary condition for silty clay loam

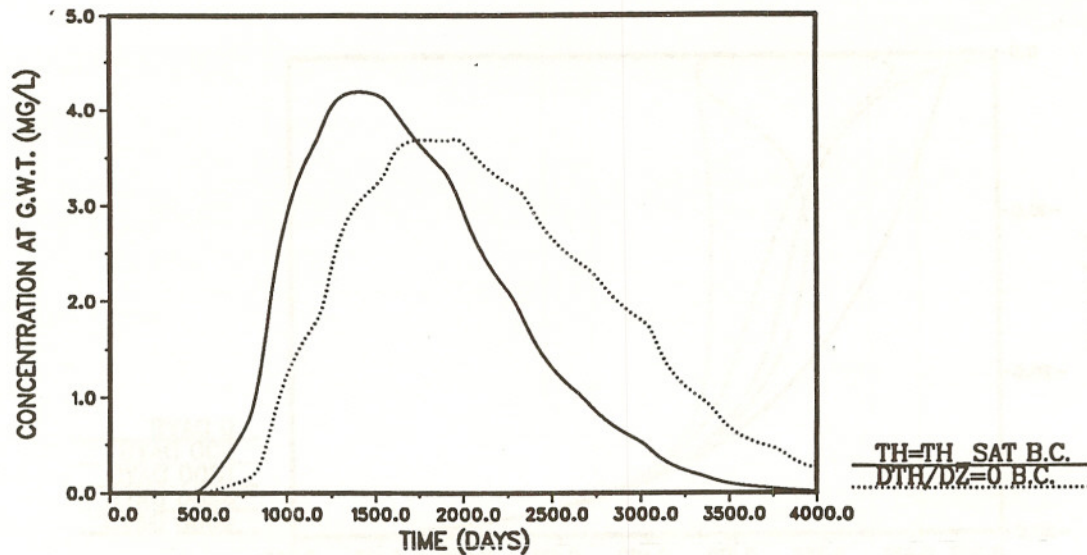


Figure 6.16: Effect of bottom boundary condition of the flow equation on liquid phase concentrations at g.w.t. for silty clay loam

zone for selected time steps. A close observation of the contamination history on the groundwater table, as shown in Figure (6.16), represents that the difference in the maximum liquid phase concentrations on the groundwater table is relatively small. This is further observed in the simulation performed for a silty clay layer. The contamination history for the silty clay layer is shown in Figure (6.17). It can be concluded that the gravity drainage condition, although it is not physically the most representative condition for the groundwater table, can be used in predicting the maximum concentrations on the groundwater table with relatively little effort and instability problems.

Effect of Climatic Conditions

The model output has been examined for different types of climatic input. First, the actual rainfall and temperature data was applied to a sandy soil contaminated with benzene. The simulation was performed for 10,000 days with spatial and time

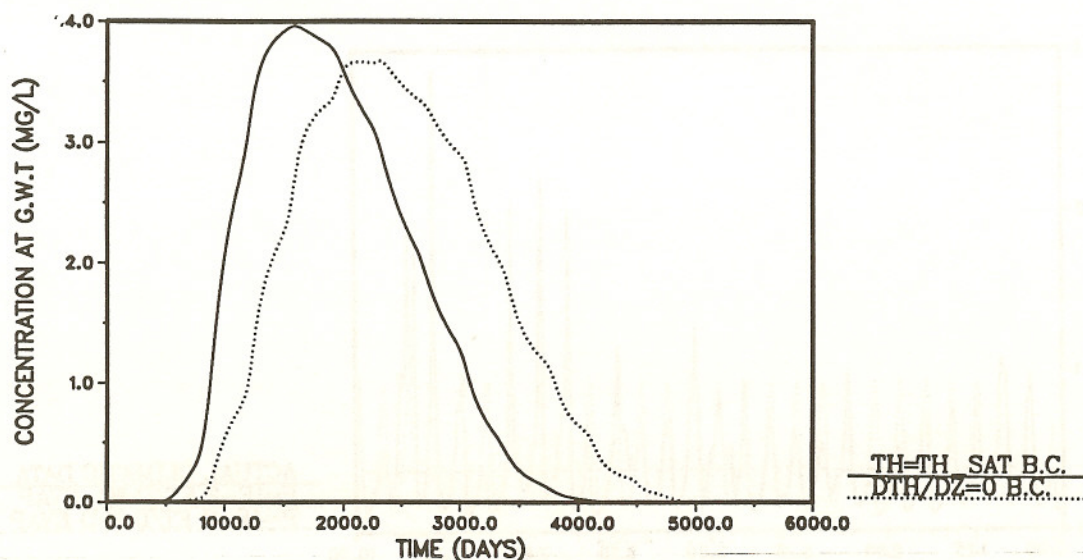


Figure 6.17: Effect of bottom boundary condition of the flow equation on liquid phase concentrations at g.w.t. for silty clay

increments of 2 feet and 5 days, respectively. The moisture fluxes at the groundwater table due to the actual climatic input is shown with a solid line in Figure (6.18). Then, the annual average rainfall for the last 30 years was applied to the same soil as a constant input with actual evapotranspiration values that were computed by the Thornthwaite's method. The dotted line in Figure (6.18) denotes the results of this simulation. Lastly, a constant value of the net infiltration, which was computed on a monthly basis by the water balance method incorporated in the model, was applied to the soil without computing the evapotranspiration values for each time step. The moisture fluxes at the groundwater table due to this constant infiltration value is denoted by the dashed line in Figure (6.18). The annual average rainfall was determined to be 3.6 feet, leading to a daily rainfall value of approximately 0.01 feet. The average annual net infiltration for sand was computed by the model as 1.41 feet, resulting the daily rainfall of approximately 0.004 feet.

Figure (6.19) illustrates the liquid phase benzene concentrations at the ground-

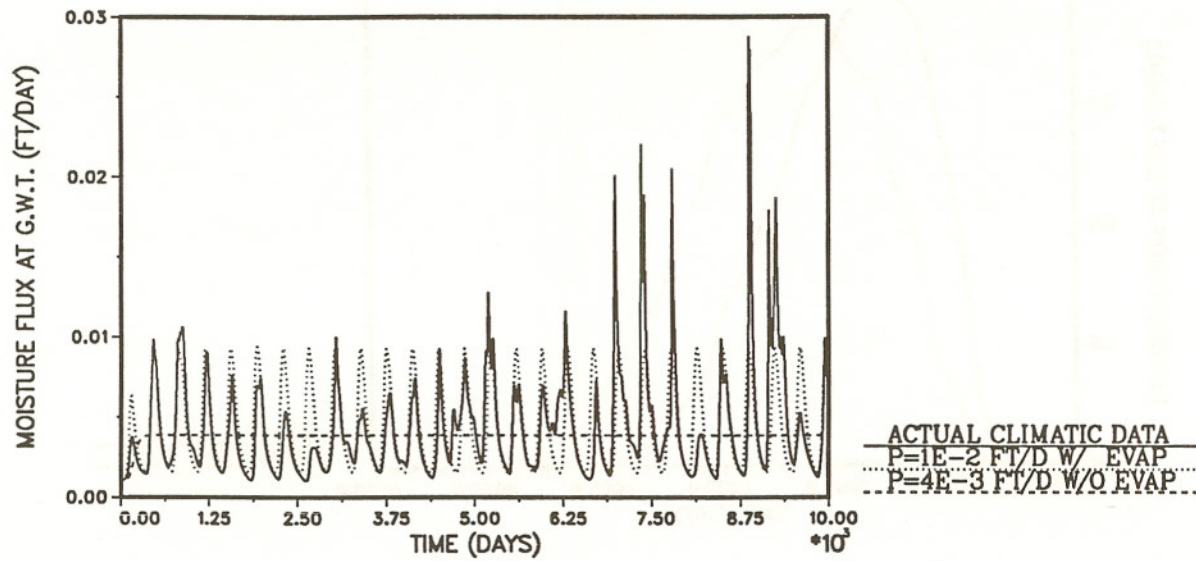


Figure 6.18: Effect of climatic input on moisture fluxes at g.w.t. for sand

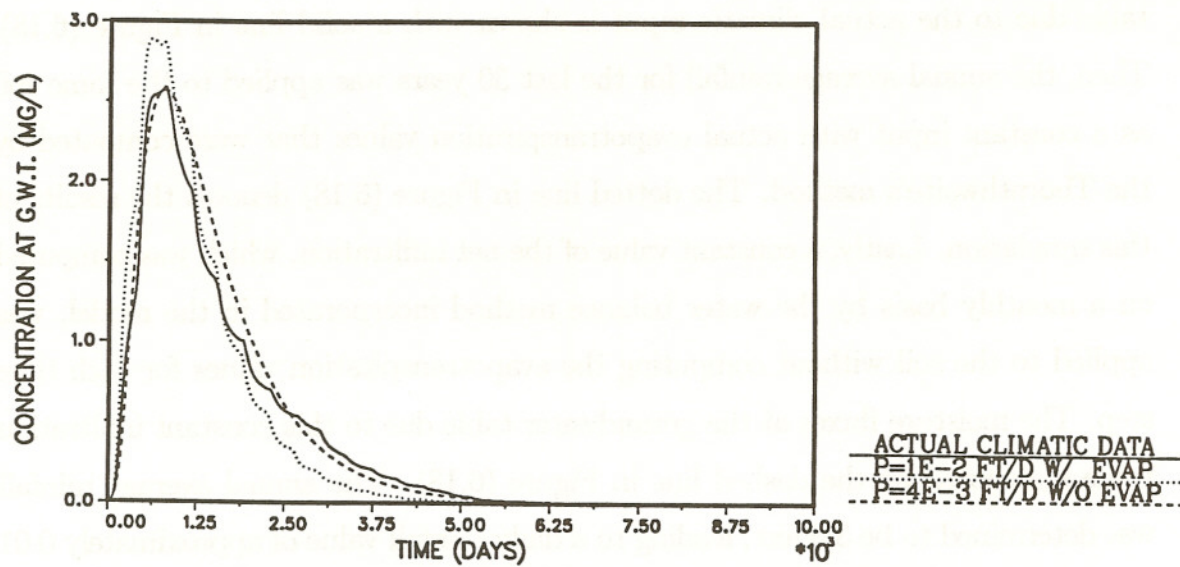


Figure 6.19: Effect of climatic input on liquid phase concentrations at g.w.t. for sand

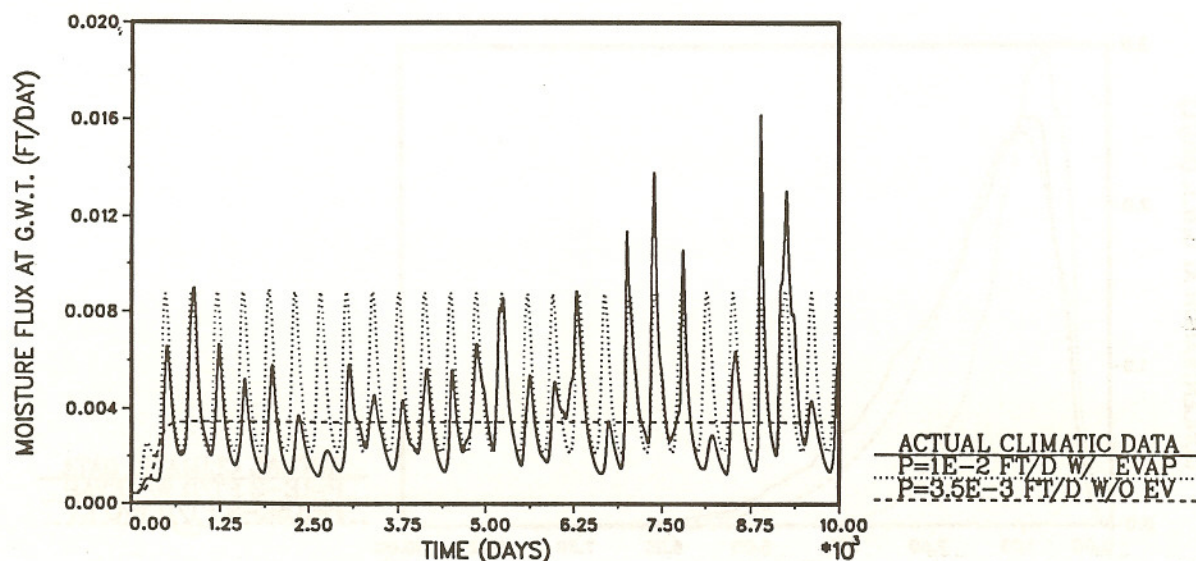


Figure 6.20: Effect of climatic input on moisture fluxes at g.w.t. for sandy loam water table for all three types of the climatic input mentioned above. The third type of rainfall input produced substantially close results to the actual climatic simulation. The annual average rainfall simulation, however, peaked at a higher maximum concentration than the other two simulations. This result was expected since the surface runoff values were not taken into account by the model for this particular simulation.

Similar simulations were performed for other types of soils with the same types of input conditions mentioned above. The only varying climatic input parameter for each soil was the annual average net infiltration value. The net infiltration is computed by the water balance method by taking the full cycle of climatic processes, such as the precipitation, evapotranspiration, and the surface runoff events, into consideration. Figures (6.20) and (6.21) represent the effect of the climatic input in a sandy loam layer contaminated with benzene. Similarly, silty clay loam and silty clay layers were examined, and results are shown in Figures (6.22), (6.23), (6.24), and (6.25).

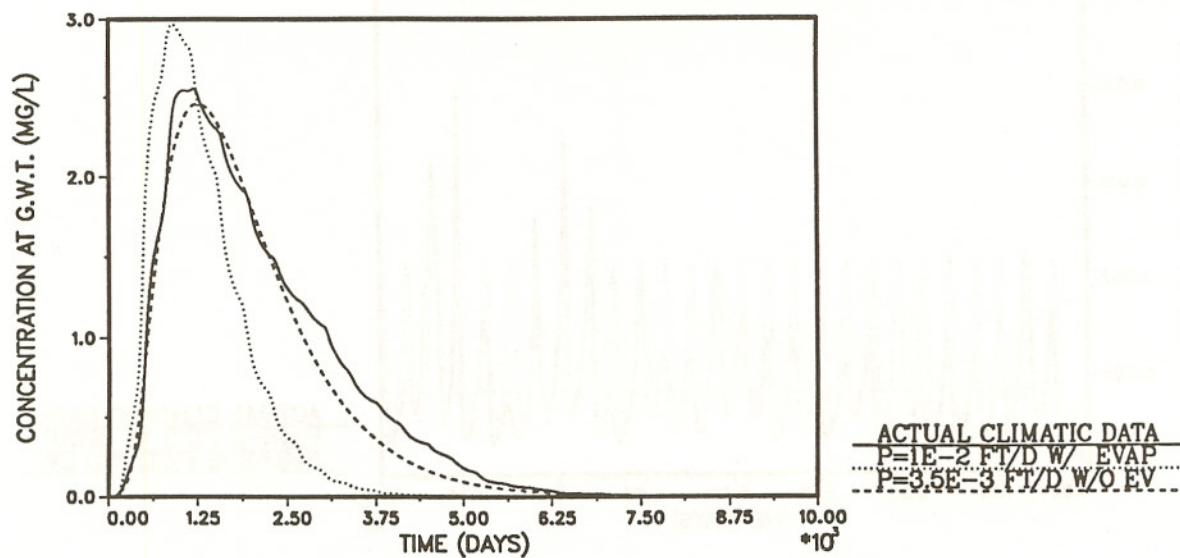


Figure 6.21: Effect of climatic input on liquid phase concentrations at g.w.t. for sandy loam

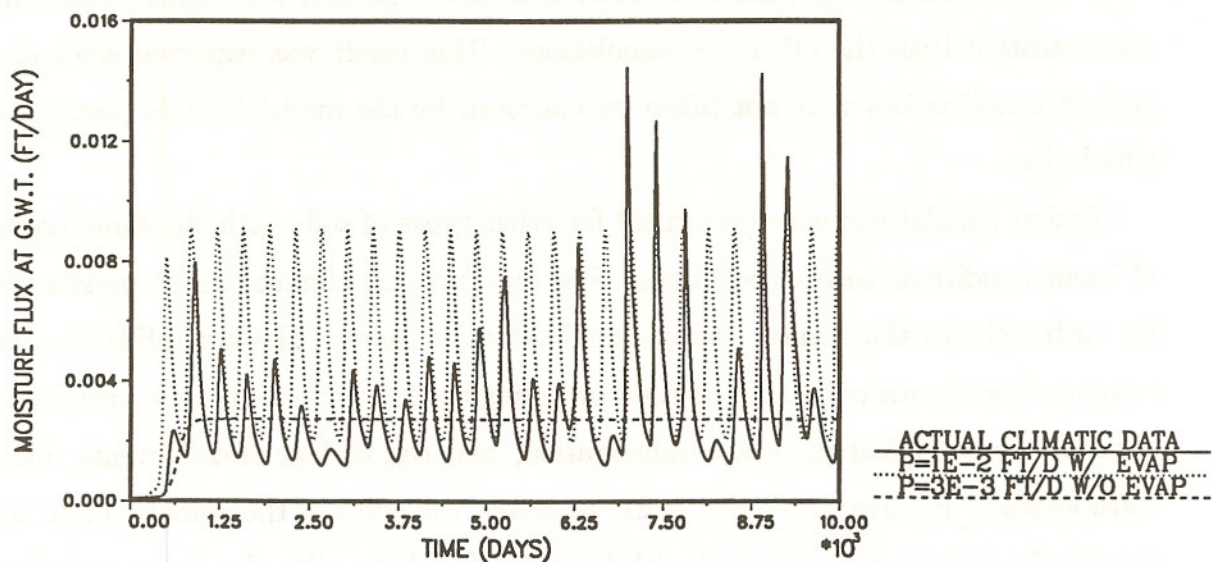


Figure 6.22: Effect of climatic input on moisture fluxes at g.w.t. for silty clay loam

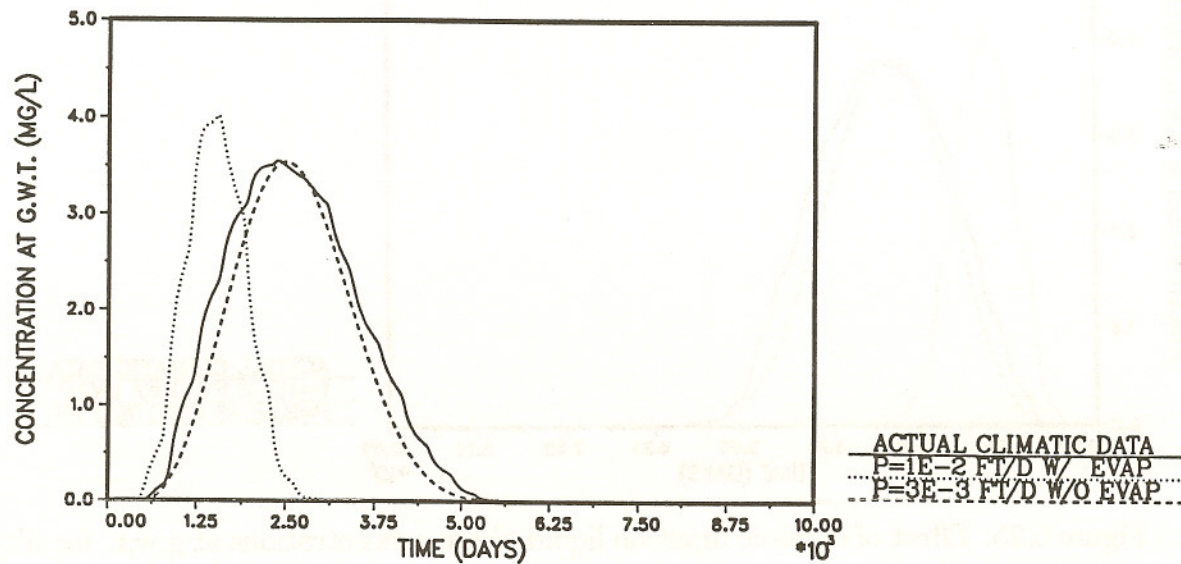


Figure 6.23: Effect of climatic input on liquid phase concentrations at g.w.t. for silty clay loam

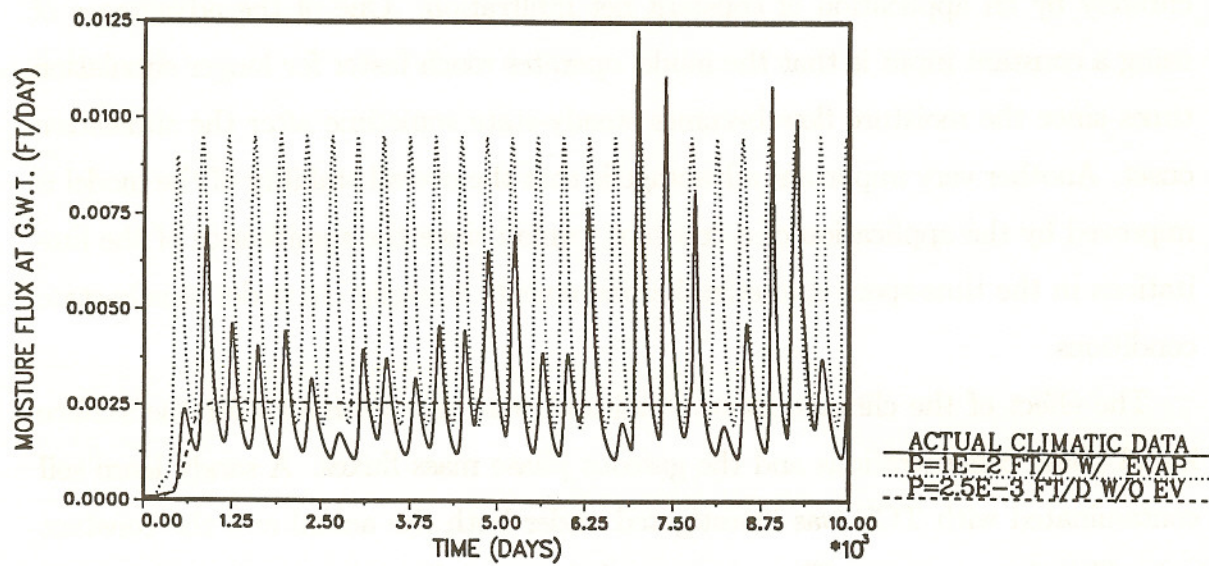


Figure 6.24: Effect of climatic input on moisture fluxes at g.w.t. for silty clay

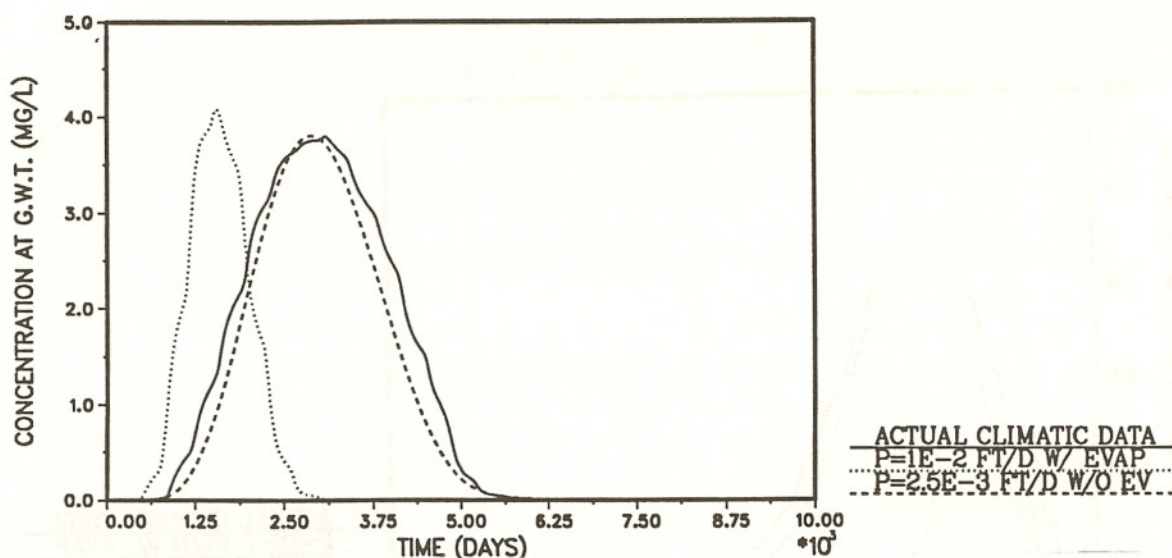


Figure 6.25: Effect of climatic input on liquid phase concentrations at g.w.t. for silty clay

Examining the simulations for each type of soil reveals that, for long term simulations, the benzene concentration at the groundwater table can be predicted accurately by an application of constant net infiltration. One of the advantages of using a constant input is that the model operates much faster for longer simulation times since the moisture flow becomes steady-state sometime after the simulation onset. Another very important advantage is that the overall stability of the model is improved by the application of a constant rainfall since the significance of the limitations in the time-space discretization increments is negligible under steady-state conditions.

The effect of the climatic input conditions were also examined for the surface liquid phase concentrations and the gaseous phase mass fluxes. A sandy loam soil contaminated with TCE was investigated under both the actual and the constant net infiltration scenarios. The unsaturated zone was discretized with $\Delta z = 0.5$ feet, and simulations were performed for 2,000 days with fully reversible adsorption. Fig-

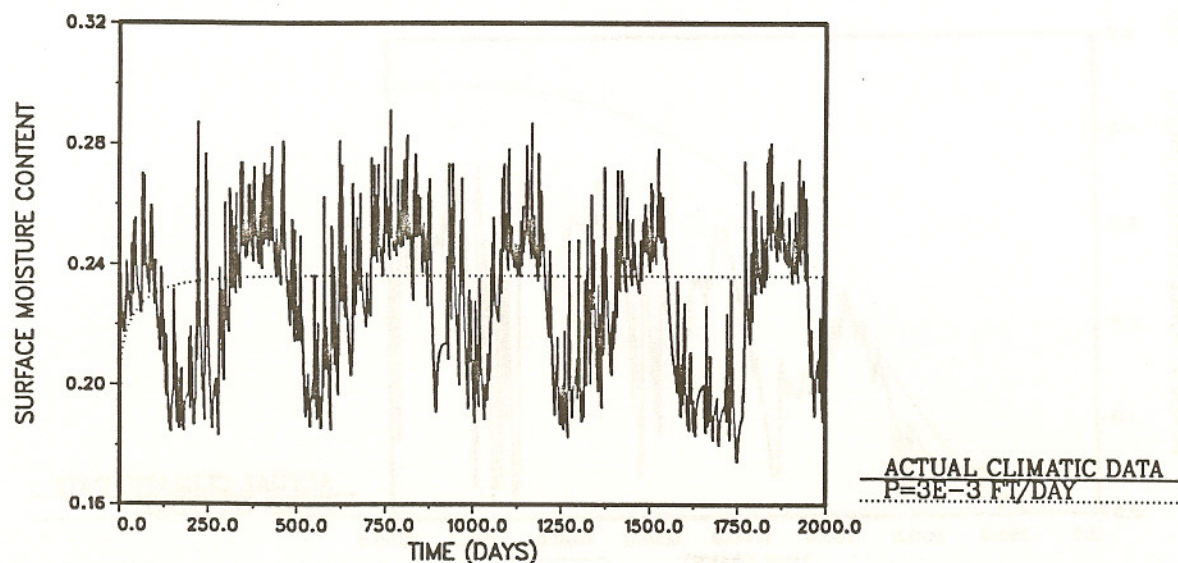


Figure 6.26: Moisture content distribution at the surface of a sandy loam layer under transient and steady-state infiltration

Figure (6.26) shows the moisture content history at the surface of the simulation domain. The dotted line represents the moisture content profile under steady-state infiltration. Figure (6.27) shows the liquid phase concentration history at the surface. As obtained in the previous simulations, the differences in concentrations for transient and steady-state infiltrations were not found to be substantial. The gaseous phase mass fluxes at the surface are shown in Figure (6.28) with respect to time. A similar simulation was performed for a sandy layer, and the results are shown in Figures (6.29) and (6.30).

Effects of Soil and Chemical Properties

The effect of various soil properties on the model output has been examined by performing simulations for the four selected types of soils contaminated with TCE. A 10,000 day simulation is shown in Figures (6.31) and (6.32) for $\Delta z=2$ ft and $\Delta t=5$ days. As expected, the hydraulic properties of the soils are affecting the

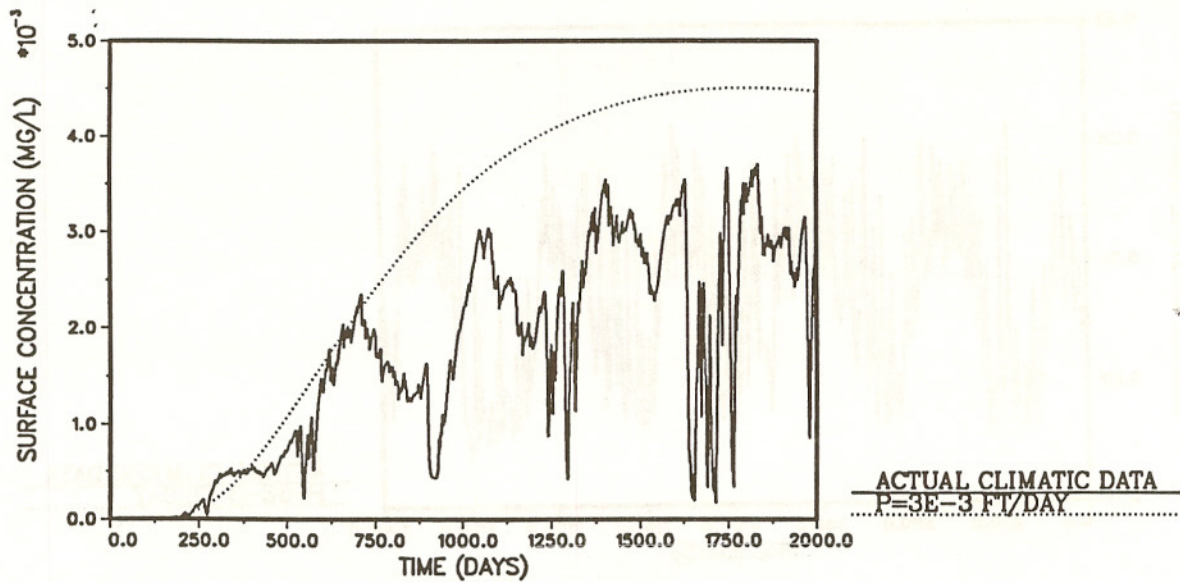


Figure 6.27: Effect of climatic input on liquid phase concentrations at the surface of a sandy loam layer

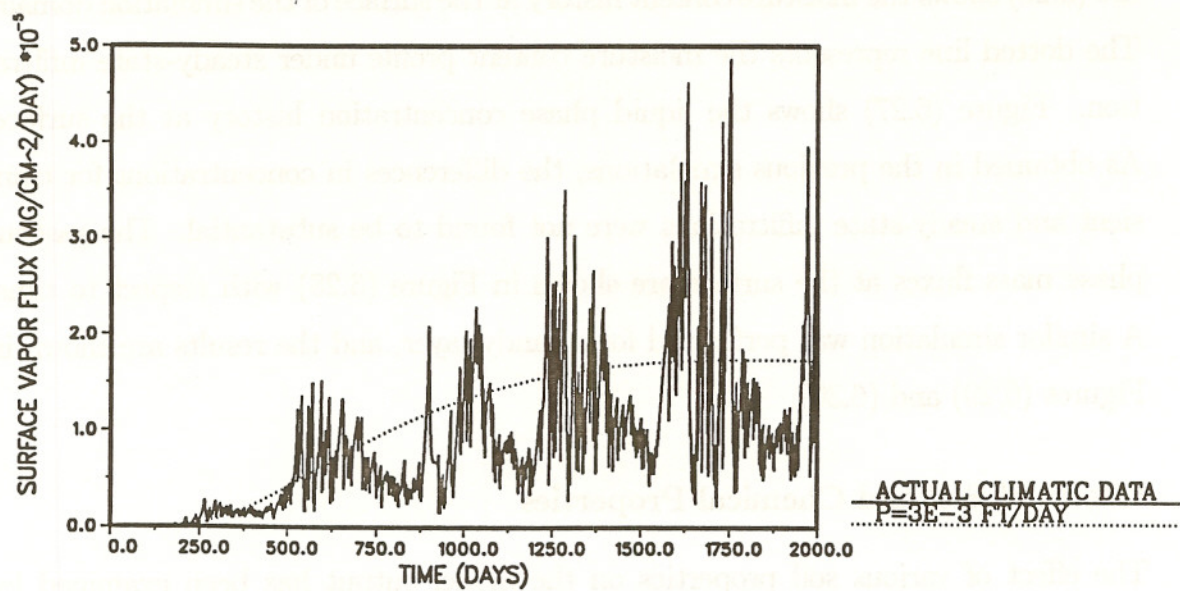


Figure 6.28: Effect of climatic input on gaseous phase fluxes at the surface of a sandy loam layer

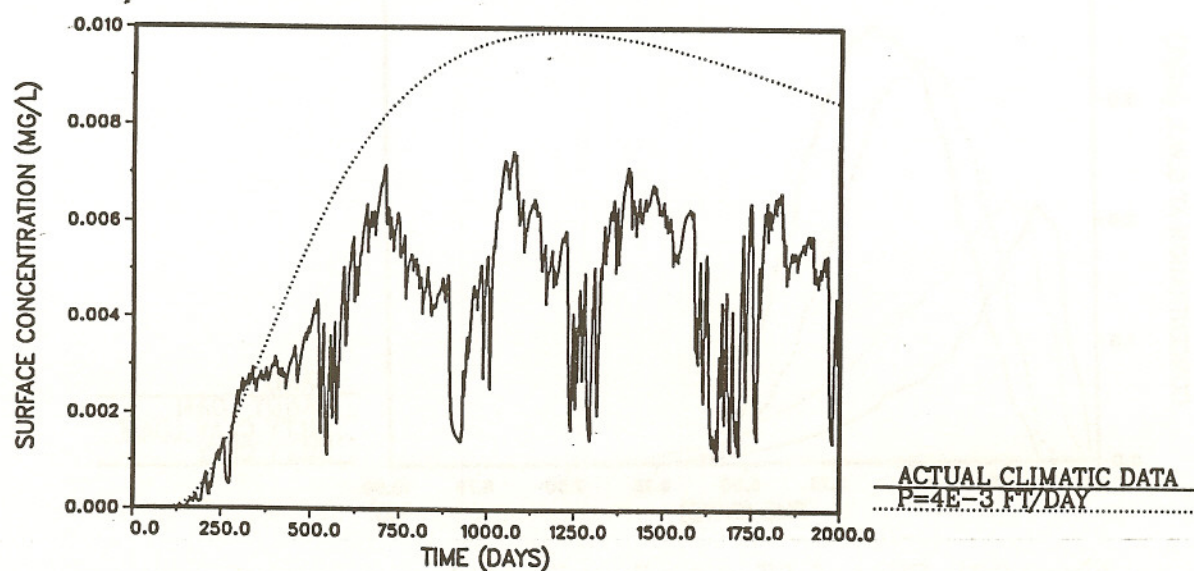


Figure 6.29: Effect of climatic input on liquid phase concentrations at the surface of a sand layer

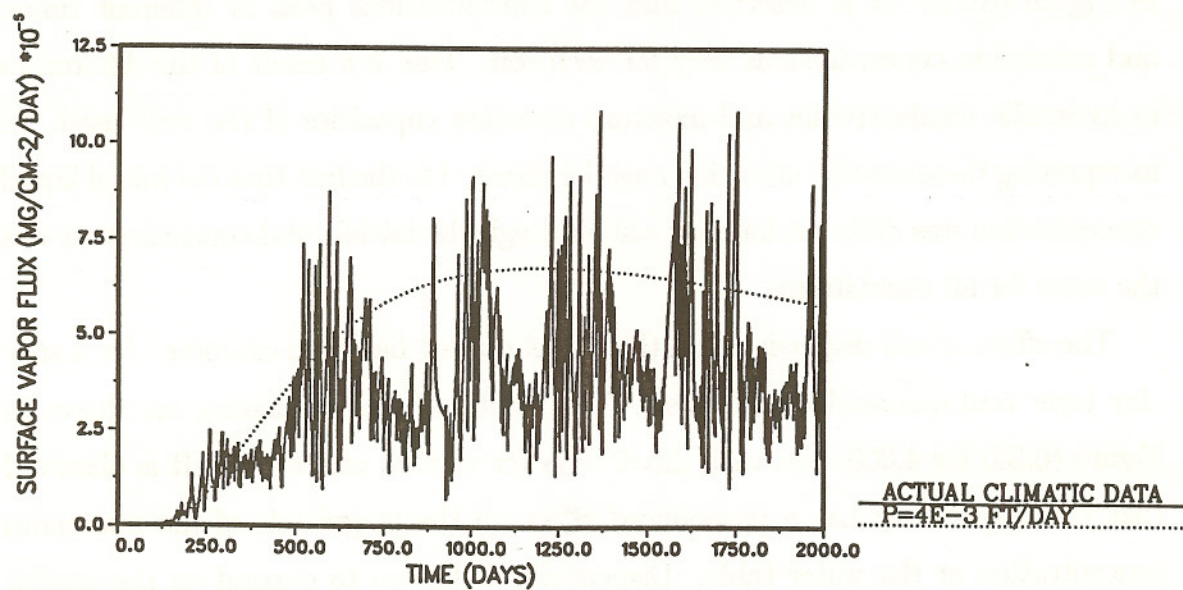


Figure 6.30: Effect of climatic input on gaseous phase fluxes at the surface of a sand layer

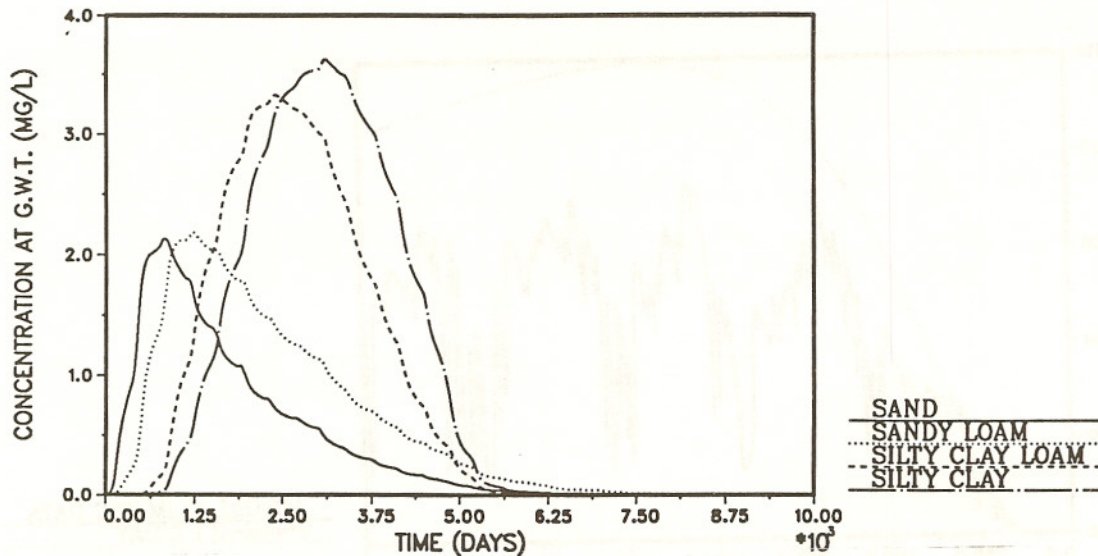


Figure 6.31: Effect of different soils on liquid phase concentrations at g.w.t.

moisture flux at the top of the groundwater table as shown in Figure (6.32). The effect on the TCE concentration at the bottom of the unsaturated soil layer is shown in Figure (6.31). It is observed that the concentrations peak at different times, and maximum concentrations vary for each soil. This is a result of the differences in hydraulic conductivities and moisture retention capacities of the soils used. In interpreting these results, attention must be directed to the fact that the initial liquid concentration was different for each soil although the initial total concentration was the same for all simulations.

The effect of soil dispersivity on the model output has been examined for a silty clay layer contaminated with toluene. The results of this simulation are shown in Figure (6.33) for 4,000 days with $\Delta t = 2$ days for various values of α . It is observed that the dispersivity has a pronounced effect on the magnitude of the maximum concentration at the water table. Dispersivity is known to depend on the spatial scale of the simulation. For surface phenomena, dispersivities of a few millimeters have been reported in the literature. For simulations in thicker soil layers, such as

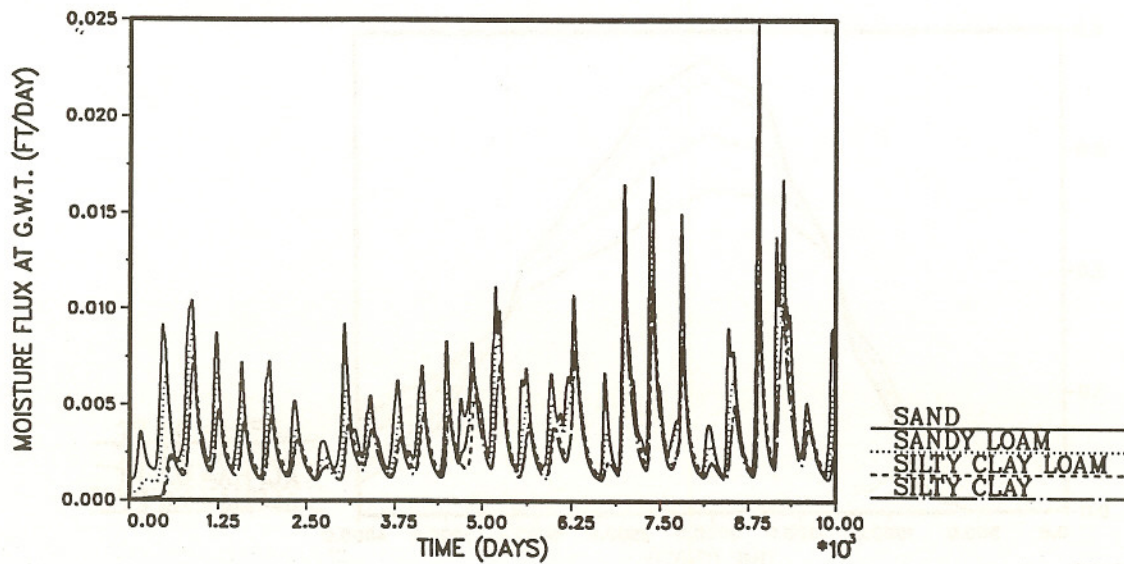


Figure 6.32: Effect of different soils on moisture fluxes at g.w.t.

the one simulated here, values in the range of 0.1 ft to 0.5 ft are recommended.

Similar simulations were performed to examine the effect of chemical constituent properties on the model output. Figure (6.34) shows three different scenarios where a sandy loam layer is contaminated with benzene, phenol, and carbon tetrachloride. The pertinent chemical properties for phenol and carbon tetrachloride are given below:

$$d_w = 7.15 \times 10^{-5} \text{ m}^2/\text{day} \text{ for phenol}$$

$$d_w = 6.61 \times 10^{-5} \text{ m}^2/\text{day} \text{ for carbon tetrachloride}$$

$$d_a = 0.622 \text{ m}^2/\text{day} \text{ for phenol}$$

$$d_a = 0.536 \text{ m}^2/\text{day} \text{ for carbon tetrachloride}$$

$$K_H = 1.89 \times 10^{-5} \text{ for phenol}$$

$$K_H = 1.0 \text{ for carbon tetrachloride}$$

Each of the runs was executed for the same initial total concentration which produced different initial liquid concentrations due to different Henry's constants. The differ-

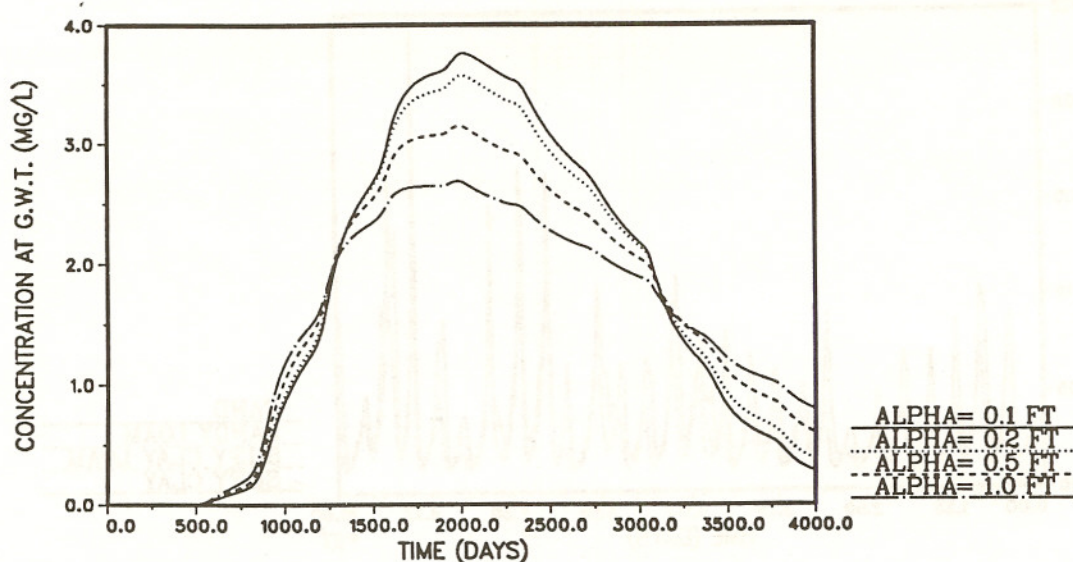


Figure 6.33: Effect of soil dispersivity on liquid phase concentrations at g.w.t. for silty clay

ences in the maximum bottom concentrations are substantial for these compounds since their Henry's constants and diffusion coefficients differ drastically.

Effect of the Top Boundary Condition for the Mass Transport Equation

The model is equipped to handle two different mass transport boundary conditions at the soil surface. These two boundary conditions represent the extreme cases of no flux of mass to the atmosphere ($\frac{\partial C_L}{\partial z} = 0$) and a maximum possible flux ($C_L = 0$) at the boundary. Figure (6.35) shows a 2,000 day simulation in a 30 feet thick sandy loam layer with the middle 10 feet contaminated with benzene for both types of boundary conditions. For this scenario, the type of boundary condition used does not influence the benzene concentration history at the top of the groundwater table. A close observation of the concentration profiles revealed that although benzene mass had migrated upward in the top 10 feet of the layer due to gaseous and liquid diffusion, the amount of mass reaching the soil surface boundary was negligible.

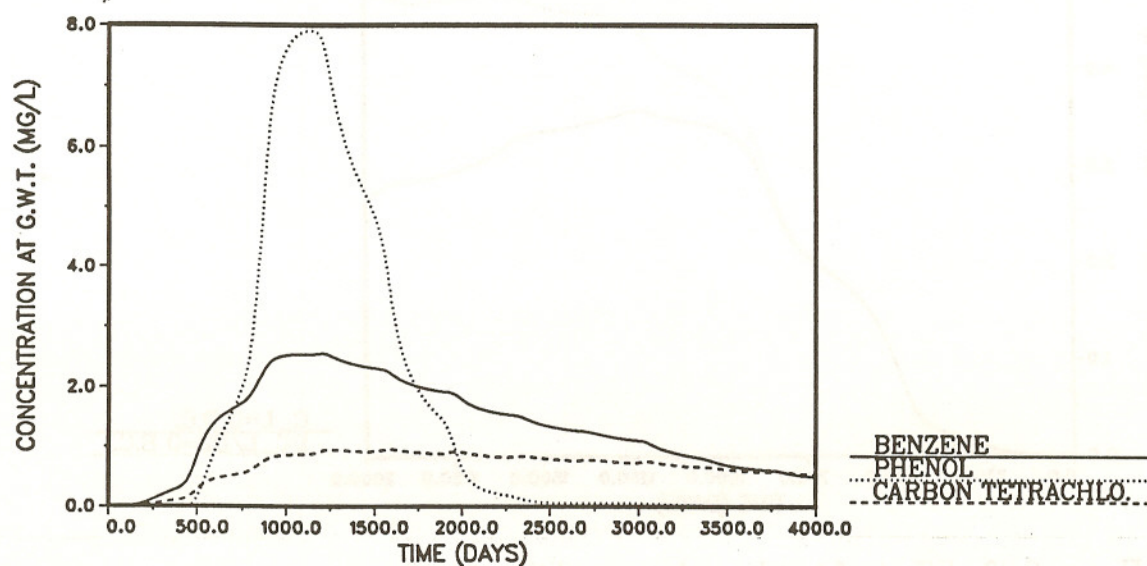


Figure 6.34: Effect of different compounds on liquid phase concentrations at g.w.t. for silty clay

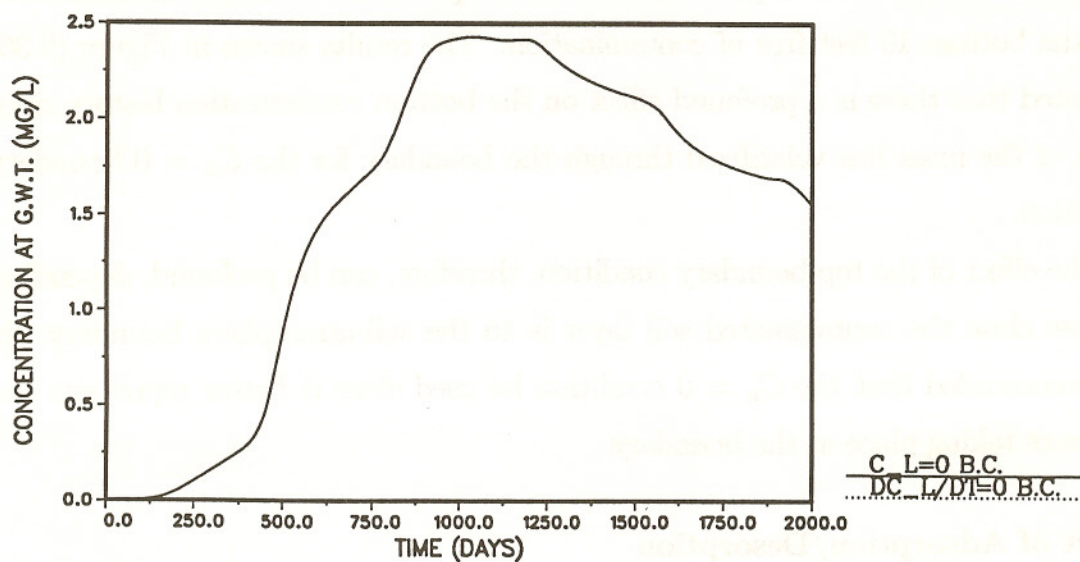


Figure 6.35: Effect of top boundary condition for the mass transport equation on liquid phase concentrations at g.w.t. for sandy loam

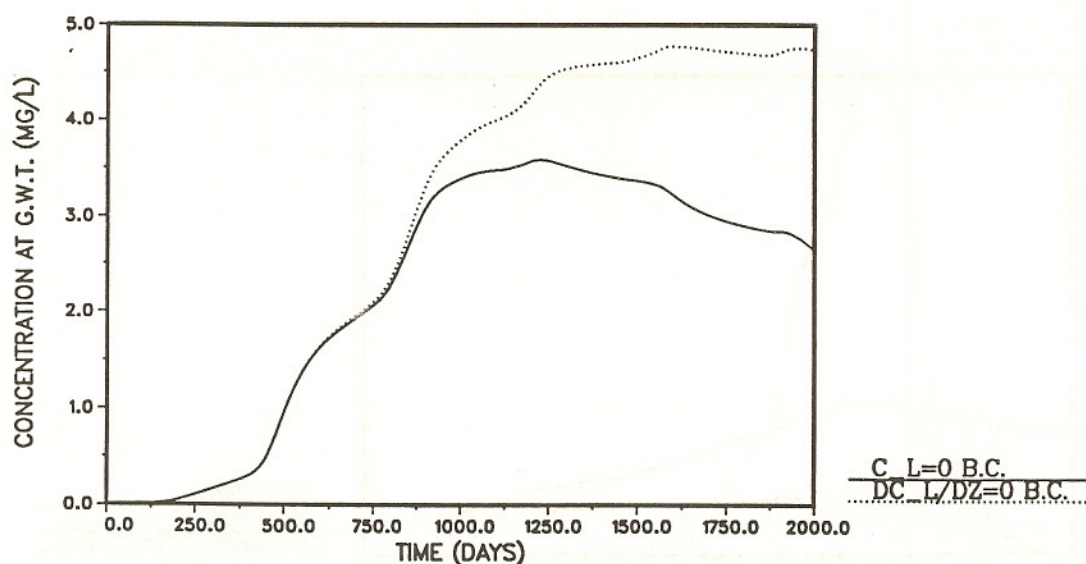


Figure 6.36: Effect of top boundary condition for the mass transport equation on liquid phase concentrations at g.w.t. for sandy loam with the top 20 feet of the layer contaminated

Another simulation was performed with the top 20 feet of the layer contaminated and the bottom 10 feet free of contamination. The results shown in Figure (6.36) indicated that there is a profound effect on the bottom concentration history since much of the mass has volatilized through the boundary for the $C_L = 0$ boundary condition.

The effect of the top boundary condition, therefore, can be profound, depending on how close the contaminated soil layer is to the soil-atmosphere boundary. It is recommended that the $C_L = 0$ condition be used since it better represents the processes taking place at the boundary.

Effect of Adsorption/Desorption

Most of the sensitivity simulations reported so far were performed without taking the sorption processes into consideration. The simulations shown in Figure (6.37)

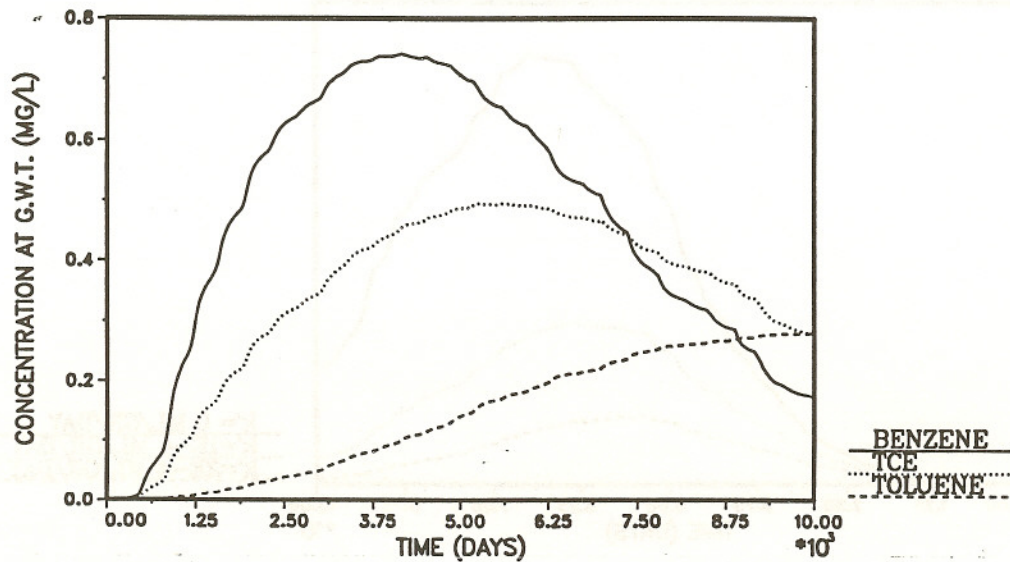


Figure 6.37: Effect of fugacity coefficient on liquid phase concentrations at g.w.t. for sandy loam

were performed for a sandy loam soil contaminated with various compounds. As expected, a retardation of the contaminant front is observed as the fugacity coefficient is increased. The maximum concentration at the water table is also affected by the fully reversible adsorption. Figure (6.38) shows a simulation where irreversible adsorption is considered in a silty clay soil. The solid line denotes no adsorption, and the dotted line shows the concentration history for the irreversible adsorption rate coefficient $k' = 1 \times 10^{-4} \text{ ml/gr} \cdot \text{day}$. The dashed line denotes the concentration history for $k' = 2 \times 10^{-4} \text{ ml/gr} \cdot \text{day}$. The maximum concentration at the groundwater is greatly influenced by k' .

Effect of Biodegradation

The model output has been found to be very sensitive on the rate coefficients of equilibrium biodegradation. All three biodegradation models, i.e. zero order, first order, and Monod kinetics, have been examined. Figure (6.39) shows the effect of

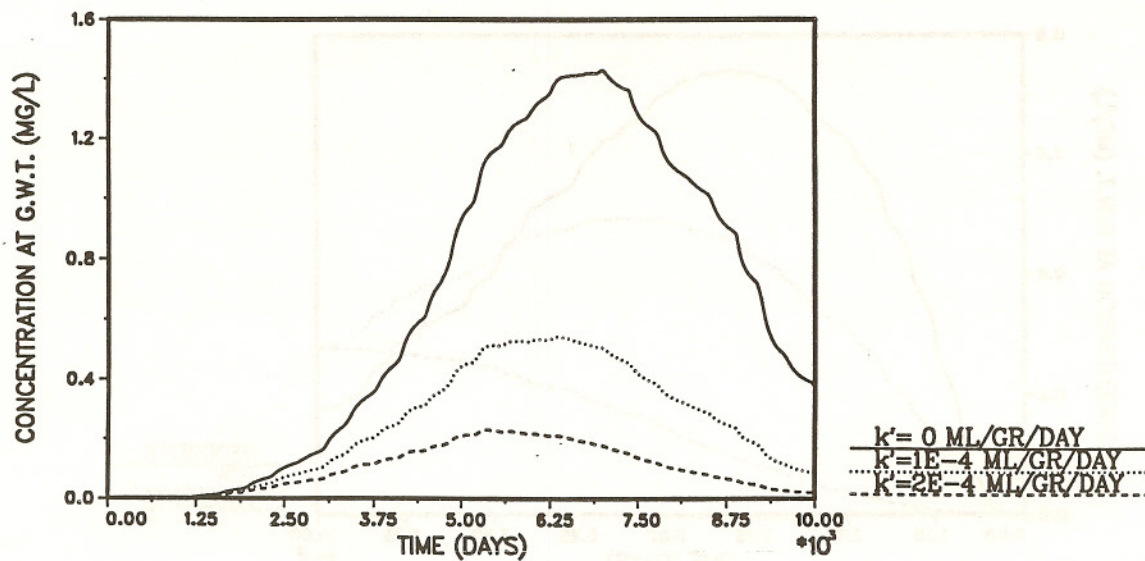


Figure 6.38: Effect of irreversible adsorption rate coefficient on liquid phase concentrations at g.w.t. for silty clay

the zero order coefficient, k_0 , on the concentration history for a silty clay loam layer contaminated with TCE. The effect of the first order reaction coefficient, k_1 , for the same contamination scenario is shown in Figure (6.40). Another simulation was performed for a sandy loam soil contaminated with benzene, TCE, and toluene. The first order equilibrium biodegradation coefficient for each of these compounds were computed by the following equation reported by Jury et al. [46]:

$$k_1 = \frac{\ln(2)}{\tau} \quad (6.1)$$

where τ is the half life of the microorganisms in the solute [days]. The following values of k_1 were computed for each compound with the τ values given by Jury et al. [46]:

$$\tau = 0.365 \times 10^3 \text{ days} \rightarrow k_1 = 1.9 \times 10^{-3} \text{ 1/day for benzene}$$

$$\tau = 0.730 \times 10^3 \text{ days} \rightarrow k_1 = 9.5 \times 10^{-4} \text{ 1/day for TCE}$$

$$\tau = 50 \text{ days} \rightarrow k_1 = 1.4 \times 10^{-2} \text{ 1/day for toluene}$$

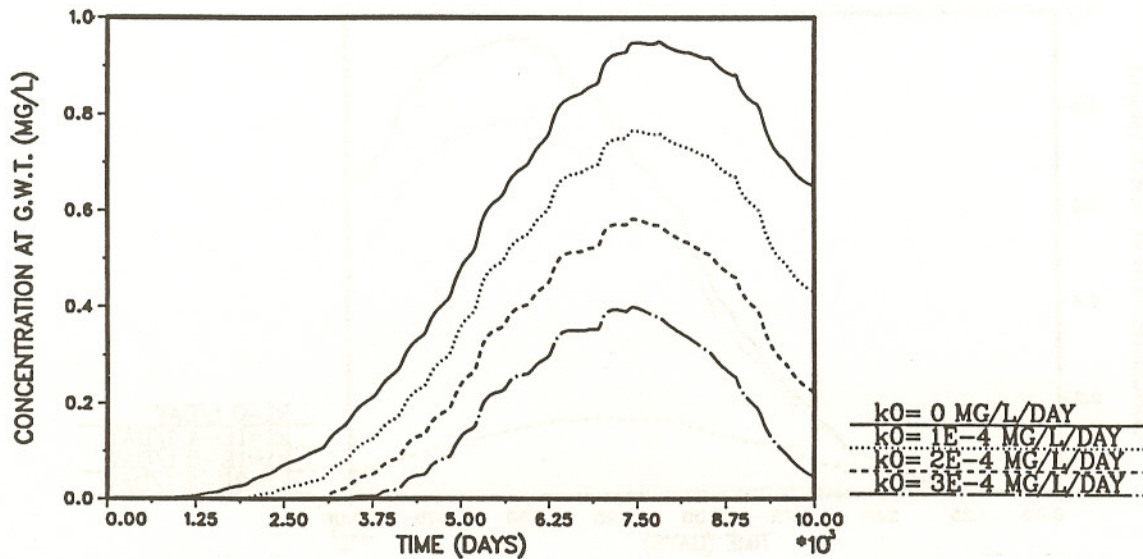


Figure 6.39: Effect of zero order biodegradation on liquid phase concentrations at g.w.t. for silty clay loam

It is observed from Figure (6.41) that the maximum liquid phase concentrations substantially differ for each of the compounds used, due to the differences in the first order biodegradation coefficients.

The Monod kinetic model was executed for a silty clay loam layer contaminated with benzene with the following values: $k_e = 0.01$ 1/day, $K_m = 100$ mg/l, $Y = 0.6$, and initial biomass concentration $X_{initial} = 1$ mg/l. A sensitivity analysis was performed for the growth rate coefficient, μ_m , and is shown in Figure (6.42).

All these simulations show that the concentration history at the bottom of the unsaturated zone is greatly influenced by the choice of the type of biodegradation model used, and the values of the coefficients of these models. It is, therefore, important that appropriate values for these coefficients are used. Unfortunately, the availability of the values for these coefficients in the literature is very limited.

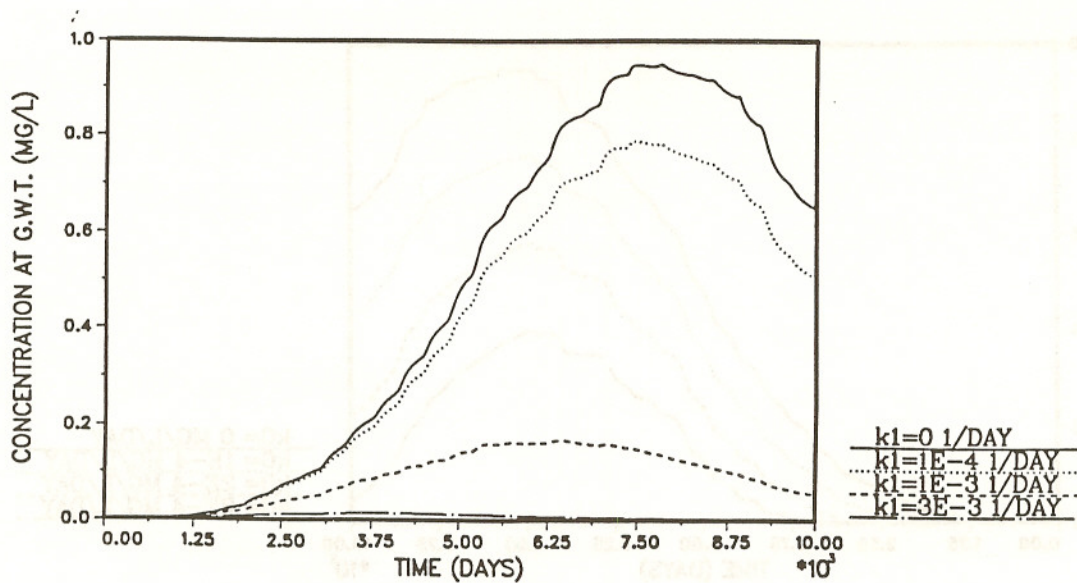


Figure 6.40: Effect of first order biodegradation on liquid phase concentrations at g.w.t. for silty clay loam

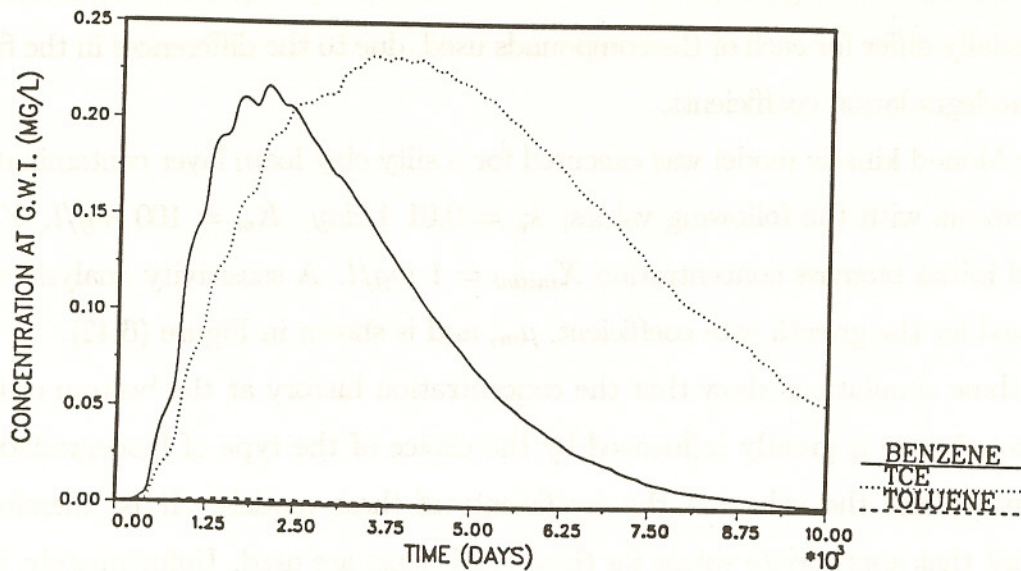


Figure 6.41: Effect of first order biodegradation on liquid phase concentrations at g.w.t. for sandy loam contaminated with different compounds

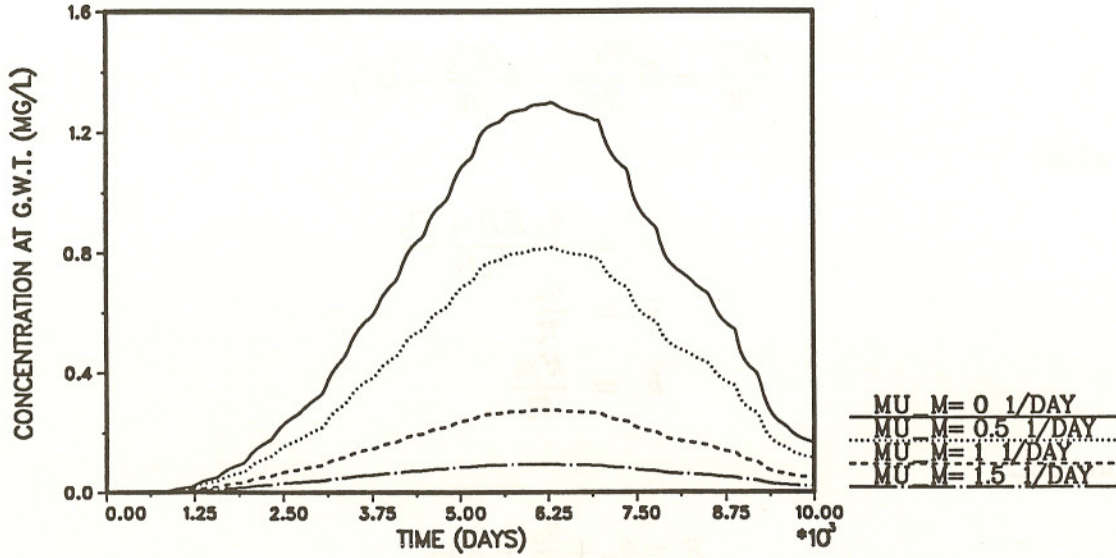


Figure 6.42: Effect of biomass growth rate on liquid phase concentrations at g.w.t. for silty clay loam

6.2 Model Verification

This section addresses a special case of groundwater contamination problem where an analytical solution exists. The governing mass transport equation is solved analytically under steady-state flow conditions for a semi-infinite domain. The mass transport equation is written without a sink term as follows:

$$\frac{\partial(\theta_w C_L)}{\partial t} + K_d \rho_b \frac{\partial C_L}{\partial t} + k' \rho_b C_L + \frac{1}{H} \frac{\partial(\theta_a C_L)}{\partial t} + \frac{\partial(q_w C_L)}{\partial z} = \frac{\partial}{\partial z} \left[\left(\theta_w E + \frac{D_a}{H} \right) \frac{\partial C_L}{\partial z} \right] \quad (6.2)$$

If the net infiltration rate through the unsaturated zone is constant and continuous with respect to time, ultimately, steady-state flow will occur. For this particular case, therefore, θ_w , θ_a , and q_w terms appearing in the governing equation given above will become constants. Hence, the equation becomes:

$$\frac{\partial C_L}{\partial t} = \bar{D} \frac{\partial^2 C_L}{\partial z^2} - \bar{v} \frac{\partial C_L}{\partial z} - \bar{k} C_L \quad (6.3)$$

where

$$\begin{aligned} \bar{D} &= \frac{\theta_w EH + D_a}{\mathcal{R}H} \\ \bar{v} &= \frac{q_w}{\mathcal{R}} \\ \bar{k} &= \frac{k' \rho_b}{\mathcal{R}} \end{aligned}$$

in which

$$\mathcal{R} = \theta_w + \frac{\theta_a}{H} + K_d \rho_b$$

For this particular problem, the simulation domain will be considered as a semi-infinite domain in the vertical axis. Namely, the following conditions will be utilized for the solution of Equation (6.3):

$$C_L(0, t) = C_0 \quad @ \quad z = 0 \quad for \quad t \geq 0 \quad (6.4)$$

$$C_L(\infty, t) = 0 \quad @ \quad z = \infty \quad for \quad t \geq 0 \quad (6.5)$$

$$C_L(z, 0) = 0 \quad for \quad t = 0 \quad (6.6)$$

The analytical solution of Equation (6.3) is obtained as follows [79]:

$$\begin{aligned} C_L(z, t) = \frac{C_0}{2} \exp \left[\frac{\bar{v}z}{2\bar{D}} \right] \left\{ \exp \left[\frac{-\sqrt{\bar{v}^2 + 4\bar{D}\bar{k}z}}{2\bar{D}} \right] \operatorname{erfc} \left[\frac{z - \sqrt{\bar{v}^2 + 4\bar{D}\bar{k}t}}{2\sqrt{\bar{D}t}} \right] + \right. \\ \left. \exp \left[\frac{\sqrt{\bar{v}^2 + 4\bar{D}\bar{k}z}}{2\bar{D}} \right] \operatorname{erfc} \left[\frac{z + \sqrt{\bar{v}^2 + 4\bar{D}\bar{k}t}}{2\sqrt{\bar{D}t}} \right] \right\} \quad (6.7) \end{aligned}$$

In order to verify the numerical scheme used in the model, the following scenario is considered: A silty clay loam layer contaminated with benzene has been investigated

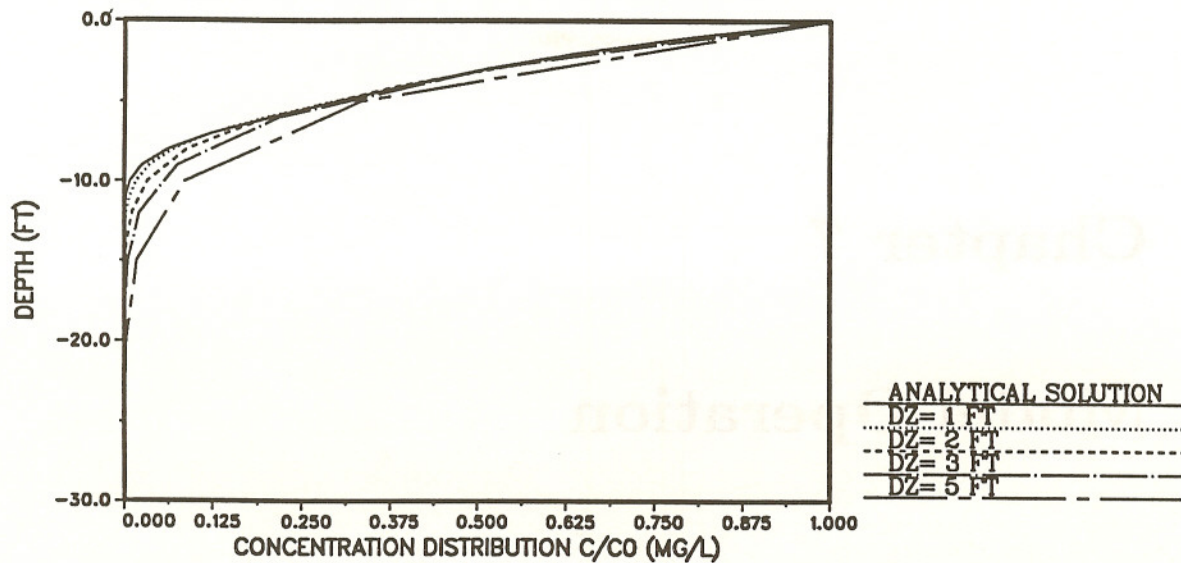


Figure 6.43: Comparison of analytical and numerical solutions of mass transport equation for a silty clay loam layer contaminated with benzene

by taking all the physicochemical processes into consideration with $k' = 0.001 \text{ ml/gr} \cdot \text{day}$. A constant rainfall of 0.007 ft/day was used for both the numerical and the analytical models. The following mass transport coefficients were computed and used in the analytical model for the steady-state volumetric moisture content of 0.3795 which was obtained by running the numerical model for 1,000 days:

$$\bar{D} = 1.68411 \times 10^{-3}$$

$$\bar{v} = 6.43993 \times 10^{-3}$$

$$\bar{k} = 1.51798 \times 10^{-3}$$

The comparison of the results at 1,000 days is shown in Figure (6.43). The numerical model predicted the concentration distribution very accurately for smaller values of Δz . When greater values of Δz were used, on the other hand, the results deviated from the analytical solution.

Chapter 7

Model Operation

7.1 General

Although the model has the flexibility to simulate a variety of situations, its main operation describes the following scenario:

A portion of the vadose zone, having thickness d_c , has been contaminated with a single organic constituent of a known concentration, C_i , as shown in Figure (7.1). Assuming that the source has been eliminated, this contaminant will move toward the groundwater table which is assumed to be free of any contamination from this constituent initially.

The concentration of the organic will reach its maximum value, C_{max} , at the groundwater surface some time later. This maximum concentration and the time that it will reach that value are predicted by the model. If C_{max} is less than the concentration allowed by regulatory standards on groundwater (C_{allow}), no remediation will be required. If, on the other hand, C_{max} exceeds C_{allow} , the model reduces the initial concentration C_i by a predetermined amount, and repeats the simulation until C_{max} becomes equal or smaller than C_{allow} . The reduction of the initial contaminant mass is accomplished in one of the following ways:

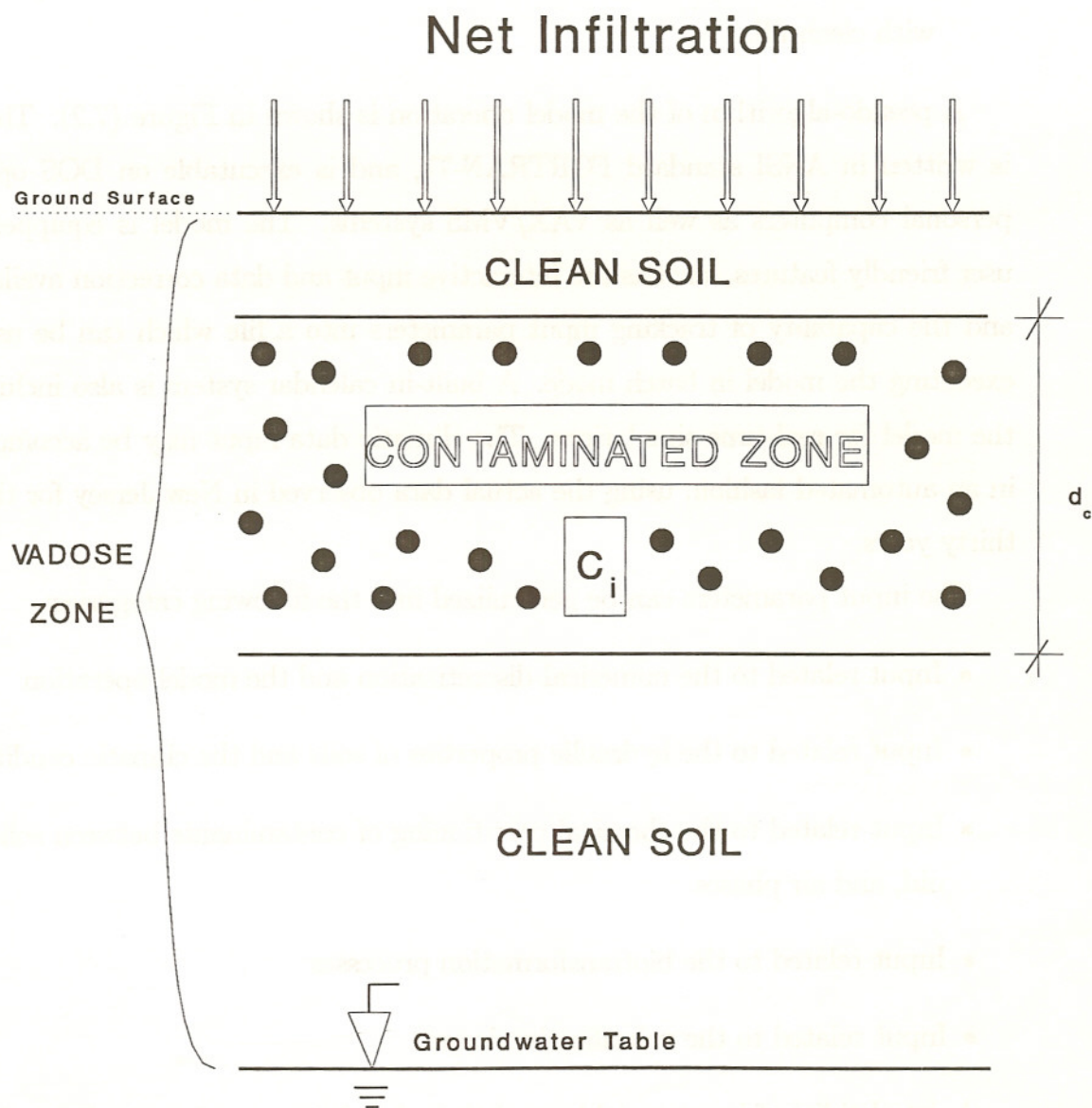


Figure 7.1: Typical scenario for model application

- a) By reducing the concentration throughout the initially contaminated zone as it would be expected in the case of in-situ remediation;
- b) By reducing the actual thickness of the initially contaminated zone as it would be expected in the case of excavation of the contaminated soil and replacement with clean fill.

A pseudo-algorithm of the model operation is shown in Figure (7.2). The code is written in ANSI standard FORTRAN-77, and is executable on DOS operated personal computers as well as VAX/VMS systems. The model is equipped with user friendly features, such as the interactive input and data correction availability, and the capability of tracking input parameters into a file which can be used for executing the model in batch mode. A built-in calendar system is also included in the model for real-time simulations. The climatic data input may be accomplished in an automated fashion, using the actual data observed in New Jersey for the last thirty years.

The input parameters can be generalized into the following categories:

- Input related to the numerical discretization and the model operation
- Input related to the hydraulic properties of soils and the climatic conditions
- Input related to the chemical partitioning of contaminants between solid, liquid, and air phases
- Input related to the biotransformation processes
- Input related to the volatilization losses

A detailed list of input variables and their definitions are given in Appendix B.

As mentioned earlier, the model works in two modes of input, i.e. interactive and batch. If the interactive mode is selected, the user will be prompted to supply

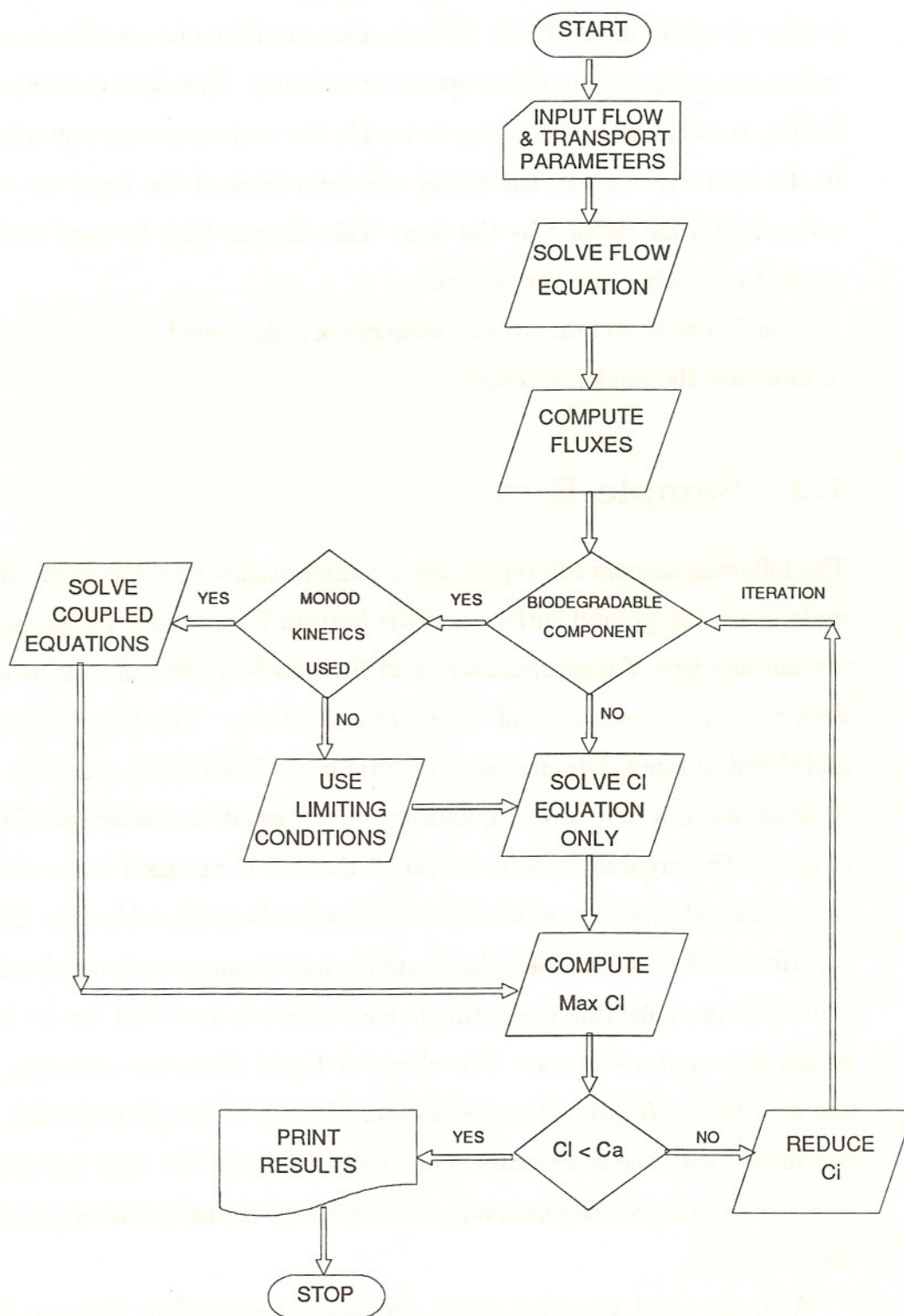


Figure 7.2: Pseudo-algorithm of the model operation

a value or values interactively. If there are more than one variable in a line of input, values are separated by either spaces or commas. The data correction subroutine, DATA, is called after each entry to enable the user to reenter any mistyped values. In the interactive mode, the model will keep track of the input by writing all the values into a file defined by the user. This file can then be used within the batch mode if successive runs are desired.

The following section gives an example of a shortened version of the main output to illustrate the model operation.

7.2 Sample Run

The following sample run represents a contamination scenario where the first 5 feet underneath the ground surface and the bottom 2 feet above the groundwater table are initially free of contamination, and the middle 13 feet of sand is contaminated with a total concentration of 1.0 mg/kg of toluene. The relevant hydrogeological and chemical input data are taken directly from Tables (6.1) and (6.2). For the sake of illustration, a first order equilibrium biodegradation coefficient of 0.0001 day^{-1} is used. The organic carbon content of the soil is assumed to be 0.5 %, and the irreversible adsorption coefficient is considered to be $0.001 \text{ ml/g}\cdot\text{day}$. The simulation is performed for a total of 400 days, and the initial concentration reduction scheme is utilized in promulgating the optimum concentration level that can be left untreated within the unsaturated zone. The allowable liquid phase concentration of toluene is assumed to be 50 ppb . The spatial discretization of the 20 feet thick vadose zone is achieved with the increments of one foot. Similarly, the time marching scheme is established with four day intervals, and the actual climatic data are used throughout the simulation.

With the input provided above, the model iterates four times to approach the

allowable total toluene concentration of 0.875 mg/kg. The following output file lists a more detailed set of results for all iterations:

SAMPLE RUN

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 = 1

HYDRAULIC PROPERTIES AND SIMULATION PARAMETERS

.....

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

DEPTH INCREMENT = 1.0000 FT

TIME INCREMENT = 4.0000 DAYS

*** OUTPUT PRINTED EVERY 100 TIME INCREMENTS ***

EPSILON = 0.001000

NUMBER OF LINES = 21

NUMBER OF TIME STEPS = 100

COEFFICIENT <AM> = 11.1000

COEFFICIENT = 4.0500

SATURATION SUCTION HEAD = 0.4000 FT

.....

• • • • •

.....

BULK WATER DIFFUSION COEFFICIENT = 0.6230E-04 M2/DAY

BULK AIR DIFFUSION COEFFICIENT = 0.7920E+00 M2/DAY
 HENRY'S CONSTANT = 0.2650
 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 0.1000E+01
 0.1000E+01 0.1000E+01 0.1000E+01 0.1000E+01 0.1000E+01 0.1000E+01
 0.1000E+01 0.1000E+01 0.1000E+01 0.1000E+01 0.1000E+01 0.1000E+01
 0.1000E+01 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 0.6134E+00
 0.6134E+00 0.6134E+00 0.6134E+00 0.6134E+00 0.6134E+00 0.6134E+00
 0.6134E+00 0.6134E+00 0.6134E+00 0.6134E+00 0.6134E+00 0.6134E+00
 0.6134E+00 0.0000E+00 0.0000E+00

***** RESULTS *****

MONTHLY MEAN TEMPERATURES (F)

.....
 JAN FEB MAR APR MAY JUN JUL AUG SEP OCT
 30.20 32.80 41.70 52.30 62.90 71.90 77.10 75.90 68.30 57.00
 NOV DEC
 46.90 35.80

CN = 72.

THF = 5.00 (%)
 THW = 2.00 (%)
 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	2.79	2.00	3.89	4.67	5.23	1.91	8.08	7.85
I	82.14	76.55	94.17	91.02	92.71	74.01	105.01	88.69
PET	0.00	0.36	15.00	45.62	91.94	132.71	160.15	143.27
I-PET	82.14	76.18	79.16	45.41	0.77	-58.71	-55.15	-54.58
S(I-PET)	0.00	0.00	0.00	0.00	0.00	58.71	113.86	168.43
ST	27.43	27.43	27.43	27.43	27.43	3.32	0.48	0.16
dST	0.00	0.00	0.00	0.00	0.00	-24.11	-2.85	-0.32
AET	0.00	0.36	15.00	45.62	91.94	98.12	107.85	89.01
PERC	82.14	76.18	79.16	45.41	0.77	0.00	0.00	0.00

	SEP	OCT	NOV	DEC	ANNUAL TOTALS
P	92.57	74.49	100.11	89.34	1097.25
RUNOFF	7.71	3.65	6.91	2.22	56.93
I	84.87	70.84	93.20	87.12	1040.32
PET	96.69	52.86	22.09	3.16	763.87
I-PET	-11.82	17.98	71.10	83.95	
S(I-PET)	180.25	0.00	0.00	0.00	
ST	0.14	18.11	27.43	27.43	214.23
dST	-0.02	17.98	9.32	0.00	0.00
AET	84.89	52.86	22.09	3.16	610.91
PERC	0.00	0.00	61.79	83.95	429.41

AVERAGE DAILY EVAPO. FOR TIME STEP 100 = 0.4111E-04 FT/DAY (2/ 1/1960)

CONCENTRATION DISTRIBUTION AT 400. DAYS MG/L

0.0000E+00 0.1961E-01 0.5204E-01 0.1001E+00 0.1622E+00 0.2326E+00
 0.3028E+00 0.3642E+00 0.4112E+00 0.4428E+00 0.4616E+00 0.4710E+00
 0.4738E+00 0.4708E+00 0.4608E+00 0.4400E+00 0.4035E+00 0.3465E+00
 0.2672E+00 0.1682E+00 0.5723E-01

MAX. CONCENTRATION= 0.5723E-01 > ALLOW. CONCENTRATION= 0.5000E-01 MG/L

NEW INITIAL LIQUID PHASE CONCENTRATION (MG/L)

 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.3067E+00
 0.3067E+00 0.3067E+00 0.3067E+00 0.3067E+00 0.3067E+00 0.3067E+00
 0.3067E+00 0.3067E+00 0.3067E+00 0.3067E+00 0.3067E+00 0.3067E+00
 0.3067E+00 0.0000E+00 0.0000E+00

ASSUMED NEW TOTAL CONCENTRATION (MG/KG)

 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 0.0000E+00 0.0000E+00

CONCENTRATION DISTRIBUTION AT 400. DAYS MG/L

0.0000E+00 0.9806E-02 0.2602E-01 0.5006E-01 0.8108E-01 0.1163E+00
 0.1514E+00 0.1821E+00 0.2056E+00 0.2214E+00 0.2308E+00 0.2355E+00
 0.2369E+00 0.2354E+00 0.2304E+00 0.2200E+00 0.2017E+00 0.1733E+00
 0.1336E+00 0.8410E-01 0.2861E-01

MAX. CONCENTRATION= 0.2861E-01 < ALLOW. CONCENTRATION= 0.5000E-01 MG/L

NEW INITIAL LIQUID PHASE CONCENTRATION (MG/L)

 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.4601E+00
 0.4601E+00 0.4601E+00 0.4601E+00 0.4601E+00 0.4601E+00 0.4601E+00
 0.4601E+00 0.4601E+00 0.4601E+00 0.4601E+00 0.4601E+00 0.4601E+00
 0.4601E+00 0.0000E+00 0.0000E+00

ASSUMED NEW TOTAL CONCENTRATION (MG/KG)

 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.7500E+00
 0.7500E+00 0.7500E+00 0.7500E+00 0.7500E+00 0.7500E+00 0.7500E+00
 0.7500E+00 0.7500E+00 0.7500E+00 0.7500E+00 0.7500E+00 0.7500E+00
 0.7500E+00 0.0000E+00 0.0000E+00

CONCENTRATION DISTRIBUTION AT 400. DAYS MG/L

0.0000E+00 0.1471E-01 0.3903E-01 0.7509E-01 0.1216E+00 0.1745E+00
 0.2271E+00 0.2731E+00 0.3084E+00 0.3321E+00 0.3462E+00 0.3532E+00
 0.3553E+00 0.3531E+00 0.3456E+00 0.3300E+00 0.3026E+00 0.2599E+00
 0.2004E+00 0.1262E+00 0.4292E-01

MAX. CONCENTRATION= 0.4292E-01 < ALLOW. CONCENTRATION= 0.5000E-01 MG/L

NEW INITIAL LIQUID PHASE CONCENTRATION (MG/L)

 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.5367E+00
 0.5367E+00 0.5367E+00 0.5367E+00 0.5367E+00 0.5367E+00 0.5367E+00
 0.5367E+00 0.5367E+00 0.5367E+00 0.5367E+00 0.5367E+00 0.5367E+00
 0.5367E+00 0.0000E+00 0.0000E+00

ASSUMED NEW TOTAL CONCENTRATION (MG/KG)

0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.8750E+00
 0.8750E+00 0.8750E+00 0.8750E+00 0.8750E+00 0.8750E+00 0.8750E+00
 0.8750E+00 0.8750E+00 0.8750E+00 0.8750E+00 0.8750E+00 0.8750E+00
 0.8750E+00 0.0000E+00 0.0000E+00

CONCENTRATION DISTRIBUTION AT 400. DAYS MG/L

0.0000E+00 0.1716E-01 0.4554E-01 0.8760E-01 0.1419E+00 0.2035E+00
 0.2650E+00 0.3187E+00 0.3598E+00 0.3875E+00 0.4039E+00 0.4121E+00
 0.4145E+00 0.4120E+00 0.4032E+00 0.3850E+00 0.3530E+00 0.3032E+00
 0.2338E+00 0.1472E+00 0.5008E-01

MAX. CONCENTRATION AT G.W.T. : 0.5008E-01 MG/L AT 400 DAYS

ALLOWABLE TOTAL CONCENTRATION (MG/KG)

0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.8750E+00
 0.8750E+00 0.8750E+00 0.8750E+00 0.8750E+00 0.8750E+00 0.8750E+00
 0.8750E+00 0.8750E+00 0.8750E+00 0.8750E+00 0.8750E+00 0.8750E+00
 0.8750E+00 0.0000E+00 0.0000E+00

MAXIMUM ALLOWABLE TOTAL CONCENTRATION= 0.8750E+00 MG/KG

EFFLUENT CONCENTRATION AT WATER TABLE

.....

AT EVERY 100 TIME STEPS

.....

TIME DAYS	DISCHARGE FT/DAY	CHEMICAL CONC. MG/L	BIOMASS CONC. MG/L
400.	0.8552E-02	0.5008E-01	0.0000E+00

DISCHARGE AND CUMM. VOL. AT WATER TABLE

.....

AT EVERY 100 TIME STEPS

.....

TIME DAYS	DISCHARGE CUBIC FT/DAY	VOLUME CUBIC FT	CUMM. VOLUME CUBIC FT
400.	0.8552E-02	0.3420E-01	0.1206E+01

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Appendix A

List of Model Input Variables

<AAKM>	Substrate concentration at 1/2 of the μ_m
<AI>	Coefficient a used in the Ragab's expression
<AKC>	Zero order biodegradation coefficient
<AKK>	Endogenous decay rate constant
<AKL>	First order biodegradation coefficient
<AKOC>	Fugacity coefficient
<AKPR>	First order irreversible adsorption rate coefficient
<AKS>	Saturated hydraulic conductivity
<ALAM>	Soil dispersivity
<ALB>	Albedo constant
<ALI>	Mean monthly leaf area index
<ALPHA>	Coefficient α used in the van Genuchten's equation
<AM>	Exponent m used in the Campbell's equation
<AMU>	Specific growth rate of microorganisms, μ_m
<AN>	Coefficient n used in the Mualem's expression
<AN2>	Exponent n used in the van Genuchten's equation
	Coefficient b used in the Clapp and Hornberger's equation
<BE>	Exponent b used in the Ragab's expression
<BET>	Coefficient β used in the Gardner's expression

<BIOMI>	Initial biomass concentration at a particular node
<CONCA>	Allowable liquid phase concentration
<CN>	SCS curve number
<CTOTAL>	Initial total concentration
<DIN>	Simulation start day
<DDA>	Bulk air diffusion coefficient of the chemical
<DDW>	Bulk water diffusion coefficient of the chemical
<DRZ>	Depth of the root zone within the surface cover
<DT>	Time increment
<DZ>	Depth increment
<DZER>	Soil diffusivity corresponding to $\theta = \theta_0$
<EPS>	Convergence criterion for the flow part
<ET>	Value of evapotranspiration rate for the particular time step
<EVTR>	Uniform rate of evapotranspiration
<GAMMA>	Coefficient γ used in the van Genuchten's equation
<HENRY>	Henry's constant, K_H
<IC1>	Main flag of the model; if IC1=0, both flow and mass transport parts will be executed; if IC1=1, only flow part will be executed

- <ICUT> Flag for concentration reduction scheme; if ICUT=0, initial concentration will be reduced; if ICUT=1, depth of contamination will be reduced
- <ID1> Flag for soil surface cover; if ID1=0, soil surface is bare; if ID1=1, soil surface has vegetation
- <ID2> Flag for Penman equation; if ID2=0, aerodynamic term in the equation is not considered; if ID2=1, aerodynamic term in the equation is considered
- <IFL1> Flag for $K - \theta$ relationship; if IFL1=1, Campbell's equation will be used; if IFL1=2, Mualem's equation will be used; if IFL1=3, Ragab's equation will be used; if IFL1=4, van Genuchten's equation will be used
- <IFL2> Flag for $D - \theta$ relationship; if IFL2=1, Clapp and Hornberger's equation will be used; if IFL2=2, Gardner's equation will be used
- <IFL3> Flag for initial moisture content distribution; if IFL3=0, initial moisture content is constant w.r.t. space; if IFL3=1, initial moisture content is variable w.r.t. space
- <IFL4> Flag for precipitation rate distribution; if IFL4=0, precipitation rate is variable w.r.t. time; if IFL4=1, precipitation rate is constant w.r.t. time; if IFL4=2, average values of precipitation data are read from the database
- <IFL5> Flag for evapotranspiration rate distribution; if IFL5=0, evapotranspiration rate is variable w.r.t. time; if IFL5=1, evapotranspiration rate will be computed by either Penman's or Thornthwaite's

- equation; if IFL5=2, evapotranspiration rate will be constant w.r.t. time
- <IFL6> Flag for printing moisture profiles; if IFL6=0, moisture profiles will be printed at a given time interval; if IFL6=1, moisture profiles will not be printed in the output file
- <IFL7> Flag for printing fluxes; if IFL7=0, moisture fluxes will be printed at a given time interval; if IFL7=1, moisture fluxes will not be printed in the output file
- <IFL8> Flag for initial total concentration distribution; if IFL8=0, initial total concentration is constant w.r.t. space; if IFL8=1, initial total concentration is variable w.r.t. space
- <IFL9> Flag for the bottom boundary condition in flow part; if IFL9=0, saturation B.C. will be used; if IFL9=1, gravity drainage B.C. will be used
- <IFL10> Flag for initial biomass concentration distribution; if IFL10=0, initial biomass concentration is constant w.r.t. space; if IFL10=1, initial biomass concentration is variable w.r.t. space
- <IFL11> Type of top B.C. for the mass transport equation; if IFL11=0, $C_L = 0$ condition is used; if IFL11=1, $\partial C_L / \partial z = 0$ condition is used
- <IFL12> Flag for biomass boundary condition; if IFL12=0, biomass B.C. is constant w.r.t. time; if IFL12=1, biomass B.C. is variable w.r.t. time

- <IFL13> Flag for biodegradation solution; if IFL13=0, Monod kinetic model is used (coupled equations); if IFL13=1, substrate limiting conditions are used
- <IFLE> Flag for evapotranspiration calculation method; if IFLE=0, Thornthwaite's expression is used; if IFLE=1, Penman's expression is used
- <IFLT> Flag for mean monthly temperatures; if IFLT=0, mean monthly temperatures are read; if IFLT=1, average values of mean monthly temperatures are used from the database
- <IMONOD> Flag for substrate limiting conditions; if IMONOD=0, zero order equilibrium is assumed, if IMONOD=1, first order equilibrium is assumed
- <INDEX> Flag for type of chemical; if INDEX=0, transport of biodegradable matter is considered; if INDEX=1, transport of nonbiodegradable matter is considered
- <INT> Printout frequency for output purposes, i.e. number of time steps at which values are printed
- <IRUN> Run number for identifying the particular run and output files
- <IUN> Flag for the units used in the model; if IUN=1, FT-DAY units are used; if IUN=2, M-DAY units are used; if IUN=3, IN-DAY units are used; if IUN=4, CM-DAY units are used
- <M> Number of time steps in the time discretization
- <MIN> Simulation start month

<N>	Number of layer interfaces in the space discretization
<OC>	Organic carbon content of the soil
<P>	Precipitation rate for the particular time step
<PR>	Uniform precipitation rate
<PSIR>	Saturation suction head
<RHO>	Soil bulk density
<RR>	Mean monthly solar radiation
<SSH>	Mean monthly percentage of daily possible sunshine
<TD>	Mean monthly dew-point temperature
<THAD>	Air-dry moisture content
<THF>	Field capacity
<THOL>	Constant value of initial moisture content w.r.t. space
<THOLD>	Value of initial moisture content for each node
<THS>	Saturated moisture content
<THW>	Wilting point of the surface soil
<THZER>	Value of θ_0
<TITLE>	A title of the particular run for output purposes
<W>	Mean monthly wind speed at the surface
<TT>	Mean monthly surface temperatures

<UNT>	String value for identifying the constituent being used
<YIN>	Simulation start year
<YEL>	Biomass yield coefficient

Appendix B

Program Listing

CC

C PROGRAM NAME: IMPACT

C VERSION: 1.1

C

C BRIEF PROGRAM DESCRIPTION: One-Dimensional Mass Transport Model
C in partially saturated soils. It
C contains two major parts:

C 1) MOISTURE TRANSPORT

C 2) MASS TRANSPORT

C

C INPUT FILES: Two modes of input:

C 1) INTERACTIVE (Menu Driven)

C 2) BATCH: An input file is read.

C The BINARY FILE (RAIN.BIN) is read

C when actual precipitation data are

C used.

C

C OUTPUT FILES: Output files will be numbered in concert with the

C run number given. The main output file is created

C as (OUTx.DAT), where x will be the run number.

C The file (BCNx.DAT) is created for values of

C bottom concentration versus time and can be used

C to plot results with any plotting routine. Similarly,

C (TCNx.DAT) is used for top concentrations. The file

C (BFXx.DAT) is created for bottom ~~fluxes~~ *moisture* versus

C time for the same purpose. If flow part is run only,

C the file (THTx.DAT) will be created for moisture

C profiles w.r.t. space for selected time steps.

C The file (TTHx.DAT) is similarly the top moisture

C content history. If the C_L=0 b.c. is used, the

C gaseous mass fluxes are written into the file

C (MFXx.DAT) w.r.t. time.

C

C SPECIAL FEATURES (LINKING INSTRUCTIONS, HARDWARE REQUIREMENTS,

C LOGICAL NAMES): This model is developed on a

C VAX/VMS system. However, it can be executed

C on an IBM compatible P.C. A math co-processor

C is strongly recommended for higher execution

C speed.

C

C


```

C
C ORIGINAL AUTHORS AND CREATION DATE: Dr. Nazmi M. Talimcioglu,
C                                     Dr. George P. Korfiatis
C                                     Stevens Institute of Technology
C                                     9/17/1990
C                                     (NJDEP Submission Date)
C

```

C H A N G E L O G

```

C      Date      | Name      | Description
C-----+-----+-----
C  9/17/1990    | N.M.T.    | Draft Version (V1.0)
C-----+-----+-----
C 11/15/1990    | N.M.T.    | Unit conversions for variables are added
C-----+-----+-----
C 11/20/1990    | N.M.T.    | LAI is removed from Thornthwaite's method
C-----+-----+-----
C 11/28/1990    | N.M.T.    | W.B.M. Method is added in subroutine EVAP
C-----+-----+-----
C 11/28/1990    | N.M.T.    | Subroutine INTPOL is added
C-----+-----+-----
C  3/27/1991    | N.M.T.    | Output units are changed to ppm for C_L
C-----+-----+-----
C-----+-----+-----

```

P R O G R A M I M P A C T

```

C-----+-----+-----
C-----+-----+-----
C
C...COMPUTER PROGRAM "IMPACT"
C
C
C
C...THIS PROGRAM MODELS THE MOISTURE FLOW AND TRANSPORT OF MASS
C...IN PARTIALLY SATURATED SOILS. IT IS SUBDIVIDED INTO TWO MAJOR
C...SUB-MODELS: THE MOISTURE MODEL YGRA AND THE SOLUTE TRANSPORT
C...MODEL SOLUTE.
C
C...THE CONTROL IC1 IS USED TO DETERMINE WHICH SUB-MODEL
C...WILL BE EXECUTED.
C-----+-----+-----
C-----+-----+-----

```

```
COMMON/BLK1/M
COMMON/BLK3/THNEW(400),THOLD(400)
COMMON/BLK4/IFL1,IFL2,AKS,THS,THF,AM,AN,AI,BE,B,THAD,AN2,AM2,
      GAMMA,ALPHA
COMMON/BLK5/PSIR,DZER,BET,THZER
COMMON/BLK6/AK(400),DIFF(400),AKM(400),AKP(400),DM(400),DP(400)
COMMON/BLK7/TH(400)
COMMON/BLK8/EPS
COMMON/BLK9/P(2234),ET(2234)
COMMON/BLK10/JT,TIME(2234)
COMMON/BLK11/QOLD(400),QNEW(400),DISCH(400)
COMMON/BLK14/DEP(400)
COMMON/BLK15/UDT,UTHO,UAKS,UDZ
COMMON/BLK16/DZ,DT
COMMON/BLK17/TITLE,IRUN,IC1,IFL8,IFL10,IFL12,
      EVTR,PR,THOL
COMMON/BLK18/AMU,AKK,AAKM,YEL
COMMON/BLK19/BIOMI(400),CTOTAL(400),CONCI(400),H,
      TMAX,INDEX
COMMON/BLK20/UNT
COMMON/BLK23/THSU(2234),D(2234),UPR
COMMON/BLK24/THAV(400),TRTH(400)
COMMON/BLK25/IT,INT
COMMON/BLK26/ICOUNT
COMMON/BLK27/VOLE(2234),VSUM(2234)
COMMON/BLK28/M
COMMON/BLK29/IUNIT,JUNIT,KUNIT
COMMON/BLK30/BELL,BOLD,BLINK,REVERS,CLEAR,HOME,NORMAL
COMMON/BLK40/TCONC(2234),BCONC(2234),BBIOM(2234),BDISCH(2234)
COMMON/BLK41/IFL3,IFL4,IFL5,IFL6,IFL7
COMMON/BLK42/IFL13,IMONOD,AKC,AKL
COMMON/BLK50/AKD,AKPR,DDW,DDA,HENRY,POROS,ALAM,RHO
COMMON/BLK51/ICUT,CONCA
COMMON/BLK52/IFL9
COMMON/BLK53/IUM
COMMON/BLK55/IFL11
COMMON/BLK56/AKOC,OC
COMMON/BLK57/FTIME
COMMON/BLK59/TTH(2,2234)
```

```
C-----
      DIMENSION THIN(400),CNOLD(400),CTEMP(400)
```



```

LOGICAL CUT,FTIME
C-----
CHARACTER*1 ANS,IRUN
CHARACTER*3 VRSN
CHARACTER*80 TITLE,FILNM1,FILNM2
CHARACTER*8 UAKS,UTHF,UTHS,UTHAD,UARE,UDZ,UDT,UPSIR,
      UDZR,UTHZ,UTHO,UPR,UET,UAMU,UAKK,UALAM
CHARACTER*12 UNT
C-----
C...ESCAPE SEQUENCE DECLARATIONS
C-----
CHARACTER ESC*1,BELL*1,CLEAR*4,NORMAL*4,BOLD*4,
      BLINK*4,REVERS*4,HOME*6
ESC      = CHAR(27)
BELL     = CHAR(7)
BOLD     = ESC//'[1m'
BLINK    = ESC//'[5m'
REVERS   = ESC//'[7m'
CLEAR    = ESC//'[2J'
HOME     = ESC//'[O;Of'
NORMAL   = ESC//'[Om'
C-----
C...SETTING PROGRAM MODE
C-----
VRSN='1.1'
C-----
1111 WRITE(6,101)CLEAR,HOME,BOLD,VRSN,NORMAL,REVERS,
      NORMAL,BOLD,NORMAL,BOLD,NORMAL,BOLD,NORMAL,
      BOLD,NORMAL,BELL,BELL
101  FORMAT(1X,3A,10X,'PROGRAM IMPACT v',2A//1X,A,
      ' TYPE ONE OF THE FOLLOWING:',A//
      5X,A,'A- RUN PROGRAM INTERACTIVELY'/
      5X,'B- RUN PROGRAM IN BATCH MODE'//
      5X,'E- EXIT',A//
      1X,'Enter ',A,'A',A,' or ',A,'B',A,' or ',A,'E',A,
      ' : ',2A,$)
      READ(5,100,ERR=1111)ANS
100  FORMAT(A)
      IF(ANS.NE.'A'.AND.ANS.NE.'a'.AND.ANS.NE.'B'.AND.ANS.NE.'b'.
      AND.ANS.NE.'E'.AND.ANS.NE.'e') GOTO 1111
      IF(ANS.EQ.'E'.OR.ANS.EQ.'e') STOP

```

```

      IF(ANS.EQ.'A'.OR.ANS.EQ.'a')THEN
          IUNIT=5
          JUNIT=6
          KUNIT=3
1112  WRITE(6,107)BELL
107   FORMAT(/1X,'ENTER THE FILE NAME TO BE CREATED FOR ',
           'BATCH INPUT : ',A,$)
      READ(6,100,ERR=1112)FILNM2
      OPEN(UNIT=KUNIT,FILE=FILNM2,STATUS='UNKNOWN')
      ELSE
          IUNIT=1
          JUNIT=2
          KUNIT=3
1113  WRITE(6,108)BELL
108   FORMAT(/1X,'ENTER THE FILE NAME TO BE READ : ',A,$)
      READ(5,100,ERR=1113)FILNM1
      OPEN(UNIT=IUNIT,FILE=FILNM1,STATUS='OLD')
      OPEN(UNIT=JUNIT,STATUS='SCRATCH')
      OPEN(UNIT=KUNIT,STATUS='SCRATCH')
      END IF

C-----
C...READ INPUT VARIABLES
C-----
10001 WRITE(JUNIT,1014)BOLD,NORMAL
1014  FORMAT(/1X,'ENTER RUN NUMBER      ',A,'<IRUN> ',A,' : ',A,$)
      READ(IUNIT,100,ERR=10001) IRUN
      IF(IUNIT.NE.1) CALL DATA
      IF(IRUN.EQ.' ') GOTO 10001
      WRITE(KUNIT,100)IRUN

C-----
C...OPEN OUTPUT FILES
C-----
      OPEN(UNIT=25,FILE='BFX'//IRUN//'.DAT',STATUS='NEW')
      OPEN(UNIT=21,FILE='OUT'//IRUN//'.DAT',STATUS='NEW')

C-----
10000 WRITE(JUNIT,1004)BOLD,NORMAL
1004  FORMAT(/1X,'ENTER PROBLEM TITLE ',A,'<TITLE> ',A,' : ',A,$)
      READ(IUNIT,100,ERR=10000) TITLE
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,100)TITLE
C-----

```



```

      WRITE(21,2043) TITLE,IUM
2043  FORMAT('1',///9X,A//9X,'RUN NO : ',A)
C-----
C...READ UNIT CONVENTION
C-----
10031 WRITE(JUNIT,1031)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,
      BOLD,NORMAL,BOLD,NORMAL,REVERS,NORMAL
1031  FORMAT(/1X,A,'ENTER',A//5X,A,'1',A,' : IF <FT-DAY>   UNITS ARE ',
      'USED'/5X,A,'2',A,' : IF <M-DAY>   UNITS ARE USED'/5X,
      A,'3',A,' : IF <INCH-DAY> UNITS ARE USED'/5X,A,'4',A,
      ' : IF <CM-DAY>   UNITS ARE USED'//1X,A,'<IUM>',A,' : ',A,$)
      READ(IUNIT,*,ERR=10031) IUM
      IF(IUNIT.NE.1) CALL DATA
10032  IF(IUM.NE.1.AND.IUM.NE.2.AND.IUM.NE.3.AND.IUM.NE.4) THEN
      WRITE(JUNIT,1032)BLINK,NORMAL,BELL,BELL
1032  FORMAT(/5X,A,'INVALID ENTRY FOR <IUM>, REENTER',A,' : ',
      2A,$)
      READ(IUNIT,*,ERR=10032)IUM
      GOTO 10032
      END IF
      WRITE(KUNIT,*) IUM
C-----
C...UNITS FOR VARIOUS VARIABLES
C-----
      IF(IUM.EQ.1) THEN
      UAKS='FT/DAY'
      UTHF='FT3/FT3'
      UTHS='FT3/FT3'
      UTHAD='FT3/FT3'
      UDZ='FT'
      UDT='DAYS'
      UPSIR='FT'
      UDZR='FT/DAY'
      UTHZ='FT3/FT3'
      UTHO='FT3/FT3'
      UPR='FT/DAY'
      UET='FT/DAY'
      UAMU='1/DAY'
      UAKK='1/DAY'
      UALAM='FT'
      END IF

```

```
IF(IUM.EQ.2) THEN
```

```
    UAKS='M/DAY'
```

```
    UTHF='M3/M3'
```

```
    UTHS='M3/M3'
```

```
    UTHAD='M3/M3'
```

```
    UDZ='M'
```

```
    UDT='DAYS'
```

```
    UPSIR='M'
```

```
    UDZR='M/DAY'
```

```
    UTHZ='M3/M3'
```

```
    UTHO='M3/M3'
```

```
    UPR='M/DAY'
```

```
    UET='M/DAY'
```

```
    UAMU='1/DAY'
```

```
    UAKK='1/DAY'
```

```
    UALAM='M'
```

```
END IF
```

```
IF(IUM.EQ.3) THEN
```

```
    UAKS='IN/DAY'
```

```
    UTHF='IN3/IN3'
```

```
    UTHS='IN3/IN3'
```

```
    UTHAD='IN3/IN3'
```

```
    UDZ='IN'
```

```
    UDT='DAYS'
```

```
    UPSIR='IN'
```

```
    UDZR='IN/DAY'
```

```
    UTHZ='IN3/IN3'
```

```
    UTHO='IN3/IN3'
```

```
    UPR='IN/DAY'
```

```
    UET='IN/DAY'
```

```
    UAMU='1/DAY'
```

```
    UAKK='1/DAY'
```

```
    UALAM='IN'
```

```
END IF
```

```
IF(IUM.EQ.4) THEN
```

```
    UAKS='CM/DAY'
```

```
    UTHF='CM3/CM3'
```

```
    UTHS='CM3/CM3'
```

```
    UTHAD='CM3/CM3'
```

```
    UDZ='CM'
```

```
    UDT='DAYS'
```



```

      UPSIR='CM'
      UDZR='CM/DAY'
      UTHZ='CM3/CM3'
      UTHO='CM3/CM3'
      UPR='CM/DAY'
      UET='CM/DAY'
      UAMU='1/DAY'
      UAKK='1/DAY'
      UALAM='CM'

      END IF

C-----
10004 WRITE(JUNIT,109)REVERS,NORMAL,BOLD,NORMAL,BOLD,
      .
      .      NORMAL,REVERS,NORMAL
109   FORMAT(/1X,A,'ENTER ONE OF THE FOLLOWING:',A//5X,
      .
      .      A,'1',A,' : FOR MOISTURE BALANCE MODEL ONLY'/
      .
      .      5X,A,'0',A,' : FOR BOTH MASS TRANSPORT AND ',
      .
      .      'MOISTURE BALANCE MODELS'//1X,A,'<IC1>',A,' : ',A,$)
      READ(IUNIT,*,ERR=10004) IC1
      IF(IUNIT.NE.1) CALL DATA
10005 IF(IC1.NE.0.AND.IC1.NE.1) THEN
      .
      .      WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
1015   FORMAT(/5X,A,'INVALID ENTRY, REENTER',A,' : ',2A,$)
      READ(IUNIT,*,ERR=10005)IC1
      GOTO 10005

      END IF

      WRITE(KUNIT,*)IC1
      IF(IC1.EQ.0) GO TO 2
      IF(IC1.GT.0) GO TO 3
2     WRITE(21,2048)
2048  FORMAT(///10X,'THIS IS A SIMULATION FOR BOTH MOISTURE ',
      .
      .      'AND SOLUTE TRANSPORT')
      GO TO 4
3     WRITE(21,2049)
2049  FORMAT(///10X,'THIS IS A SIMULATION FOR MOISTURE ',
      .
      .      'TRANSPORT ONLY')
4     WRITE(21,2000)
2000  FORMAT('1',///20X,'***** INPUT DATA FOR SUBPROGRAM YGRA *****')
      WRITE(21,2011)
2011  FORMAT(27X,'.....')
C-----
C...READ AND PRINT FLAGS

```

```

C-----
C
C...IFL1 IS USED TO DETERMINE WHICH FUNCTION WILL BE USED
C...TO EVALUATE THE K VS THETA RELATIONSHIP
C
C...IFL2 IS USED TO DETERMINE WHICH FUNCTION WILL BE USED TO
C...EVALUATE THE D VS THETA RELATIONSHIP
C
C...IFL3 IS USED TO DETERMINE HOW THE INITIAL MOISTURE VALUES
C...WILL BE READ.
C
C...IFL4 IS USED TO DETERMINE HOW THE PRECIPITATION VALUES
C...WILL BE READ
C
C...IFL5 IS USED TO DETERMINE HOW THE EVAPOTRANSPIRATION VALUES
C...WILL BE READ
C
C...IFL6 IS USED TO DETERMINE IF THE MOISTURE PROFILE VALUES
C...WILL BE PRINTED OR NOT
C
C...IFL7 IS USED TO DETERMINE IF THE MOISTURE FLUX VALUES
C...WILL BE PRINTED OR NOT
C
C...IFL8 IS USED TO DETERMINE HOW INITIAL CONCENTRATION WILL BE READ
C
C...IFL9 IS USED TO DETERMINE WHAT KIND OF BOTTOM BC IS USED FOR
C...FLOW EQUATION
C
C...IFL10 IS USED TO DETERMINE HOW INITIAL CONCENTRATION OF
C...MICROORGANISM WILL BE READ
C
C...IFL11 IS USED TO SWITCH TOP B.C. FOR MASS TRANSPORT EQUATION
C
C...IFL12 IS USED TO EXERCISE CONCENTRATION REDUCTION SCHEME
C-----
      WRITE(JUNIT,1016)CLEAR,HOME,BOLD,NORMAL,BELL,BELL
1016  FORMAT(1X,2A,20X,A,'INPUT FLAGS',3A//)
C-----
10006 WRITE(JUNIT,1017)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,
      BOLD,NORMAL,BOLD,NORMAL,REVERS,NORMAL
1017  FORMAT(/1X,A,'ENTER',A//5X,A,'1',A,': IF CAMPBELL'S ',

```



```

      '      K-THETA RELATIONSHIP IS USED'/5X,A,'2',A,
      ': IF MUALEM''S      K-THETA RELATIONSHIP IS USED'/
      5X,A,'3',A,'': IF RAGAB''S      K-THETA RELATIONSHIP ',
      'IS USED'/5X,A,'4',A,'': IF van GENUCHTEN''S K-THETA ',
      'RELATIONSHIP IS USED'//1X,A,'<IFL1>',A,' : ', $)
      READ(IUNIT,*,ERR=10006)IFL1
      IF(IUNIT.NE.1) CALL DATA
10007 IF(IFL1.NE.1.AND.IFL1.NE.2.AND.IFL1.NE.3.AND.IFL1.NE.4) THEN
      WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
      READ(IUNIT,*,ERR=10007)IFL1
      GOTO 10007
      END IF
      WRITE(KUNIT,*)IFL1
      IF(IFL1.EQ.4) THEN
      IFL2=3
      GO TO 10010
      END IF
C-----
10008 WRITE(JUNIT,1018)REVERS,NORMAL,BOLD,NORMAL,BOLD,
      NORMAL,REVERS,NORMAL
1018  FORMAT(/1X,A,'ENTER',A//5X,A,'1',A,'': IF CLAPP & HORNBERGER''S ',
      'D-THETA RELATIONSHIP IS USED'/5X,A,'2',A,
      ': IF GARDNER''S      D-THETA RELATIONSHIP IS USED'
      //1X,A,'<IFL2>',A,' : ', $)
      READ(IUNIT,*,ERR=10008)IFL2
      IF(IUNIT.NE.1) CALL DATA
10009 IF(IFL2.NE.1.AND.IFL2.NE.2) THEN
      WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
      READ(IUNIT,*,ERR=10009)IFL2
      GOTO 10009
      END IF
      WRITE(KUNIT,*)IFL2
C-----
10010 WRITE(JUNIT,1019)REVERS,NORMAL,BOLD,NORMAL,BOLD,
      NORMAL,REVERS,NORMAL
1019  FORMAT(/1X,A,'ENTER',A//5X,A,'0',A,'': IF INITIAL ',
      'MOISTURE CONTENT IS CONSTANT W.R.T. SPACE'/
      5X,A,'1',A,'': IF INITIAL MOISTURE CONTENT ',
      'IS VARIABLE W.R.T. SPACE'//1X,A,'<IFL3>',A,
      ' : ', $)
      READ(IUNIT,*,ERR=10010)IFL3

```

```

      IF(IUNIT.NE.1) CALL DATA
10011 IF(IFL3.NE.O.AND.IFL3.NE.1) THEN
      WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
      READ(IUNIT,*,ERR=10011)IFL3
      GOTO 10011
    END IF
    WRITE(KUNIT,*)IFL3
C-----
10012 WRITE(JUNIT,1020)REVERS,NORMAL,BOLD,NORMAL,BOLD,
      .
      .      NORMAL,BOLD,NORMAL,REVERS,NORMAL
1020  FORMAT(/1X,A,'ENTER',A//5X,A,'O',A,': IF PRECIPITATION ',
      .
      .      'RATE IS VARIABLE W.R.T. TIME'/5X,A,'1',A,
      .
      .      ': IF PRECIPITATION RATE IS CONSTANT W.R.T. TIME'/
      .
      .      5X,A,'2',A,': IF PRECIPITATION RATE WILL BE COMPUTED BY ',
      .
      .      'SUBROUTINE PREP'//
      .
      .      1X,A,'<IFL4>',A,' : ', $)
      READ(IUNIT,*,ERR=10012)IFL4
      IF(IUNIT.NE.1) CALL DATA
10013 IF(IFL4.NE.O.AND.IFL4.NE.1.AND.IFL4.NE.2) THEN
      WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
      READ(IUNIT,*,ERR=10013)IFL4
      GOTO 10013
    END IF
    WRITE(KUNIT,*)IFL4
C-----
10014 WRITE(JUNIT,1021)REVERS,NORMAL,BOLD,NORMAL,BOLD,
      .
      .      NORMAL,BOLD,NORMAL,REVERS,NORMAL
1021  FORMAT(/1X,A,'ENTER',A//5X,A,'O',A,': IF ',
      .
      .      'EVAPOTRANSPIRATION RATE IS VARIABLE W.R.T. TIME'/
      .
      .      5X,A,'1',A,': IF EVAPOTRANSPIRATION RATE WILL ',
      .
      .      'BE COMPUTED BY SUBROUTINE EVAP'/5X,A,'2',A,
      .
      .      ': IF EVAPOTRANSPIRATION RATE IS CONSTANT W.R.T. ',
      .
      .      'TIME'//1X,A,'<IFL5>',A,' : ', $)
      READ(IUNIT,*,ERR=10014)IFL5
      IF(IUNIT.NE.1) CALL DATA
10015 IF(IFL5.NE.O.AND.IFL5.NE.1.AND.IFL5.NE.2) THEN
      WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
      READ(IUNIT,*,ERR=10015)IFL5
      GOTO 10015
    END IF
    WRITE(KUNIT,*)IFL5

```



```

C-----
10016 WRITE(JUNIT,1022)REVERS,NORMAL,BOLD,NORMAL,BOLD,
      .
      .      NORMAL,REVERS,NORMAL
1022  FORMAT(/1X,A,'ENTER',A//5X,A,'O',A,' : IF MOISTURE PROFILE ',
      .
      .      'WILL BE PRINTED AT EACH TIME STEP'/5X,A,'1',A,
      .
      .      ' : IF MOISTURE PROFILE WILL NOT BE PRINTED'//1X,
      .
      .      A,'<IFL6>',A,' : ',A,$)
      READ(IUNIT,*,ERR=10016)IFL6
      IF(IUNIT.NE.1) CALL DATA
10017 IF(IFL6.NE.0.AND.IFL6.NE.1) THEN
      .
      .      WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
      .
      .      READ(IUNIT,*,ERR=10017)IFL6
      .
      .      GOTO 10017
      .
      .      END IF
      .
      .      WRITE(KUNIT,*)IFL6
C-----
10018 WRITE(JUNIT,1023)REVERS,NORMAL,BOLD,NORMAL,BOLD,
      .
      .      NORMAL,REVERS,NORMAL
1023  FORMAT(/1X,A,'ENTER',A//5X,A,'O',A,' : IF MOISTURE FLUX ',
      .
      .      'WILL BE PRINTED AT EACH TIME STEP'/5X,A,'1',A,
      .
      .      ' : IF MOISTURE FLUX WILL NOT BE PRINTED'//1X,
      .
      .      A,'<IFL7>',A,' : ',A,$)
      READ(IUNIT,*,ERR=10018)IFL7
      IF(IUNIT.NE.1) CALL DATA
10019 IF(IFL7.NE.0.AND.IFL7.NE.1) THEN
      .
      .      WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
      .
      .      READ(IUNIT,*,ERR=10019)IFL7
      .
      .      GOTO 10019
      .
      .      END IF
      .
      .      WRITE(KUNIT,*)IFL7
C-----
10071 WRITE(JUNIT,1079)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,
      .
      .      REVERS,NORMAL
1079  FORMAT(/1X,A,'ENTER TYPE OF BOTTOM B.C. FOR FLOW ',
      .
      .      'EQUATION',A//5X,A,'O',A,' : SATURATION ',
      .
      .      'CONDITION [THETA=THETA_sat]'/
      .
      .      5X,A,'1',A,' : GRAVITY FLOW CONDITION [d(THETA)/d(Z)=0]',
      .
      .      //1X,A,'<IFL9>',A,' : ',A,$)
      READ(IUNIT,*,ERR=10071) IFL9
      IF(IUNIT.NE.1) CALL DATA
10072 IF(IFL9.NE.0.AND.IFL9.NE.1) THEN

```

```

        WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
        READ(IUNIT,*,ERR=10072)IFL9
        GOTO 10072
    END IF
    WRITE(KUNIT,*)IFL9
C-----
    IF(IC1.NE.1) THEN
C-----
10055 WRITE(JUNIT,1063)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,
        REVERS,NORMAL
1063  FORMAT(/1X,A,'ENTER',A//5X,A,'O',A,': IF CONSTITUENT '
        'IS BIODEGRADABLE'/5X,A,'1',A,': IF CONSTITUENT IS ',
        'NONBIODEGRADABLE'/1X,A,'<INDEX>',A,': ',A,$)
        READ(IUNIT,*,ERR=10055)INDEX
        IF(IUNIT.NE.1) CALL DATA
10056 IF(INDEX.NE.0.AND.INDEX.NE.1) THEN
        WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
        READ(IUNIT,*,ERR=10056)INDEX
        GOTO 10056
    END IF
    WRITE(KUNIT,*)INDEX
C-----
10022  WRITE(JUNIT,1025)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,
        REVERS,NORMAL
1025  FORMAT(/1X,A,'ENTER TYPE OF TOP B.C. FOR MASS TRANSPORT ',
        'EQUATION',A//5X,A,'O',A,': ZERO LIQUID PHASE ',
        'CONCENTRATION [CL=0]'/5X,A,'1',A,': NO MASS FLUX ',
        'CONDITION          [d(CL)/d(Z)=0]')//
        1X,A,'<IFL11>',A,': ',A,$)
        READ(IUNIT,*,ERR=10022) IFL11
        IF(IUNIT.NE.1) CALL DATA
10023  IF(IFL11.NE.0.AND.IFL11.NE.1) THEN
        WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
        READ(IUNIT,*,ERR=10023)IFL11
        GOTO 10023
    END IF
    WRITE(KUNIT,*)IFL11
C-----
10020  WRITE(JUNIT,1024)REVERS,NORMAL,BOLD,NORMAL,BOLD,
        NORMAL,REVERS,NORMAL
1024  FORMAT(/1X,A,'ENTER',A//5X,A,'O',A,': IF INITIAL ',

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      'TOTAL CONCENTRATION IS CONSTANT ',
      'W.R.T. SPACE'/5X,A,'1',A,'': IF INITIAL ',
      'TOTAL CONCENTRATION IS VARIABLE ',
      'W.R.T. SPACE'//1X,A,'<IFL8>',A,' : ', $)
      READ(IUNIT,*,ERR=10020)IFL8
      IF(IUNIT.NE.1) CALL DATA
10021  IF(IFL8.NE.0.AND.IFL8.NE.1) THEN
          WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
          READ(IUNIT,*,ERR=10021)IFL8
          GOTO 10021
      END IF
      WRITE(KUNIT,*)IFL8
C-----
      IF(INDEX.EQ.0) THEN
C-----
10100  WRITE(JUNIT,1010)REVERS,NORMAL,BOLD,NORMAL,
          BOLD,NORMAL,REVERS,NORMAL
1010  FORMAT(/1X,A,'ENTER',A//5X,A,'0',A,'': IF MONOD KINETICS ',
          'ARE ASSUMED (COUPLED EQUATIONS)'/5X,A,'1',A,
          ': IF EQUILIBRIUM CONDITIONS ARE ASSUMED ',
          '(SINGLE EQUATION)'/1X,A,'<IFL13>',A,' : ', $)
      READ(IUNIT,*,ERR=10100)IFL13
      IF(IUNIT.NE.1) CALL DATA
10101  IF(IFL13.NE.0.AND.IFL13.NE.1) THEN
          WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
          READ(IUNIT,*,ERR=10101)IFL13
          GOTO 10101
      END IF
      WRITE(KUNIT,*)IFL13
C-----
      IF(IFL13.EQ.1) THEN
C-----
10102  WRITE(JUNIT,1011)REVERS,NORMAL,BOLD,NORMAL,
          BOLD,NORMAL,REVERS,NORMAL
1011  FORMAT(/1X,A,'ENTER',A//5X,A,'0',A,'': IF ZERO',
          ' ORDER KINETICS ARE USED (Rs=k0)'/
          5X,A,'1',A,'': IF FIRST ORDER KINETICS ARE USED ',
          '(Rs=k1*C_L)'/1X,A,'<IMONOD>',A,' : ', $)
      READ(IUNIT,*,ERR=10102)IMONOD
      IF(IUNIT.NE.1) CALL DATA
10103  IF(IMONOD.NE.0.AND.IMONOD.NE.1) THEN

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        WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
        READ(IUNIT,*,ERR=10103)IMONOD
        GOTO 10103
    END IF
    WRITE(KUNIT,*)IMONOD
C-----
    ELSE
C-----
10024    WRITE(JUNIT,1026)REVERS,NORMAL,BOLD,NORMAL,BOLD,
        NORMAL,REVERS,NORMAL
10026    FORMAT(/1X,A,'ENTER',A//5X,A,'O',A,': IF INITIAL ',
        'BIOMASS CONCENTRATION IS CONSTANT ',
        'W.R.T. SPACE'/5X,A,'1',A,': IF INITIAL ',
        'BIOMASS CONCENTRATION IS VARIABLE ',
        'W.R.T. SPACE'//1X,A,'<IFL10>',A,': ',A,$)
        READ(IUNIT,*,ERR=10024)IFL10
        IF(IUNIT.NE.1) CALL DATA
10025    IF(IFL10.NE.0.AND.IFL10.NE.1) THEN
        WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
        READ(IUNIT,*,ERR=10025)IFL10
        GOTO 10025
    END IF
    WRITE(KUNIT,*)IFL10
    END IF
C-----
    END IF
C-----
10028    WRITE(JUNIT,1028)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,
        REVERS,NORMAL
10028    FORMAT(/1X,A,'ENTER',A//5X,A,'O',A,': IF CONCENTRATION ',
        'REDUCTION SCHEME IS NOT EXERCISED'/5X,A,'1',A,
        ': IF CONCENTRATION REDUCTION SCHEME IS EXERCISED'//
        1X,A,'<IFL12>',A,': ',A,$)
        READ(IUNIT,*,ERR=10028) IFL12
        IF(IUNIT.NE.1) CALL DATA
10029    IF(IFL12.NE.0.AND.IFL12.NE.1) THEN
        WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
        READ(IUNIT,*,ERR=10029)IFL12
        GOTO 10029
    END IF
    WRITE(KUNIT,*)IFL12

```



```

C-----
      IF(IFL12.EQ.1) THEN
C-----
10002      WRITE(JUNIT,1013)REVERS,NORMAL,BOLD,NORMAL,
           BOLD,NORMAL,REVERS,NORMAL
1013      FORMAT(/1X,A,'ENTER',A//5X,A,'O',A,': FOR INITIAL ',
           'CONCENTRATION REDUCTION'/5X,A,'1',A,
           ': FOR CONTAMINATION DEPTH REDUCTION'//1X,
           A,'<ICUT>',A,' : ',,$)
      READ(IUNIT,*,ERR=10002) ICUT
      IF(IUNIT.NE.1) CALL DATA
10003      IF(ICUT.NE.0.AND.ICUT.NE.1) THEN
           WRITE(JUNIT,1015)BLINK,NORMAL,BELL,BELL
           READ(IUNIT,*,ERR=10003) ICUT
           GOTO 10003
      END IF
      WRITE(KUNIT,*)ICUT
C-----
10069      WRITE(JUNIT,1077)BOLD,NORMAL
1077      FORMAT(/1X,'ENTER THE ALLOWABLE LIQUID PHASE ',
           'CONCENTRATION IN [ppb] ',A,'<CONCA>',A,' : ',,$)
      READ(IUNIT,*,ERR=10069)CONCA
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)CONCA
C-----
C...CONVERT Calow [ppb] TO APPROPRIATE UNITS
C-----
      IF(IUN.EQ.1) CONCA=2.83168E-5*CONCA
      IF(IUN.EQ.2) CONCA=1E-3*CONCA
      IF(IUN.EQ.3) CONCA=1.6387E-8*CONCA
      IF(IUN.EQ.4) CONCA=1E-9*CONCA
C-----
      END IF
C-----
      END IF
C-----
      WRITE(21,2001) IFL1,IFL2,IFL3,IFL4,IFL5,IFL6,IFL7,
           IFL8,IFL9,IFL10,IFL11,IFL12
2001      FORMAT(/2X,'FLAG1 =',I2,5X,'FLAG2 =',I2,5X,'FLAG3 =',
           I2,5X,'FLAG4 =',I2/2X,'FLAG5 =',I2,5X,'FLAG6 =',
           I2,5X,'FLAG7 =',I2,5X,'FLAG8 =',I2/2X,'FLAG9 =',

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      I2,5X,'FLAG10=',I2,5X,'FLAG11=',I2,5X,'FLAG12=',I2)
C-----
C...READ CHARACTERISTIC VALUES FOR PARTICULAR SOIL ZONE
C
C...AKS IS THE SATURATED HYDRAULIC CONDUCTIVITY
C...THF IS THE FIELD CAPACITY MOISTURE CONTENT
C...THS IS THE SATURATION MOISTURE CONTENT
C...THAD IS THE AIR-DRY MOISTURE CONTENT
C-----
      WRITE(21,2044)
      WRITE(21,2045)
2044  FORMAT(///10X,'HYDRAULIC PROPERTIES AND SIMULATION PARAMETERS')
2045  FORMAT(10X,'.....'//)
      WRITE(JUNIT,1029)CLEAR,HOME,BOLD,NORMAL,BELL,BELL
1029  FORMAT(1X,2A,10X,A,'INPUT SOIL PARAMETERS',3A//)
10030 WRITE(JUNIT,1030)REVERS,NORMAL,BOLD,NORMAL,BOLD,
      NORMAL,BOLD,NORMAL,BOLD,NORMAL,
      REVERS,NORMAL
1030  FORMAT(/1X,A,'ENTER',A//5X,'THE VALUE OF SATURATED ',
      'HYDRAULIC CONDUCTIVITY',T55,A,'<AKS>',A/5X,
      'THE VALUE OF FIELD CAPACITY MOISTURE CONTENT',
      T55,A,'<THF>',A/5X,'THE VALUE OF SATURATION ',
      'MOISTURE CONTENT',T55,A,'<THS>',A/5X,
      'THE VALUE OF AIR-DRY MOISTURE CONTENT',T55,
      A,'<THAD>',A//1X,A,'RESPECTIVELY',A,' : ',A,$)
      READ(IUNIT,*,ERR=10030)AKS,THF,THS,THAD
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)AKS,THF,THS,THAD
C-----
      WRITE(21,2002)AKS,UAKS,THF,UTHF,THS,UTHS,THAD,UTHAD
2002  FORMAT(/2X,'SATURATED HYDRAULIC CONDUCTIVITY =' ,F10.4,2X,
      A//2X,'FIELD CAPACITY MOISTURE CONTENT =' ,F10.4,2X,
      A//2X,'SATURATION MOISTURE CONTENT =' ,F10.4,2X,
      A//2X,'AIR-DRY MOISTURE CONTENT =' ,F10.4,2X,A)
C-----
C...READ SPATIAL AND TIME INCREMENTS
C-----
10037 WRITE(JUNIT,1037)REVERS,NORMAL,BOLD,NORMAL,
      BOLD,NORMAL,REVERS,NORMAL
1037  FORMAT(/1X,A,'ENTER',A//5X,'DEPTH INCREMENT',T25,
      A,'<DZ>',A/5X,'TIME INCREMENT',T25,A,'<DT>',A

```



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      //1X,A,'RESPECTIVELY',A,' : ',,$)
      READ(IUNIT,*,ERR=10037)DZ,DT
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)DZ,DT
      WRITE(21,2003) DZ,UDZ,DT,UDT
2003  FORMAT(/2X,'DEPTH INCREMENT           =' ,F10.4,2X,A/
      /2X,'TIME INCREMENT           =' ,F10.4,2X,A)
C-----
10040 WRITE(JUNIT,1040)BOLD,NORMAL
1040  FORMAT(/1X,'ENTER THE VALUE OF PRINTOUT FREQUENCY ',
      '(TIME INTERVAL) ',A,'<INT>',A,' : ',,$)
      READ(IUNIT,*,ERR=10040)INT
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)INT
      WRITE(21,2009)INT
2009  FORMAT(/5X,'*** OUTPUT PRINTED EVERY ',I5,
      ' TIME INCREMENTS ***')
C-----
C...READ CONVERGENCE CRITERIA
C
C...EPS IS THE ITERATION CONVERGENCE CRITERION
C-----
10041 WRITE(JUNIT,1041)BOLD,NORMAL
1041  FORMAT(/1X,'ENTER THE VALUE OF ITERATION CONVERGENCE ',
      'CRITERION ',A,'<EPS>',A,' : ',,$)
      READ(IUNIT,*,ERR=10041)EPS
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)EPS
      IF(EPS.EQ.0.0)EPS=0.001
      WRITE(21,2020)EPS
2020  FORMAT(/2X,'EPSILON           =' ,F13.6)
C-----
C...READ NUMBER OF LAYER INTERFACES AND NUMBER OF TIME STEPS
C
C...N IS THE NUMBER OF LAYER INTERFACES ,NUMBER OF LAYERS IS N-1
C...M IS THE NUMBER OF TIME STEPS
C-----
10042 WRITE(JUNIT,1042)REVERS,NORMAL,BOLD,NORMAL,BOLD,
      NORMAL,REVERS,NORMAL
1042  FORMAT(/1X,A,'ENTER',A//5X,'NUMBER OF NODES OR LAYER ',
      'INTERFACES',T50,A,'<N>',A/5X,'NUMBER OF TIME ',

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```

      'STEPS',T50,A,'<M>',A//1X,A,'RESPECTIVELY',A,
      ' : ',,$)
      READ(IUNIT,*,ERR=10042)N,M
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)N,M
      WRITE(21,2004)N,M
2004  FORMAT(/2X,'NUMBER OF LINES           =',I6/
      /2X,'NUMBER OF TIME STEPS          =',I6)
      NM=N-1
C-----
C...READ PARAMETERS REQUIRED FOR COMPUTATION OF K AND D
C-----
      IF(IFL1.EQ.1) GO TO 102
      IF(IFL1.EQ.2) GO TO 103
      IF(IFL1.EQ.3) GO TO 104
      IF(IFL1.EQ.4) GO TO 111
102  WRITE(JUNIT,1043)BOLD,NORMAL
1043  FORMAT(/1X,'ENTER THE VALUE OF EXPONENT M IN ',
      'CAMPBELL'S K-THETA EXPRESSION ',A,'<AM>',
      A,' : ',,$)
      READ(IUNIT,*,ERR=102)AM
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)AM
      WRITE(21,2013)AM
2013  FORMAT(/2X,'COEFFICIENT <AM>           =',F10.4)
      GO TO 200
C-----
103  WRITE(JUNIT,1044)BOLD,NORMAL
1044  FORMAT(/1X,'ENTER THE VALUE OF n IN MUALEM'S ',
      'K-THETA EXPRESSION ',A,'<AN>',A,' : ',,$)
      READ(IUNIT,*,ERR=103)AN
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)AN
      WRITE(21,2014)AN
2014  FORMAT(/2X,'COEFFICIENT <AN>           =',F10.4)
      GO TO 200
C-----
104  WRITE(JUNIT,1045)REVERS,NORMAL,BOLD,NORMAL,BOLD,
      NORMAL,REVERS,NORMAL
1045  FORMAT(/1X,A,'ENTER',A//5X,'COEFFICIENT A',T55,A,'<AI>',
      A/5X,'AND EXPONENT b IN RAGAB'S K-THETA ',

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      'EXPRESSION',T55,A,'<BE>',A//1X,A,
      'RESPECTIVELY',A,' : ', '$)
      READ(IUNIT,*,ERR=104)AI,BE
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)AI,BE
      WRITE(21,2015)AI,BE
2015  FORMAT(/2X,'COEFFICIENT <AI>                =',F10.4/
      /2X,'COEFFICIENT <BE>                =',F10.4)
      GO TO 200

C-----
111  WRITE(JUNIT,1080)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,BOLD,
      NORMAL,REVERS,NORMAL
1080  FORMAT(/1X,A,'ENTER van GENUCHTEN PARAMETERS',A//5X,'GAMMA',T30,
      A,'<GAMMA>',A/5X,'EXPONENT n',T30,A,'<AN2>',A/5X,'ALPHA',
      T30,A,'<ALPHA>',A//1X,A,'RESPECTIVELY',A,' : ', '$)
      READ(IUNIT,*,ERR=111)GAMMA,AN2,ALPHA
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)GAMMA,AN2,ALPHA
      WRITE(21,2021)GAMMA,AN2,ALPHA
2021  FORMAT(/2X,'COEFFICIENT <GAMMA>            =',F10.4/
      /2X,'COEFFICIENT <AN2>                =',F10.4/
      /2X,'COEFFICIENT <ALPHA>            =',F10.4)
      AN2=1-1/AN2
      GO TO 201
200  IF(IFL2.EQ.1) GO TO 105
      IF(IFL2.EQ.2) GO TO 106

C-----
105  WRITE(JUNIT,1046)REVERS,NORMAL,BOLD,NORMAL,BOLD,
      NORMAL,REVERS,NORMAL
1046  FORMAT(/1X,A,'ENTER',A//5X,'THE COEFFICIENT b AND',
      T70,A,'<B>',A/5X,'THE VALUE OF SATURATION ',
      'SUCTION HEAD IN CAMPBELL'S EXPRESSION',
      T70,A,'<PSIR>',A//1X,A,'RESPECTIVELY',A,
      ' : ', '$)
      READ(IUNIT,*,ERR=105)B,PSIR
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)B,PSIR
      WRITE(21,2016)B,PSIR,UPSIR
2016  FORMAT(/2X,'COEFFICIENT <B>                =',F10.4/
      /2X,'SATURATION SUCTION HEAD            =',F10.4,2X,A)
      BP=B+1

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```

      GO TO 201
C-----
106  WRITE(JUNIT,1048)REVERS,NORMAL,BOLD,NORMAL,
      .
      .      BOLD,NORMAL,BOLD,NORMAL,REVERS,NORMAL
1048  FORMAT(/1X,A,'ENTER',A//5X,'THE VALUE OF DIFFUSIVITY ',
      .      'CORRESPONDING TO THETA=THETA_O',T65,A,'<DZER>',
      .      A/5X,'THE VALUE OF COEFFICIENT BETA',T65,
      .      A,'<BET>',A/5X,'AND THE VALUE OF THETA_O IN ',
      .      'GARDNER'S EXPRESSION',T65,A,'<THZER>',
      .      A//1X,A,'RESPECTIVELY',A,' : ',A,$)
      READ(IUNIT,*,ERR=106)DZER,BET,THZER
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)DZER,BET,THZER
      WRITE(21,2017)DZER,UDZR,BET,THZER,UTHZ
2017  FORMAT(/2X,'D_ZERO'                                =',F10.4,2X,A/
      .      /2X,'COEFFICIENT <BET>'                    =',F10.4/
      .      /2X,'THETA_ZERO'                            =',F10.4,2X,A)
C-----
C...READ INITIAL VALUES OF MOISTURE
C-----
201  IF(IFL3.EQ.0) GO TO 202
C-----
      DO 11 IJ=1,N
10047 WRITE(JUNIT,1052)IJ,BOLD,IJ,NORMAL
1052  FORMAT(/1X,'ENTER THE VALUE OF INITIAL MOISTURE ',
      .      'CONTENT FOR MODE ',I3,2X,A,'<THOLD('',I3,'')>',
      .      A,' : ',A,$)
      READ(IUNIT,*,ERR=10047)THOLD(IJ)
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)THOLD(IJ)
11    CONTINUE
      GO TO 203
C-----
202  WRITE(JUNIT,1053)BOLD,NORMAL
1053  FORMAT(/1X,'ENTER THE CONSTANT VALUE OF INITIAL ',
      .      'MOISTURE CONTENT ',A,'<THOL>',A,' : ',A,$)
      READ(IUNIT,*,ERR=202)THOL
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)THOL
      DO 204 I=1,N
204  THOLD(I)=THOL

```



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203  CONTINUE
      WRITE(21,2005) UTHO
2005  FORMAT(/30X,'INITIAL MOISTURE CONTENT',2X,'(',A,
      .      ')/30X,'.....')
      IF(IFL3.EQ.0) THEN
          WRITE(21,2018) THOLD(1)
2018  FORMAT(23X,F10.4,3X,'CONSTANT FOR ALL NODES')
      ELSE
          WRITE(21,2006) (THOLD(I),I=1,N)
2006  FORMAT(1X,10F10.4)
      END IF
C-----
      BP=B+1
C-----
C...READ PRECIPITATION RATES
C
C...P IS THE PRECIPITATION RATE PER TIME STEP
C-----
      IF(IFL4.GT.0) GO TO 206
C-----
      DO 12 IJ=1,N
10050 WRITE(JUNIT,1056)IJ,BOLD,IJ,NORMAL
1056  FORMAT(/1X,'ENTER THE VALUE OF PRECIPITATION RATE ',
      .      'FOR TIME STEP ',I3,2X,A,'<P(',I3,')>',A,' : ',%)
      READ(IUNIT,*,ERR=10050)P(IJ)
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)P(IJ)
12    CONTINUE
      GO TO 410
C-----
206  IF(IFL4.EQ.2) THEN
      CALL PREP
      GOTO 410
      END IF
C-----
      WRITE(JUNIT,1057)BOLD,NORMAL
1057  FORMAT(/1X,'ENTER THE UNIFORM PRECIPITATION RATE ',
      .      A,'<PR>',A,' : ',%)
      READ(IUNIT,*,ERR=206)PR
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)PR

```

APPENDIX B. PROGRAM LISTING

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```

      DO 207 JP=1,M
207   P(JP)=PR
C-----
410   WRITE(21,2007) UPR
2007  FORMAT(/32X,'INFILTRATION RATE',2X,'(',A,')'
      /32X,'.....'/)
      IF(IFL4.EQ.1) THEN
          WRITE(21,2019)P(1)
2019   FORMAT(23X,F10.4,3X,'CONSTANT FOR ALL TIME STEPS')
      ELSE
          WRITE(21,2006) (P(JP), JP=1,M)
      END IF
C-----
C...READ EVAPOTRANSPIRATION RATES
C
C...ET IS THE EVAPOTRANSPIRATION RATE PER TIME STEP
C-----
      IF(IFL5.EQ.1) GO TO 213
      IF(IFL5.EQ.2) GO TO 209
C-----
      DO 13 IJ=1,M
10053 WRITE(JUNIT,1060)IJ,BOLD,IJ,NORMAL
1060  FORMAT(/1X,'ENTER EVAPOTRANSPIRATION RATE FOR TIME STEP ',
      I3,2X,A,'<ET(',I3,')>',A,' : ',,$)
      READ(IUNIT,*,ERR=10053)ET(IJ)
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)ET(IJ)
13    CONTINUE
      GO TO 208
C-----
209   WRITE(JUNIT,1061)BOLD,NORMAL
1061  FORMAT(/1X,'ENTER THE UNIFORM RATE OF EVAPOTRANSPIRATION ',
      A,'<EVTR>',A,' : ',,$)
      READ(IUNIT,*,ERR=209)EVTR
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)EVTR
      DO 210 JP=1,M
210   ET(JP)=EVTR
208   WRITE(21,2022)UET
2022  FORMAT(/30X,'EVAPOTRANSPIRATION RATE',2X,'(',A,')'
      /30X,'.....'/)

```



```

      IF(IFL5.EQ.2) THEN
        WRITE(21,2019) ET(1)
      ELSE
        WRITE(21,2006) (ET(JP),JP=1,M)
      END IF
213  CONTINUE
      WRITE(21,2028)
2028 FORMAT(///)
C-----
      IF(IC1.GT.0) GOTO 7700
C-----
      WRITE(21,700)
700  FORMAT('1',///20X,'***** INPUT DATA FOR MASS TRANSPORT ',
           'MODEL *****'/20X,
           ' .....'//)
C-----
      H=DT
      TMAX=DT*M
C-----
10057 WRITE(JUNIT,1064)BOLD,NORMAL
1064 FORMAT(/1X,'ENTER TYPE OF CONSTITUENT CONSIDERED ',A,
           '<UNT>',A,' : ',,$)
      READ(IUNIT,100,ERR=10057)UNT
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,100)UNT
C-----
      IF(IFL8.EQ.1) GO TO 3013
C-----
10060 WRITE(JUNIT,1067)BOLD,NORMAL
1067 FORMAT(/1X,'ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN ',
           '[MG/KG] ',A,'<CTOTAL(1)>',A,' : ',,$)
      READ(IUNIT,*,ERR=10060)CTOTAL(1)
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*) CTOTAL(1)
      DO 3014 I=2,N
3014  CTOTAL(I)=CTOTAL(1)
      IF(IFL11.EQ.0) CTOTAL(1)=0.0
      GOTO 3005
C-----
3013  CTOTAL(1)=0.0
      NMN=1

```

APPENDIX B. PROGRAM LISTING

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```

      IF(IFL11.EQ.0) NMN=2
      DO 16 IJ=NMN,N
10062 WRITE(JUNIT,1069)(IJ-1)*DZ,UDZ,BOLD,IJ,NORMAL
1069  FORMAT(/1X,'ENTER THE VALUE OF INITIAL TOTAL CONCENTRATION IN ',
           ' [MG/KG] ' /1X,'AT DEPTH ',F6.2,1X,A,T58,A,'<CTOTAL(' ,I3,
           ')>',A,' : ',,$)
      READ(IUNIT,*,ERR=10062)CTOTAL(IJ)
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*) CTOTAL(IJ)
16   CONTINUE
C-----
3005  WRITE(JUNIT,1071)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,
           BOLD,NORMAL,BOLD,NORMAL,REVERS,NORMAL
1071  FORMAT(/1X,A,'ENTER',A//5X,'BULK WATER DIFFUSION ',
           ' COEFFICIENT IN [M^2/DAY]',T55,A,'<DDW>',A/5X,
           ' BULK AIR  DIFFUSION COEFFICIENT IN [M^2/DAY]',
           T55,A,'<DDA>',A/5X,'HENRY'S CONSTANT ',
           '[GASEOUS/LIQUID]',T55,A,'<HENRY>',A/5X,
           ' FUGACITY COEFFICIENT IN [ML/GR]',T55,A,'<AKOC>',
           A//1X,A,'RESPECTIVELY',A,' : ',,$)
      READ(IUNIT,*,ERR=3005)DDW,DDA,HENRY,AKOC
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)DDW,DDA,HENRY,AKOC
C-----
C...CONVERT DDA AND DDW TO APPROPRIATE UNITS, INVERT HENRY'S CONSTANT
C-----
      IF(IUN.EQ.1) THEN
          DDA=10.76391*DDA
          DDW=10.76391*DDW
      ELSE
          IF(IUN.EQ.3) THEN
              DDA=1550.0031*DDA
              DDW=1550.0031*DDW
          ELSE
              IF(IUN.EQ.4) THEN
                  DDA=1E4*DDA
                  DDW=1E4*DDW
              END IF
          END IF
      END IF
      END IF
C-----

```



```

HENRY=1./HENRY
C-----
10036 WRITE(JUNIT,1036)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,
      BOLD,NORMAL,BOLD,NORMAL,REVERS,NORMAL
1036  FORMAT(/1X,A,'ENTER',A//5X,'DESORPTION COEFFICIENT OF ',
      'SOIL IN [ML/GR/DAY] ',T55,A,'<AKPR>',
      A/5X,'ORGANIC CARBON CONTENT OF SOIL IN [%] ',
      T55,A,' <OC>',A/5X,'DISPERSIVITY OF SOIL ',
      T55,A,'<ALAM>',A/5X,'BULK DENSITY OF SOIL ',
      ' IN [GR/CM3] ',T55,A,' <RHO>',A//1X,A,
      ' RESPECTIVELY',A,' : ', $)
      READ(IUNIT,*,ERR=10036)AKPR,OC,ALAM,RHO
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)AKPR,OC,ALAM,RHO
C-----
C...COMPUTE ADSORPTION COEFFICIENT IN ML/GR
C-----
      OC=OC/100.
      AKD=OC*AKOC
C-----
C...CONVERT RHO, AKPR, AND AKD TO APPROPRIATE UNITS
C-----
      IF(IUN.EQ.1) THEN
          RHO=2.8316847E4*RHO
          AKPR=3.53146E-5*AKPR
          AKD=3.53146E-5*AKD
      ELSE
          IF(IUN.EQ.2) THEN
              RHO=1E6*RHO
              AKPR=1E-6*AKPR
              AKD=1E-6*AKD
          ELSE
              IF(IUN.EQ.3) THEN
                  RHO=16.387064*RHO
                  AKPR=6.10237E-2*AKPR
                  AKD=6.10237E-2*AKD
              END IF
          END IF
      END IF
C-----
C...ASSIGN POROSITY FOR EACH SOIL

```

```

C-----
      POROS=THS
C-----
C...CONVERT TOTAL CONC. TO APPROPRIATE UNITS
C-----
      DO 17 JJ=1,N
17      CTEMP(JJ)=1E-6*RHO*CTOTAL(JJ)
C-----
C...CONVERT TOTAL CONC. TO LIQUID PHASE CONC.
C-----
      DO 94 KK=1,N
94      CONCI(KK)=CTEMP(KK)*HENRY/((HENRY-1)*THOLD(KK)+
          HENRY*RHO*AKD+POROS)
C-----
      IF(INDEX.EQ.1)GO TO 244
C-----
      IF(IFL13.EQ.1) THEN
          IF(IMONOD.EQ.0) THEN
10104      WRITE(JUNIT,1012)BOLD,NORMAL
1012      FORMAT(/1X,'ENTER ZERO ORDER MONOD COEFFICIENT',
          ' FOR SOIL IN [MG/L/DAY]',2X,A,
          '<AKC>',A,' : ', '$)
          READ(IUNIT,*,ERR=10104)AKC
          IF(IUNIT.NE.1) CALL DATA
          WRITE(KUNIT,*)AKC
          ELSE
10105      WRITE(JUNIT,1050)BOLD,NORMAL
1050      FORMAT(/1X,'ENTER FIRST ORDER MONOD COEFFICIENT',
          ' FOR SOIL IN [1/DAY]',2X,A,'<AKL>',A,
          ' : ', '$)
          READ(IUNIT,*,ERR=10105)AKL
          IF(IUNIT.NE.1) CALL DATA
          WRITE(KUNIT,*)AKL
          END IF
C-----
      ELSE
C-----
10065      WRITE(JUNIT,1073)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,
          BOLD,NORMAL,BOLD,NORMAL,REVERS,NORMAL
1073      FORMAT(/1X,A,'ENTER',A//5X,'SPECIFIC GROWTH RATE OF ',
          'MICROORGANISMS IN [1/DAY]',T58,A,'<AMU>',A/5X,

```



```

      'ENDOGENEOUS DECAY RATE CONSTANT IN [1/DAY]',T58,A,
      '<AKK>',A/5X,'SUBSTRATE CONCENTRATION AT 1/2 OF ',
      '<AMU> IN [MG/L]',T58,A,'<AAKM>',A/5X,
      'BIOMASS YIELD COEFFICIENT',T58,A,'<YEL>',A/1X,A,
      'RESPECTIVELY',A,' : ',)$)
      READ(IUNIT,*,ERR=10065)AMU,AKK,AAKM,YEL
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)AMU,AKK,AAKM,YEL
      END IF
C-----
      IF(IFL13.EQ.1) GOTO 3012
C-----
      IF(IFL10.EQ.1) GO TO 3010
C-----
10068 WRITE(JUNIT,1076)BOLD,NORMAL
1076  FORMAT(/1X,'ENTER THE CONSTANT VALUE OF INITIAL BIOMASS ',
      'CONC. [MG/L] ',A,'<BIOMI(1)>',A,' : ',)$)
      READ(IUNIT,*,ERR=10068)BIOMI(1)
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)BIOMI(1)
C-----
      DO 3017 I=2,N
3017  BIOMI(I)=BIOMI(1)
C-----
      GO TO 3012
C-----
3010  DO 19 IJ=1,N
10070 WRITE(JUNIT,1078)(IJ-1)*DZ,UDZ,BOLD,IJ,NORMAL
1078  FORMAT(/1X,'ENTER THE VALUE OF INITIAL BIOMASS CONC. ',
      '[MG/L] '/1X,'AT DEPTH ',F6.2,1X,A,T55,A,'<BIOMI(',I3,
      ')>',A,' : ',)$)
      READ(IUNIT,*,ERR=10070)BIOMI(IJ)
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)BIOMI(IJ)
19    CONTINUE
C-----
3012  WRITE(21,719)
719   FORMAT(20X,'THIS IS A SIMULATION FOR BIODEGRADABLE MATTER'//)
      WRITE(21,900)INT,UNT
900   FORMAT(10X,'PRINTOUT FREQUENCY                =',I5//
      '      10X,'NATURE OF THE SUBSTRATE            =',1X,A/)

```

```

C-----
      IF(IFL13.EQ.0) THEN
C-----
      WRITE(21,901)AMU,UAMU,AKK,UAKK,AAKM,'MG/L',YEL
901  FORMAT(10X,'BIOMASS SPECIFIC GROWTH RATE           =',E14.4,2X,A//
      .      10X,'ENDOGENOUS DECAY CONSTANT           =',E14.4,2X,A//
      .      10X,'SUBSTRATE CONC. AT 1/2 OF MU_m       =',E14.4,2X,A//
      .      10X,'BIOMASS YIELD COEFFICIENT           =',E14.4//)
C-----
C...CONVERT AAKM TO APPROPRIATE UNITS
C-----
      IF(IUN.EQ.1) AAKM=2.83168E-2*AAKM
      IF(IUN.EQ.3) AAKM=1.6387E-5*AAKM
      IF(IUN.EQ.4) AAKM=1E-6*AAKM
C-----
      ELSE
C-----
      IF(IMONOD.EQ.0) WRITE(21,903)AKC,'MG/L ',UAMU
903  FORMAT(10X,'ZERO ORDER MONOD COEFF. FOR SOIL ',
      .      '      =',E14.4,2X,2A//)
      IF(IMONOD.EQ.1) WRITE(21,904)AKL,UAMU
904  FORMAT(10X,'FIRST ORDER MONOD COEFF. FOR SOIL ',
      .      '      =',E14.4,2X,A//)
C-----
C...CONVERT AKC TO APPROPRIATE UNITS
C-----
      IF(IUN.EQ.1) THEN
        AKC=2.83168E-2*AKC
      ELSE
        IF(IUN.EQ.3) THEN
          AKC=1.6387E-5*AKC
        ELSE
          IF(IUN.EQ.4) THEN
            AKC=1E-6*AKC
          END IF
        END IF
      END IF
C-----
      END IF
C-----
      IF(IUN.EQ.1) THEN

```



```

WRITE(21,902) AKOC,'ML/GR',ALAM,UALAM,
      2.8316847E4*AKD,'ML/GR',
      2.8316847E4*AKPR,'ML/GR ',UAKK,
      9.2903E-2*DDW,'M2/DAY',9.2903E-2*DDA,'M2/DAY',
      1/HENRY,3.53146E-5*RHO,'GR/CM3'
ELSE
  IF(IUN.EQ.2) THEN
    WRITE(21,902) AKOC,'ML/GR',ALAM,UALAM,
      1E6*AKD,'ML/GR',
      1E6*AKPR,'ML/GR ',UAKK,
      DDW,'M2/DAY',DDA,'M2/DAY',
      1/HENRY,1E-6*RHO,'GR/CM3'
  ELSE
    IF(IUN.EQ.3) THEN
      WRITE(21,902) AKOC,'ML/GR',ALAM,UALAM,
      16.387064*AKD,'ML/GR',
      16.387064*AKPR,'ML/GR ',UAKK,
      6.4516E-4*DDW,'M2/DAY',6.4516E-4*DDA,
      'M2/DAY',1/HENRY,6.10237E-2*RHO,
      'GR/CM3'
    ELSE
      IF(IUN.EQ.4) THEN
        WRITE(21,902) AKOC,'ML/GR',ALAM,UALAM,
          AKD,'ML/GR',AKPR,'ML/GR ',
          UAKK,1E-4*DDW,'M2/DAY',1E-4*DDA,
          'M2/DAY',1/HENRY,RHO,'GR/CM3'
      END IF
    END IF
  END IF
END IF
902  FORMAT(/20X,'SOIL '//
      10X,'FUGACITY COEFFICIENT           =' ,E14.4,2X,A//
      10X,'SOIL DISPERSIVITY              =' ,F10.4,2X,A//
      10X,'FIRST ORDER ADSORPTION COEFFICIENT =' ,E14.4,2X,A//
      10X,'FIRST ORDER DESORPTION COEFFICIENT =' ,E14.4,2X,2A//
      10X,'BULK WATER DIFFUSION COEFFICIENT =' ,E14.4,2X,A//
      10X,'BULK AIR DIFFUSION COEFFICIENT  =' ,E14.4,2X,A//
      10X,'HENRY'S CONSTANT                =' ,F10.4//
      10X,'SOIL BULK DENSITY               =' ,E14.4,2X,A)
C-----
WRITE(21,251)

```

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```

251  FORMAT(//22X,'INITIAL TOTAL CONCENTRATION',2X,
      '(MG/KG)'/
      22X,'.....'//)
C-----
      IF(IFL8.EQ.0) THEN
C-----
          WRITE(21,261) CTOTAL(2)
261  FORMAT(20X,E15.4,3X,'CONSTANT FOR ALL NODES')
C-----
          ELSE
C-----
          WRITE(21,260) (CTOTAL(I),I=1,N)
260  FORMAT(1X,8E15.4)
C-----
          END IF
C-----
          WRITE(21,250)
250  FORMAT(//22X,'INITIAL LIQUID PHASE CONCENTRATION',2X,
      '(MG/L)'/
      22X,'.....'//)
C-----
      IF(IFL8.EQ.0) THEN
C-----
          IF(IUN.EQ.1) WRITE(21,261) 35.314667*CONCI(2)
          IF(IUN.EQ.2) WRITE(21,261) CONCI(2)
          IF(IUN.EQ.3) WRITE(21,261) 61023.744*CONCI(2)
          IF(IUN.EQ.4) WRITE(21,261) 1E6*CONCI(2)
C-----
          ELSE
C-----
          IF(IUN.EQ.1) WRITE(21,260) (35.314667*CONCI(I),I=1,N)
          IF(IUN.EQ.2) WRITE(21,260) (CONCI(I),I=1,N)
          IF(IUN.EQ.3) WRITE(21,260) (61023.744*CONCI(I),I=1,N)
          IF(IUN.EQ.4) WRITE(21,260) (1E6*CONCI(I),I=1,N)
C-----
          END IF
C-----
      IF(IFL13.EQ.0) THEN
C-----
          WRITE(21,270)
270  FORMAT(//20X,'INITIAL BIOMASS CONCENTRATION',2X,

```



```

      '(MG/L)')/
      20X,'.....')/
    IF(IFL10.EQ.0) THEN
      WRITE(21,261) BIOMI(1)
    ELSE
      WRITE(21,260) (BIOMI(I),I=1,N)
    END IF

C-----
C...CONVERT BIOMASS CONCENTRATION TO APPROPRIATE UNITS
C-----

    DO 21 JJ=1,N
      IF(IUN.EQ.1) BIOMI(JJ)=2.83168E-2*BIOMI(JJ)
      IF(IUN.EQ.3) BIOMI(JJ)=1.6387E-5*BIOMI(JJ)
      IF(IUN.EQ.4) BIOMI(JJ)=1E-6*BIOMI(JJ)
21   CONTINUE
C-----

    END IF
C-----

    GO TO 424
C-----

244  WRITE(21,720)
720  FORMAT(20X,'THIS IS A SIMULATION FOR NONBIODEGRADABLE MATTER'//)
      WRITE(21,900) INT,UNT
C-----

    IF(IUN.EQ.1) THEN
      WRITE(21,902) AKOC,'ML/GR',ALAM,UALAM,
        .      2.8316847E4*AKD,'ML/GR',
        .      2.8316847E4*AKPR,'ML/GR ',UAKK,
        .      9.2903E-2*DDW,'M2/DAY',9.2903E-2*DDA,'M2/DAY',
        .      1/HENRY,3.53146E-5*RHO,'GR/CM3'
    ELSE
      IF(IUN.EQ.2) THEN
        WRITE(21,902) AKOC,'ML/GR',ALAM,UALAM,
          .      1E6*AKD,'ML/GR',
          .      1E6*AKPR,'ML/GR ',UAKK,
          .      DDW,'M2/DAY',DDA,'M2/DAY',
          .      1/HENRY,1E-6*RHO,'GR/CM3'
      ELSE
        IF(IUN.EQ.3) THEN
          WRITE(21,902) AKOC,'ML/GR',ALAM,UALAM,
            .      16.387064*AKD,'ML/GR',

```

```

        16.387064*AKPR,'ML/GR ',UAKK,
        6.4516E-4*DDW,'M2/DAY',6.4516E-4*DDA,
        'M2/DAY',1/HENRY,6.10237E-2*RHO,
        'GR/CM3'
    ELSE
        IF(IUM.EQ.4) THEN
            WRITE(21,902) AKOC,'ML/GR',ALAM,UALAM,
            AKD,'ML/GR',AKPR,'ML/GR ',
            UAKK,1E-4*DDW,'M2/DAY',1E-4*DDA,
            'M2/DAY',1/HENRY,RHO,'GR/CM3'
        END IF
    END IF
END IF
WRITE(21,251)
C-----
    IF(IFL8.EQ.0) THEN
        WRITE(21,261) CTOTAL(2)
    ELSE
        WRITE(21,260) (CTOTAL(I),I=1,N)
    END IF
    WRITE(21,250)
C-----
    IF(IFL8.EQ.0) THEN
C-----
        IF(IUM.EQ.1) WRITE(21,261) 35.314667*CONCI(2)
        IF(IUM.EQ.2) WRITE(21,261) CONCI(2)
        IF(IUM.EQ.3) WRITE(21,261) 61023.744*CONCI(2)
        IF(IUM.EQ.4) WRITE(21,261) 1E6*CONCI(2)
C-----
    ELSE
C-----
        IF(IUM.EQ.1) WRITE(21,260) (35.314667*CONCI(I),I=1,N)
        IF(IUM.EQ.2) WRITE(21,260) (CONCI(I),I=1,N)
        IF(IUM.EQ.3) WRITE(21,260) (61023.744*CONCI(I),I=1,N)
        IF(IUM.EQ.4) WRITE(21,260) (1E6*CONCI(I),I=1,N)
C-----
    END IF
C-----
424  CONTINUE
7700 WRITE(21,2008)

```



```

2008  FORMAT('1',/////35X,19H***** RESULTS *****)
      WRITE(21,2010)
2010  FORMAT(20X,'.....')

```

C-----C...START COMPUTATION C-----

```

      ICOUNT=0
      FTIME=.TRUE.
      IF(IC1.GT.0) GO TO 83

```

C-----C...REDUCTION SCHEME

888 IF(FTIME) THEN

```

C-----
      NZT=0
      NZB=0
      DO 3016 KK=1,N
        CNOLD(KK)=CONCI(KK)
3016   THIN(KK)=THOLD(KK)
        CMAX=CONCI(1)
      DO 3021 KK=2,N
3021   IF(CONCI(KK).GT.CMAX) CMAX=CONCI(KK)
        DCONC=CMAX
      DO 3022 KK=1,N
3022   IF(CONCI(KK).NE.0.) GOTO 3023
3023   NZT=KK
      DO 3024 KK=NZT,N
3024   IF(CONCI(KK).EQ.0.) GOTO 3025
3025   NZB=KK-1

```

C-----ELSE

```

C-----
      IF((NZB-NZT).LE.1) THEN
        WRITE(6,3031) BOLD,NORMAL
3031   FORMAT(/5X,A,'ALL OF THE CONTAMINATED SOIL MUST BE ',
           'EXCAVATED!',A/)
        WRITE(21,3032)
3032   FORMAT(/5X,'ALL OF THE CONTAMINATED SOIL MUST BE ',
           'EXCAVATED!'/)
        STOP
      END IF

```

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```

C-----
      DO 3018 KK=1,N
3018      THOLD(KK)=THIN(KK)
          DCONC=DCONC/2.
          NDZ=(NZB-NZT)/2
C-----
      IF(CUT) THEN
C-----
          IF(IUM.EQ.1) WRITE(6,272)35.314667*BCMAX,35.314667*CONCA
          IF(IUM.EQ.2) WRITE(6,272)BCMAX,CONCA
          IF(IUM.EQ.3) WRITE(6,272)61023.744*BCMAX,61023.744*CONCA
          IF(IUM.EQ.4) WRITE(6,272)1E6*BCMAX,1E6*CONCA
C-----
          IF(IUM.EQ.1) WRITE(21,272)35.314667*BCMAX,35.314667*CONCA
          IF(IUM.EQ.2) WRITE(21,272)BCMAX,CONCA
          IF(IUM.EQ.3) WRITE(21,272)61023.744*BCMAX,61023.744*CONCA
          IF(IUM.EQ.4) WRITE(21,272)1E6*BCMAX,1E6*CONCA
C-----
272      FORMAT(/1X,'MAX. CONCENTRATION= ',E10.4,' > ',
              'ALLOW. CONCENTRATION= ',E10.4,1X,'MG/L'/)
C-----
      IF(ICUT.EQ.0) THEN
          DO 3019 KK=NZT,NZB
              CONCI(KK)=CONCI(KK)-DCONC
3019      IF(CONCI(KK).LT.0.) CONCI(KK)=0.0
          ELSE
              NZT=NZT+NDZ
              DO 3027 KK=1,NZT-1
3027      CONCI(KK)=0.0
              DO 3028 KK=NZT,NZB
3028      CONCI(KK)=CNOLD(KK)
          END IF
C-----
      ELSE
C-----
          IF(IUM.EQ.1) WRITE(6,273)35.314667*BCMAX,35.314667*CONCA
          IF(IUM.EQ.2) WRITE(6,273)BCMAX,CONCA
          IF(IUM.EQ.3) WRITE(6,273)61023.744*BCMAX,61023.744*CONCA
          IF(IUM.EQ.4) WRITE(6,273)1E6*BCMAX,1E6*CONCA
C-----
          IF(IUM.EQ.1) WRITE(21,273)35.314667*BCMAX,35.314667*CONCA

```



```

      IF(IUN.EQ.2) WRITE(21,273)BCMAX,CONCA
      IF(IUN.EQ.3) WRITE(21,273)61023.744*BCMAX,61023.744*CONCA
      IF(IUN.EQ.4) WRITE(21,273)1E6*BCMAX,1E6*CONCA
C-----
273      FORMAT(/1X,'MAX. CONCENTRATION= ',E10.4,' < ',
             'ALLOW. CONCENTRATION= ',E10.4,1X,'MG/L'/)
C-----
      IF(ICUT.EQ.0) THEN
        DO 3020 KK=WZT,WZB
3020      CONCI(KK)=CONCI(KK)+DCONC
        ELSE
          WZT=WZT-NDZ
          DO 3029 KK=1,WZT-1
3029      CONCI(KK)=0.0
          DO 3030 KK=WZT,WZB
3030      CONCI(KK)=CWOLD(KK)
        END IF
C-----
      END IF
C-----
      WRITE(21,271)
271      FORMAT(/20X,'NEW INITIAL LIQUID PHASE CONCENTRATION',2X,
             '(MG/L)'/
             20X,'-----'/)
C-----
      IF(IUN.EQ.1) WRITE(21,260) (35.314667*CONCI(JJ),JJ=1,N)
      IF(IUN.EQ.2) WRITE(21,260) (CONCI(JJ),JJ=1,N)
      IF(IUN.EQ.3) WRITE(21,260) (61023.744*CONCI(JJ),JJ=1,N)
      IF(IUN.EQ.4) WRITE(21,260) (1E6*CONCI(JJ),JJ=1,N)
C-----
      DO 3026 JJ=1,N
        CTEMP(JJ)=(THIN(JJ)+(POROS-THIN(JJ))/HENRY+
                  RHO*AKD)*CONCI(JJ)
        CTOTAL(JJ)=1E6*CTEMP(JJ)/RHO
3026      CONTINUE
C-----
      WRITE(21,275)
275      FORMAT(/20X,'ASSUMED NEW TOTAL CONCENTRATION',
             2X,'(MG/KG)'/
             20X,'-----'/)
      WRITE(21,260) (CTOTAL(JJ),JJ=1,N)

```

```

C-----
      END IF
C-----
C...SOLVE BOTH FLOW AND MASS TRANSPORT EQUATION
C-----
      ICOUNT=0
      CALL SOLUTE
C-----
      GO TO 97
C-----
83  OPEN(UNIT=22,FILE='THT'//IRUN//'.DAT',STATUS='NEW')
      OPEN(UNIT=28,FILE='TTH'//IRUN//'.DAT',STATUS='NEW')
C-----
      DO 95 JT=1,M
      TIME(JT+1)=FLOAT(JT)*DT
      D(JT)=DIFF(1)
      THSU(JT)=THOLD(1)
      ICOUNT=ICOUNT+1
C-----
C...SOLVE FLOW EQUATION
C-----
      CALL YGRA
C-----
      BDISCH(JT)=DISCH(N)
C-----
C...OPTIONAL OUTPUT FOR GRAPHICAL REPRESENTATION OF THETA DISTRIBUTION
C-----
      WRITE(28,2222)TIME(JT+1),THNEW(2)
      IF (ICOUNT/INT*INT.EQ.ICOUNT) THEN
        WRITE(22,2221)TIME(JT)+DT,UDT
2221  FORMAT(10X,'TIME=',F6.0,1X,A)
        DO 777 IJ=1,N
777   WRITE(22,2222)THNEW(IJ),-1*DEP(IJ)
2222  FORMAT(1X,F10.4,1X,F10.4)
      END IF
C-----
      DO 80 I=1,N
      THOLD(I)=THNEW(I)
80   QOLD(I)=QNEW(I)
C-----
95  CONTINUE

```



```

97'  CONTINUE
C-----
      IF(IC1.GT.0)GO TO 90
C-----
C...COMPUTE MAXIMUM CONCENTRATION
C-----
      BCMAX=BCONC(1)
      MAXM=0
      DO 93, I=1,M
        IF(BCONC(I+1).GT.BCMAX) THEN
          BCMAX=BCONC(I+1)
          MAXM=I*DT
        END IF
93  CONTINUE
C-----
      IF(IFL12.EQ.0.OR.ABS(BCMAX-CONCA)/CONCA.LE.0.1) GOTO 91
      IF(BCMAX.GT.CONCA) THEN
        CUT=.TRUE.
      ELSE
        IF(FTIME) GOTO 91
        CUT=.FALSE.
      END IF
      FTIME=.FALSE.
      GOTO 888
C-----
91  OPEN(UNIT=23,FILE='BCM'//IRUN//'.DAT',STATUS='NEW')
      OPEN(UNIT=27,FILE='TCN'//IRUN//'.DAT',STATUS='NEW')
      IF(IFL11.EQ.0) THEN
        OPEN(UNIT=29,FILE='MFX'//IRUN//'.DAT',STATUS='NEW')
      END IF
C-----
      IF(IUN.EQ.1) WRITE(21,2037) 35.314667*BCMAX,MAXM
      IF(IUN.EQ.2) WRITE(21,2037) BCMAX,MAXM
      IF(IUN.EQ.3) WRITE(21,2037) 61023.744*BCMAX,MAXM
      IF(IUN.EQ.4) WRITE(21,2037) 1E6*BCMAX,MAXM
C-----
2037  FORMAT('1',10X,'MAX. CONCENTRATION AT G.W.T. : ',
           'E15.4,1X,'MG/L',', AT ',I5,' DAYS')
C-----
      IF(IFL12.EQ.1) THEN
C-----

```

APPENDIX B. PROGRAM LISTING

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```

      WRITE(21,276)
276   FORMAT(/20X,'ALLOWABLE TOTAL CONCENTRATION',
           2X,'(MG/KG)'/
           20X,'-----')/)
      WRITE(21,260) (CTOTAL(JJ),JJ=1,N)
      DMAX=CTOTAL(1)
C-----
      DO 92 JJ=2,N
92    IF(CTOTAL(JJ).GT.DMAX) DMAX=CTOTAL(JJ)
C-----
      WRITE(6,2038)DMAX
      WRITE(21,2038)DMAX
2038  FORMAT(/1X,'MAXIMUM ALLOWABLE TOTAL CONCENTRATION= ',
           E10.4,' MG/KG'/)
C-----
      END IF
C-----
      WRITE(21,2029)
2029  FORMAT(/20X,'EFFLUENT CONCENTRATION AT WATER TABLE')
      WRITE(21,2030)
2030  FORMAT(20X,'.....')/)
      WRITE(21,2031)INT
2031  FORMAT(26X,'AT EVERY ',I4,' TIME STEPS'/)
      WRITE(21,2030)
      IF(INDEX.EQ.0) GO TO 850
      WRITE(21,2032) UDT,UAKS,'MG/L'
2032  FORMAT(/15X,'TIME',1X,A,5X,'DISCHARGE',1X,A,5X,
           'CHEMICAL CONC.',1X,A/)
      DO 96 JT=1,M
C-----
      IF (JT/INT*INT.EQ.JT) THEN
C-----
          IF(IUM.EQ.1) WRITE(21,2033) TIME(JT+1),BDISCH(JT),
              35.314667*BCONC(JT+1)
          IF(IUM.EQ.2) WRITE(21,2033) TIME(JT+1),BDISCH(JT),BCONC(JT+1)
          IF(IUM.EQ.3) WRITE(21,2033) TIME(JT+1),BDISCH(JT),
              61023.744*BCONC(JT+1)
          IF(IUM.EQ.4) WRITE(21,2033) TIME(JT+1),BDISCH(JT),
              1E6*BCONC(JT+1)
2033  FORMAT(15X,F6.0,12X,E15.4,12X,E15.4)
C-----

```



```

      END IF
C-----
C...COMPUTE GASEOUS PHASE MASS FLUXES AT TOP OF THE SOIL [MG/CM^2/DAY]
C-----
      IF(IFL11.EQ.0) THEN
          AVTH=(2*POROS-TTH(1,JT+1)-TTH(2,JT+1))/2.
          QGAS=DDA/HENRY*AVTH**(10./3.)/POROS**2*TCNC(JT+1)/DZ
          IF(IUM.EQ.1) WRITE(29,2036) TIME(JT+1),1E3*QGAS/30.48**2
          IF(IUM.EQ.2) WRITE(29,2036) TIME(JT+1),QGAS/10.
          IF(IUM.EQ.3) WRITE(29,2036) TIME(JT+1),1E3*QGAS/2.54**2
          IF(IUM.EQ.4) WRITE(29,2036) TIME(JT+1),1E3*QGAS
      END IF
C-----
C...OPTIONAL OUTPUT FOR TOP AND BOTTOM CONCENTRATION TRACER
C-----
      IF(IUM.EQ.1) THEN
          WRITE(23,2036) TIME(JT+1),35.314667*BCNC(JT+1)
          WRITE(27,2036) TIME(JT+1),35.314667*TCNC(JT+1)
      ELSE
          IF(IUM.EQ.2) THEN
              WRITE(23,2036) TIME(JT+1),BCNC(JT+1)
              WRITE(27,2036) TIME(JT+1),TCNC(JT+1)
          ELSE
              IF(IUM.EQ.3) THEN
                  WRITE(23,2036) TIME(JT+1),61023.744*BCNC(JT+1)
                  WRITE(27,2036) TIME(JT+1),61023.744*TCNC(JT+1)
              ELSE
                  IF(IUM.EQ.4) THEN
                      WRITE(23,2036) TIME(JT+1),1E6*BCNC(JT+1)
                      WRITE(27,2036) TIME(JT+1),1E6*TCNC(JT+1)
                  END IF
              END IF
          END IF
      END IF
      END IF
      END IF
96   CONTINUE
2036  FORMAT(1X,F6.0,1X,E15.4)
C-----
      GO TO 90
850  WRITE(21,2034) UDT,UAKS,'MG/L','MG/L'
2034  FORMAT(/5X,'TIME',1X,A,5X,'DISCHARGE',1X,A,5X,
           'CHEMICAL CONC.',1X,A,5X,'BIOMASS CONC.',1X,A)

```

APPENDIX B. PROGRAM LISTING

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```

DO 99 JT=1,M
C-----
  IF (JT/INT*INT.EQ.JT) THEN
C-----
    IF(IUM.EQ.1) WRITE(21,2035) TIME(JT+1),BDISCH(JT),
      35.314667*BCONC(JT+1),
      35.314667*BBIOM(JT+1)
    IF(IUM.EQ.2) WRITE(21,2035) TIME(JT+1),BDISCH(JT),
      BCONC(JT+1),BBIOM(JT+1)
    IF(IUM.EQ.3) WRITE(21,2035) TIME(JT+1),BDISCH(JT),
      61023.744*BCONC(JT+1),
      61023.744*BBIOM(JT+1)
    IF(IUM.EQ.4) WRITE(21,2035) TIME(JT+1),BDISCH(JT),
      1E6*BCONC(JT+1),1E6*BBIOM(JT+1)
2035    FORMAT(5X,F6.0,12X,E15.4,12X,E15.4,12X,E15.4)
C-----
    END IF
C-----
C...COMPUTE GASEOUS PHASE MASS FLUXES AT TOP OF THE SOIL [MG/CM^2/DAY]
C-----
  IF(IFL11.EQ.0) THEN
    AVTH=(2*POROS-TTH(1,JT+1)-TTH(2,JT+1))/2.
    QGAS=DDA/HENRY*AVTH**(10./3.)/POROS**2*TCONC(JT+1)/DZ
    IF(IUM.EQ.1) WRITE(29,2036) TIME(JT+1),1E3*QGAS/30.48**2
    IF(IUM.EQ.2) WRITE(29,2036) TIME(JT+1),QGAS/10.
    IF(IUM.EQ.3) WRITE(29,2036) TIME(JT+1),1E3*QGAS/2.54**2
    IF(IUM.EQ.4) WRITE(29,2036) TIME(JT+1),1E3*QGAS
  END IF
C-----
  IF(IUM.EQ.1) THEN
    WRITE(23,2036) TIME(JT+1),35.314667*BCONC(JT+1)
    WRITE(27,2036) TIME(JT+1),35.314667*TCONC(JT+1)
  ELSE
    IF(IUM.EQ.2) THEN
      WRITE(23,2036) TIME(JT+1),BCONC(JT+1)
      WRITE(27,2036) TIME(JT+1),TCONC(JT+1)
    ELSE
      IF(IUM.EQ.3) THEN
        WRITE(23,2036) TIME(JT+1),61023.744*BCONC(JT+1)
        WRITE(27,2036) TIME(JT+1),61023.744*TCONC(JT+1)
      ELSE

```



```

        IF(IUN.EQ.4) THEN
            WRITE(23,2036) TIME(JT+1),1E6*BCONC(JT+1)
            WRITE(27,2036) TIME(JT+1),1E6*TCONC(JT+1)
        END IF
    END IF
END IF
END IF
C-----
99  CONTINUE
C-----
        IF(IFL11.EQ.0) CLOSE (UNIT=29)
        CLOSE (UNIT=23)
90  DO 992 JT=2,M
992  VOLE(JT)=(BDISCH(JT)+BDISCH(JT-1))*DT/2.
        VOLE(1)=BDISCH(1)*DT
        WRITE(21,2220)
2220 FORMAT('1',20X,'DISCHARGE AND CUMM. VOL. AT ',
        'WATER TABLE')
        WRITE(21,2030)
        WRITE(21,2031)INT
        WRITE(21,2030)
        WRITE(21,2052) UDT,UAKS,UDZ,UDZ
2052 FORMAT(/5X,'TIME',1X,A,5X,'DISCHARGE CUBIC',1X,A,8X,
        'VOLUME CUBIC',1X,A,2X,'CUMM. VOLUME CUBIC',1X,A/)
        VSS=0.0
        DO 991 JT=1,M
        VSS=VSS+VOLE(JT)
        VSUM(JT)=VSS
C-----
C...OPTIONAL OUTPUT FOR BOTTOM FLUXES
C-----
        WRITE(25,2036) TIME(JT+1),BDISCH(JT)
C-----
        IF (JT/INT*INT.EQ.JT) THEN
            WRITE(21,2053) TIME(JT+1),BDISCH(JT),VOLE(JT),VSUM(JT)
2053  FORMAT(5X,F6.0,12X,E15.4,15X,E15.4,10X,E15.4)
        END IF
991  CONTINUE
C-----
C...END OF EXECUTION
C-----

```

APPENDIX B. PROGRAM LISTING

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```
WRITE(6,2054)BOLD,NORMAL,BELL
2054 FORMAT(/10X,A,'END OF EXECUTION',2A/)
```

C-----

C...CLOSE FILES

C-----

```
CLOSE (UNIT=21)
CLOSE (UNIT=22)
CLOSE (UNIT=25)
CLOSE (UNIT=27)
CLOSE (UNIT=28)
CLOSE (UNIT=IUNIT)
CLOSE (UNIT=JUNIT)
CLOSE (UNIT=KUNIT)
END
```



```

C-----
C-----
      SUBROUTINE YGRA
C-----
C-----
      COMMON/BLK1/M
      COMMON/BLK3/THNEW(400),THOLD(400)
      COMMON/BLK4/IFL1,IFL2,AKS,THS,THF,AM,AN,AI,BE,B,THAD,AN2,AM2,
           GAMMA,ALPHA
      COMMON/BLK5/PSIR,DZER,BET,THZER
      COMMON/BLK6/AK(400),DIFF(400),AKM(400),AKP(400),DM(400),DP(400)
      COMMON/BLK7/TH(400)
      COMMON/BLK8/EPS
      COMMON/BLK9/P(2234),ET(2234)
      COMMON/BLK10/JT,TIME(2234)
      COMMON/BLK11/QOLD(400),QNEW(400),DISCH(400)
      COMMON/BLK13/IT2
      COMMON/BLK14/DEP(400)
      COMMON/BLK15/UDT,UTHO,UAKS,UDZ
      COMMON/BLK16/DZ,DT
      COMMON/BLK24/THAV(400),TRTH(400)
      COMMON/BLK25/IT,INT
      COMMON/BLK26/ICOUNT
      COMMON/BLK28/M
      COMMON/BLK30/BELL,BOLD,BLINK,REVERS,CLEAR,HOME,NORMAL
      COMMON/BLK40/TCONC(2234),BCONC(2234),BBIOM(2234),BDISCH(2234)
      COMMON/BLK41/IFL3,IFL4,IFL5,IFL6,IFL7
      COMMON/BLK52/IFL9
      COMMON/BLK57/FTIME
C-----
      LOGICAL FTIME
      CHARACTER*8 UDT,UTHO,UDZ,UAKS
      CHARACTER ESC*1,BELL*1,CLEAR*4,NORMAL*4,BOLD*4,
           BLINK*4,REVERS*4,HOME*6
C-----
      NM=N-1
      BP=B+1
C-----
C...START SOLUTION OF NUMERICAL EQUATIONS
C-----
      IF(IFL5.NE.1) GO TO 801

```

```

C-----
      IF(.NOT.FTIME) GOTO 801
      CALL EVAP
C-----
801  CONTINUE
      DO 310 I=1,N
310  THNEW(I)=THOLD(I)
C-----
C...COUNTER FOR NUMBER OF ITERATIONS
C-----
40   IT=0
      IT2=0
C-----
C...COMPUTE APPROXIMATIONS TO K AND D
C
C...CHECKS TO TRANSFER CONTROL TO FLUXEQ OR TO CONSMO
C-----
41   DO 43 I=1,N
      IF(THNEW(I).GE.THS) THNEW(I)=THS
      IF(THNEW(I).LE.THAD) THNEW(I)=THAD
43   CONTINUE
C-----
C...OPTIONAL COUNTER FOR DEBUGGING
C-----
      IJK=IJK+1
      WRITE(6,7878)REVERS,IJK,NORMAL
7878  FORMAT('+',A,'TOTAL ITERATIONS IN YGRA= ',I6,A)
C-----
      IF(THNEW(1).LT.THS.AND.THNEW(1).GT.THAD) GO TO 44
      QINC=P(JT)-ET(JT)
      IF(THNEW(1).EQ.THS.AND.QINC.GE.AKS) GO TO 25
      IF(THNEW(1).EQ.THAD.AND.QINC.LE.O.) GO TO 25
C-----
C...SUBROUTINE FOR FLUX BOUNDARY CONDITION
C-----
44   CALL FLUXEQ
C-----
C...COMPARE TRIAL THETAS WITH ASSUMED ONES
C-----
42   DO 345 I=1,N
      DEL=TH(I)-THNEW(I)

```



```

      DELTH=ABS(DEL)
      IF(DELTH.GT.EPS) GO TO 49
345  CONTINUE
      GO TO 55
49   IT=IT+1
      DO 350 I=1,N
      TRTH(I)=THNEW(I)
350  THNEW(I)=TH(I)
      IF(IT.GE.20) GO TO 81
      GO TO 41
C-----
C...SUBROUTINE FOR CONSTANT MOISTURE BOUNDARY CONDITION
C-----
25   CALL CONSMO
C-----
      DO 400 I=1,N
      DEL=TH(I)-THNEW(I)
      DELTH=ABS(DEL)
      IF(DELTH.GT.EPS) GO TO 449
400  CONTINUE
      GO TO 55
449  IT2=IT2+1
      DO 450 I=1,N
      TRTH(I)=THNEW(I)
450  THNEW(I)=TH(I)
      IF(IT2.GE.20) GO TO 81
      GO TO 25
C-----
C...COMPUTE K's AND D's
C-----
55   DO 60 I=1,N
60   THNEW(I)=TH(I)
      IF(IFL1.EQ.1) GO TO 75
      IF(IFL1.EQ.2) GO TO 80
      IF(IFL1.EQ.3) GO TO 85
      IF(IFL1.EQ.4) GO TO 86
C-----
75   DO 20 I=1,N
20   AK(I)=AKS*(THNEW(I)/THS)**AM
      GO TO 90
C-----

```

```

80' DO 30 I=1,N
30 AK(I)=AKS*((THNEW(I)-THF)/(THS-THF))**AM
GO TO 90

C-----
85 DO 95 I=1,N
95 AK(I)=AI*(THNEW(I)**BE)
GO TO 90

C-----
86 DO 96 I=1,N
IF(THNEW(I).GE.TH) THNEW(I)=THS-0.001
IF(THNEW(I).LE.TH) THNEW(I)=THF+0.001
SE=(THNEW(I)-THF)/(THS-THF)
96 AK(I)=AKS*SE**GAMMA*(1-(1-SE**(1/AM2))**AM2)**2

C-----
90 IF(IFL2.EQ.1) GO TO 91
IF(IFL2.EQ.2) GO TO 92
IF(IFL2.EQ.3) GO TO 98

C-----
91 DO 93 I=1,N
93 DIFF(I)=AK(I)*B*PSIR/THS*(THS/THNEW(I))**BP
GO TO 65

C-----
92 DO 94 I=1,N
94 DIFF(I)=DZER*EXP(BET*(THNEW(I)-THZER))
GO TO 65

C-----
98 DO 83 I=1,N
SE=(THNEW(I)-THF)/(THS-THF)
83 DIFF(I)=AK(I)/(ALPHA*(AM2-1)*(THS-THF))*(1-SE**(1/AM2))**
(-AM2)*SE**(-1/AM2)

C-----
C..COMPUTATION OF THE MOISTURE FLUX
C-----
65 SUM2=0.0
DO 58 I=1,N
DEP(I)=SUM2
58 SUM2=SUM2+DZ

C-----
DO 61 I=2,NM
IM=I-1
IP=I+1

```



```

C-----
      DTHDZ=(2.*DEP(I)*((THNEW(IM)/((DEP(IM)-DEP(I))*DEP(IM)-
      DEP(IP))))+(THNEW(I)/((DEP(I)-DEP(IM))*DEP(I)-
      DEP(IP))))+(THNEW(IP)/((DEP(IP)-DEP(IM))*DEP(IP)-
      DEP(I))))+(THNEW(IM)/((DEP(IM)-DEP(I))*DEP(IM)-
      DEP(I))))-((THNEW(IM)*DEP(I)+DEP(IM)))/
      ((DEP(IM)-DEP(I))*DEP(IM)-DEP(IP)))-((THNEW(I)*
      DEP(I)+DEP(IM)))/((DEP(I)-DEP(IM))*DEP(I)-
      DEP(IP)))-((THNEW(IP)*DEP(I)+DEP(IM)))/((DEP(IP)-
      DEP(IM))*DEP(IP)-DEP(I))))
C-----
      IF(IFL1.EQ.4) THEN
        IF(THNEW(I).GE.THS-0.001) DTHDZ=0.0
      ELSE
        IF(THNEW(I).GE.THS) DTHDZ=0.0
      END IF
C-----
      QNEW(I)=AK(I)-(DIFF(I)*DTHDZ)
C-----
      IF(IFL9.EQ.0) THEN
        QNEW(I)=AK(I)-DIFF(I)*(THNEW(I)-THNEW(IM))/(DZ)
      END IF
C-----
      IF(THNEW(I).EQ.THAD) QNEW(I)=0.0
      TIEF=THNEW(I)-THF
      IF(TIEF.LT.0.000001) QNEW(I)=0.0
      DISCH(I)=QNEW(I)
61  CONTINUE
C-----
      QNEW(N)=AK(N)-DIFF(N)*((THNEW(N)-THNEW(NM))/DZ)
      IF(IFL1.EQ.4) THEN
        IF(THNEW(1).GE.THS-0.001) QNEW(1)=AKS
      ELSE
        IF(THNEW(1).GE.THS) QNEW(1)=AKS
      END IF
C-----
      IF(THNEW(1).EQ.THAD) QNEW(1)=0.0
      IF(THNEW(1).GT.THAD.AND.THNEW(1).LT.THS) QNEW(1)=P(JT)-ET(JT)
      DISCH(1)=QNEW(1)
      DISCH(N)=QNEW(N)
C-----

```

C..COMPUTATION OF THE MASS BALANCE RESIDUAL

```

C-----
      SUM=0.0
      DO 56 I=2,NM
56      SUM=SUM+(TH(I)-THOLD(I))
      SUM=(SUM+(TH(1)-THOLD(1)+TH(N)-THOLD(N))/2)*DZ
      TIEN=THNEW(N)-THF
      IF(TIEN.LE.0.000001) QNEW(N)=0.0
      TOTAC=(P(JT)-ET(JT)-0.5*(QNEW(N)+QOLD(N)))*DT
      RES=TOTAC-SUM
C-----
      IF(ICOUNT/INT*INT.NE.ICOUNT) GO TO 101
      IF(IFL6.EQ.0) THEN
          WRITE(21,2010) TIME(JT+1),UDT,UTHO
2010      FORMAT(///20X,'MOISTURE DISTRIBUTION AT ',F6.0,3X,A,3X,A/)
          WRITE(21,2026) (THNEW(I),I=1,N)
2026      FORMAT(10F10.5)
          WRITE(21,2009) IT
2009      FORMAT(///2X,'NO. OF ITERATIONS IN SUBROUTINE FLUXEQ = ',I2/)
          WRITE(21,2024) IT2
2024      FORMAT(2X,'NO. OF ITERATIONS IN SUBROUTINE CONSMO = ',I2/)
          WRITE(21,2018) RES,UDZ
2018      FORMAT(2X,'MASS BALANCE RESIDUAL                = ',E13.5,
                2X,A/)
      END IF
      IF(IFL7.EQ.0) THEN
          WRITE(21,2013) TIME(JT+1),UAKS
2013      FORMAT(///20X,'FLOW RATE DISTRIBUTION AT ',F6.0,3X,
                'DAYS IN',1X,A/)
          WRITE(21,2011) (QNEW(I),I=1,N)
2011      FORMAT(8E15.4)
      END IF
      GO TO 101
81      WRITE(6,2012)
2012      FORMAT(/5X,'*** NO CONVERGENCE ***'//
                1X,'CHECK INPUT RELATED TO FLOW PART'/)
      STOP
101      RETURN
      END

```



```

C-----
C-----
      SUBROUTINE EVAP
C-----
C-----
C...THIS SUBROUTINE COMPUTES THE EVAPOTRANSPIRATION RATE BY EITHER
C...PENMAN'S OR THORNTHWAITES'S THEORY, AND ADJUSTS THE POTENTIAL
C...EVAPOTRANSPIRATION VALUES BY THE WATER BALANCE METHOD.
C-----

      COMMON/BLK1/M
      COMMON/BLK4/IFL1,IFL2,AKS,THS,THF,AM,AN,AT,BE,B,THAD,AN2,AM2,
      .
      .      GAMMA,ALPHA
      COMMON/BLK9/P(2234),ET(2234)
      COMMON/BLK10/JT,TIME(2234)
      COMMON/BLK16/DZ,DT
      COMMON/BLK21/IFLE,IFLT,ID1,ID2,RR(12),ALB,TD(12),W(12),
      .
      .      SSH(12),ALI(12),DIN,MIN,YIN,TT(12),THW,DRZ
      COMMON/BLK23/THSU(2234),D(2234),UPR
      COMMON/BLK25/IT,INT
      COMMON/BLK28/M
      COMMON/BLK29/IUNIT,JUNIT,KUNIT
      COMMON/BLK30/BELL,BOLD,BLINK,REVERS,CLEAR,HOME,NORMAL
      COMMON/BLK41/IFL3,IFL4,IFL5,IFL6,IFL7
      COMMON/BLK53/IUM
      COMMON/BLK54/CN
C-----

      DIMENSION BB(12),PE(12),APE(12),RNF(11170),DIPET(12),
      .
      .      SIPET(12),RAV(12),AINF(12),PAV(12),RRAV(30,12),
      .
      .      ST(12),DST(12),PERC(12),IDUR(12)
      CHARACTER BELL*1,CLEAR*4,NORMAL*4,BOLD*4,BLINK*4,REVERS*4,
      .
      .      HOME*6,UPR*8
      INTEGER DAY,MONTH,YEAR,OLDM,OLDY,DIN,MIN,YIN
      REAL II
C-----
C...THORNTHWAITE MODIFICATION PARAMETERS FOR NORTHERN LATITUDE 40
C-----

      DATA BB/0.84,0.83,1.03,1.11,1.24,1.25,1.27,1.18,1.04,0.96,
      .
      .      0.83,0.81/
C-----
C...AVERAGE PRECIPITATION VALUES FOR THE LAST 30 YEARS IN [100*In]
C-----

```

```

DATA PAV/334.3667,309.2333,386.0667,376.7667,385.6000,298.9000,
      445.2333,380.1000,364.4667,293.2667,394.1333,351.7333/
C-----
C...DURATION OF MONTHS OF A YEAR (DAYS)
C-----
DATA IDUR/31,28,31,30,31,30,31,31,30,31,30,31/
C-----
C...READ DATA
C-----
      IF(JT.GT.1) GO TO 15
C-----
C...SET INPUT DAY, MONTH, AND YEAR OF SIMULATION
C-----
      DIN=1
      MIN=1
      YIN=1959
C-----
C...CHECK CURVE NUMBER TO PREVENT SINGULARITIES
C-----
103  IF(CM.EQ.0) THEN
      WRITE(JUNIT,1021) BOLD,NORMAL
1021  FORMAT(/1X,'ENTER THE SCS SOIL CURVE NUMBER ',A,'<CN>',A,
           ' : ',,$)
      READ(IUNIT,*,ERR=103) CM
      IF(IUNIT.NE.1) CALL DATA
10022 IF(CM.LE.0.OR.CM.GT.100) THEN
      WRITE(JUNIT,1022)BLINK,NORMAL,BELL,BELL
1022  FORMAT(/5X,A,'INVALID ENTRY FOR <CN>, REENTER : ',
           A,' : ',2A,$)
      READ(IUNIT,*,ERR=10022) CM
      GOTO 10022
      END IF
      WRITE(KUNIT,*) CM
      END IF
C-----
10011 WRITE(JUNIT,111)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,BOLD,
      NORMAL
111  FORMAT(/1X,A,'ENTER ONE OF THE FOLLOWING:',A//5X,A,'0',A,
           ': IF THORNTWHAITE'S EQUATIONS ARE USED'/5X,A,'1',A,
           ': IF PENMAN'S EQUATIONS ARE USED'//1X,A,
           '<IFLE>',A,' : ',,$)

```



```

      READ(IUNIT,*,ERR=10011)IFLE
      IF(IUNIT.NE.1) CALL DATA
10012 IF(IFLE.NE.0.AND.IFLE.NE.1) THEN
      WRITE(JUNIT,112)BLINK,NORMAL,BELL,BELL
112   FORMAT(/5X,A,'INVALID ENTRY FOR <IFLE>, REENTER',A,' : ',2A,$)
      READ(IUNIT,*,ERR=10012) IFLE
      GOTO 10012
    END IF
    WRITE(KUNIT,*) IFLE
C-----
    IF(IFL4.EQ.2) THEN
C-----
      DAY=DIN
      MONTH=MIN
      YEAR=YIN
C-----
    ELSE
C-----
10015   WRITE(JUNIT,118)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,
      BOLD,NORMAL,REVERS,NORMAL
118   FORMAT(/1X,A,'ENTER SIMULATION STARTING DATE',A//5X,
      'DAY',T25,A,'<DIN>',A/5X,'MONTH',T25,A,'<MIN>',
      A/5X,'YEAR',T25,A,'<YIN>',A//1X,A,
      'RESPECTIVELY',A,' : ',2A,$)
      READ(IUNIT,*,ERR=10015) DIN,MIN,YIN
      IF(IUNIT.NE.1) CALL DATA
10016   IF(DIN.GT.31.OR.DIN.LT.1) THEN
      WRITE(JUNIT,120)BLINK,NORMAL,BELL,BELL
120   FORMAT(/5X,A,'INVALID ENTRY FOR <DIN>, REENTER',A,
      ' : ',2A,$)
      READ(IUNIT,*,ERR=10016) DIN
      GOTO 10016
    END IF
10017   IF(MIN.GT.12.OR.MIN.LT.1) THEN
      WRITE(JUNIT,121)BLINK,NORMAL,BELL,BELL
121   FORMAT(/5X,A,'INVALID ENTRY FOR <MIN>, REENTER',
      A,' : ',2A,$)
      READ(IUNIT,*,ERR=10017) MIN
      GOTO 10017
    END IF
    WRITE(KUNIT,*) DIN,MIN,YIN

```

```

      DAY=DIN
      MONTH=MIN
      YEAR=YIN
C-----
      END IF
C-----
10014  WRITE(JUNIT,122)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,
      REVERS,NORMAL
122    FORMAT(/1X,A,'ENTER',A//5X,A,'O',A,': IF MONTHLY MEAN ',
      'TEMPERATURES ARE SUPPLIED BY USER'/5X,A,'1',A,
      ': IF THE AVERAGE VALUES OF THE LAST 30 YEARS ',
      'ARE USED'/1X,A,'<IFLT>',A,': ',A)
      READ(IUNIT,*,ERR=10014) IFLT
      IF(IUNIT.NE.1) CALL DATA
10018  IF(IFLT.NE.0.AND.IFLT.NE.1) THEN
      WRITE(JUNIT,119)BLINK,NORMAL,BELL,BELL
119    FORMAT(/5X,A,'INVALID ENTRY FOR <IFLT>, REENTER',A,
      ' : ',2A,$)
      READ(IUNIT,*,ERR=10018) IFLT
      GOTO 10018
      END IF
      WRITE(KUNIT,*) IFLT
C-----
      IF(IFLT.EQ.0) THEN
C-----
      DO 28 IJ=1,12
10013  WRITE(JUNIT,113)IJ,BOLD,IJ,NORMAL
113    FORMAT(/1X,'ENTER THE MEAN MONTHLY TEMPERATURE IN ',
      'FAHRENHEIT FOR MONTH ',I2,2X,A,'<TT(',I2,')>',A,
      ' : ',A)
      READ(IUNIT,*,ERR=10013) TT(IJ)
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*) TT(IJ)
28     CONTINUE
C-----
      ELSE
C-----
      C...AVERAGE MONTHLY MEAN TEMPERATURES FOR THE LAST 30 YEARS
C-----
      TT(1)=30.2
      TT(2)=32.8

```



```

      TT(3)=41.7
      TT(4)=52.3
      TT(5)=62.9
      TT(6)=71.9
      TT(7)=77.1
      TT(8)=75.9
      TT(9)=68.3
      TT(10)=57.
      TT(11)=46.9
      TT(12)=35.8

C-----
      END IF

C-----
C...PRINT YEARLY TEMPERATURE VALUES
C-----
      WRITE(21,114)
114   FORMAT(/30X,'MONTHLY MEAN TEMPERATURES (F)'/
      30X,'.....'//
      4X,'JAN',4X,'FEB',4X,'MAR',4X,'APR',4X,'MAY',4X,'JUN',
      4X,'JUL',4X,'AUG',4X,'SEP',4X,'OCT',4X,'NOV',4X,'DEC'/)
      WRITE(21,115) (TT(I),I=1,12)
115   FORMAT(5(2X,F5.2),3X,F5.2,3(2X,F5.2),1X,F5.2,2X,F5.2,3X,F5.2)

C-----
C...READ INPUT RELATED TO WATER BALANCE METHOD
C-----
10019  WRITE(JUNIT,1015)BOLD,NORMAL
1015   FORMAT(/1X,'ENTER WILTING POINT OF THE SOIL IN [%]' ,A,
      '<THW>',A,' : ',A)
      READ(IUNIT,*,ERR=10019) THW
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*) THW

C-----
10020  WRITE(JUNIT,1019)BOLD,NORMAL
1019   FORMAT(/1X,'ENTER THE DEPTH OF ROOT ZONE ',A,'<DRZ>',A,
      ' : ',A)
      READ(IUNIT,*,ERR=10020) DRZ
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*) DRZ

C-----
C...CONVERT DRZ TO [M]
C-----

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```

      IF(IUN.EQ.1) DRZ=0.3048*DRZ
      IF(IUN.EQ.3) DRZ=0.0254*DRZ
      IF(IUN.EQ.4) DRZ=0.01*DRZ
C-----
C...CONVERT TEMPERATURE VALUES TO CELSIUS
C-----
      DO 32 IJ=1,12
          TT(IJ)=(TT(IJ)-32.)*5./9.
          IF(TT(IJ).LT.0) TT(IJ)=0.0
32      CONTINUE
C-----
      IF(IFLE.EQ.1) THEN
C-----
10000    WRITE(JUNIT,100)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,
          BOLD,NORMAL,BOLD,NORMAL,BOLD,NORMAL,BOLD,
          NORMAL,REVERS,NORMAL
100      FORMAT(/1X,A,'ENTER',A//5X,A,'O',A,
          ' : IF SOIL SURFACE IS ',
          'BARE'/5X,A,'1',A,' : IF SOIL SURFACE HAS ',
          'VEGETATION',T75,A,'<ID1>',A//5X,A,'O',A,
          ' : IF AERODYNAMIC TERM IN PENMAN'S EQ IS NOT ',
          'CONSIDERED'/5X,A,'1',A,' : IF AERODYNAMIC TERM ',
          'IN PENMAN'S EQ IS CONSIDERED',T75,A,'<ID2>',A//1X,A,
          'RESPECTIVELY',A,' : ',A,$)
      READ(IUNIT,*,ERR=10000)ID1,ID2
      IF(IUNIT.NE.1) CALL DATA
10001    IF(ID1.NE.0.AND.ID1.NE.1) THEN
          WRITE(JUNIT,101)BLINK,NORMAL,BELL,BELL
101      FORMAT(/5X,A,'INVALID ENTRY FOR <ID1>, REENTER',A,
          ' : ',2A,$)
          READ(IUNIT,*,ERR=10001)ID1
          GOTO 10001
      END IF
10002    IF(ID2.NE.0.AND.ID2.NE.1) THEN
          WRITE(JUNIT,102)BLINK,NORMAL,BELL,BELL
102      FORMAT(/5X,A,'INVALID ENTRY FOR <ID2>, REENTER',A,
          ' : ',2A,$)
          READ(IUNIT,*,ERR=10002)ID2
          GOTO 10002
      END IF
      WRITE(KUNIT,*)ID1,ID2

```



```

C-----
      DO 22 IJ=1,12
10005  WRITE(JUNIT,105)IJ,BOLD,IJ,NORMAL
105    FORMAT(/1X,'ENTER THE VALUE OF MEAN SOLAR RADIATION ',
           ' [mm WATER] FOR MONTH ',I2,2X,A,'<RR(',I2,')> ',
           A,' : ',,$)
      READ(IUNIT,*,ERR=10005)RR(IJ)
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)RR(IJ)
22     CONTINUE
      WRITE(21,1007)
1007    FORMAT(/10X,'MEAN MONTHLY SOLAR RADIATION IN MM WATER ',
           'EVAPORATED PER DAY'/)
      WRITE(21,1005) (RR(JL),JL=1,12)
1005    FORMAT(1X,8F10.4)
C-----
10006  WRITE(JUNIT,106)BOLD,NORMAL
106    FORMAT(/1X,'ENTER THE VALUE OF ALBEDO COEFFICIENT ',A,
           '<ALB>',A,' : ',,$)
      READ(IUNIT,*,ERR=10006)ALB
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)ALB
      WRITE(21,1008) ALB
1008    FORMAT(/10X,'ALBEDO =',2X,F10.4)
C-----
      IF(ID2.EQ.0) GO TO 10
C-----
      DO 23 IJ=1,12
10007  WRITE(JUNIT,107)IJ,BOLD,IJ,NORMAL
107    FORMAT(/1X,'ENTER THE VALUE OF MEAN DEW-POINT TEMP. ',
           ' IN [F] FOR MONTH ',I2,2X,A,'<TD(',I2,')> ',A,' : ',,$)
      READ(IUNIT,*,ERR=10007)TD(IJ)
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)TD(IJ)
23     CONTINUE
      WRITE(21,1009)
1009    FORMAT(/10X,'MEAN MONTHLY DEW POINT TEMPERATURE IN ',
           'DEGREES FAHRENHEIT'/)
      WRITE(21,1005) (TD(JL),JL=1,12)
C-----
C...CONVERT DEW-POINT TEMP. TO CELSIUS

```

```

C-----
      DO 21 IJ=1,12
          TD(IJ)=(TD(IJ)-32)*5/9.
21      CONTINUE
C-----
      DO 24 IJ=1,12
10008    WRITE(JUNIT,108)IJ,BOLD,IJ,NORMAL
108      FORMAT(/1X,'ENTER THE VALUE OF MEAN WIND SPEED IN [mph] ',
          'FOR MONTH ',I2,2X,A,'<W(',I2,')>',A,' : ', $)
      READ(IUNIT,*,ERR=10008)W(IJ)
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)W(IJ)
24      CONTINUE
      WRITE(21,1010)
1010     FORMAT(/25X,'MEAN MONTHLY WIND SPEED IN MPH'/)
      WRITE(21,1005) (W(JL),JL=1,12)
C-----
      DO 26 IJ=1,12
10009    WRITE(JUNIT,109)IJ,BOLD,IJ,NORMAL
109      FORMAT(/1X,'ENTER THE VALUE OF MEAN DAILY ',
          'SUNSHINE IN [%] FOR MONTH ',I2,2X,A,'<SSH(',
          I2,')>',A,' : ', $)
      READ(IUNIT,*,ERR=10009)SSH(IJ)
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)SSH(IJ)
26      CONTINUE
      WRITE(21,1011)
1011     FORMAT(/20X,'MEAN MONTHLY PERCENT OF DAILY POSSIBLE ',
          'SUNSHINE'/)
      WRITE(21,1005) (SSH(JL),JL=1,12)
C-----
10      IF(ID1.EQ.0) GO TO 16
C-----
      DO 27 IJ=1,12
10010    WRITE(JUNIT,110)IJ,BOLD,IJ,NORMAL
110      FORMAT(/1X,'ENTER THE VALUE OF MEAN LEAF ARE INDEX FOR ',
          'MONTH ',I2,2X,A,'<ALI(',I2,')>',A,' : ', $)
      READ(IUNIT,*,ERR=10010)ALI(IJ)
      IF(IUNIT.NE.1) CALL DATA
      WRITE(KUNIT,*)ALI(IJ)
27      CONTINUE

```



```

      WRITE(21,1012)
1012  FORMAT(//25X,'MEAN MONTHLY LEAF AREA INDECES'//)
      WRITE(21,1005) (ALI(JL),JL=1,12)

C-----
C...COMPUTE THE CONSTANT RATE EVAP. IN [MM] USING PENMAN'S EQUATIONS
C-----
16    DO 11 IJ=1,12
      IF(TT(IJ).EQ.0) GOTO 11

C-----
      IF(ID2.EQ.0) GO TO 20

C-----
C...COMPUTE SATURATION VAPOR PRESSURES
C-----
      EA=33.8639*((0.00738*TT(IJ)+0.8072)**8.-0.000019*ABS(1.8*
        TT(IJ)+48.)+0.001316)*(760./1013.25)
      ED=33.8639*((0.00738*TD(IJ)+0.8072)**8.-0.000019*ABS(1.8*
        TD(IJ)+48.)+0.001316)*(760./1013.25)
      SS=SSH(IJ)/100.

C-----
C...LATENT HEAT OF VAPORIZATION ,HV, IN CAL/GR FOR T IN CELSIUS
C-----
      HV=597.3-0.564*TT(IJ)

C-----
C...WATER DENSITY RHO=0.998 GR/CM3,SIGMA=11.71E-8 CAL/(CM2 DAY K4)
C...COMPUTE BOLTZMANN CONSTANT, NET SOLAR RADIATION, DAILY EVAPORATION
C-----
      BT=(11.71E-8*(273.+TT(IJ))**4.)/(0.998*HV))*10.
      HO=RR(IJ)*(1.-ALB)*(0.18+0.55*SS)-BT*(0.56-0.092*(ED**5))*
        (.1+.9*SS)
      WW=W(IJ)*24.
      AEV=.35*(EA-ED)*(1.+0.0098*WW)

C-----
      GO TO 25

C-----
20    HO=RR(IJ)*(1.-ALB)

C-----
25    DELT=422.22*(5205./(TT(IJ)+273)**2)*EXP(13.95-5205./
      (TT(IJ)+273))
      IF(ID2.EQ.0) AEV=0.0

C-----
C...COMPUTE POTENTIAL EVAP. -- PSYCHROMETRIC CONSTANT = 0.27 [MM HG/F]

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```

C-----
      PEV=((DELT*HO+.27*AEV)/(.27+DELT))*IDUR(IJ)
C-----
      IF(ID1.EQ.0) GO TO 35
      SEVP=PEV*EXP(-0.4*ALI(IJ))
C-----
35      IF(ID1.EQ.0) THEN
          PE(IJ)=PEV
      ELSE
          EPL=PEV*ALI(IJ)/3.
          PE(IJ)=SEVP+EPL
          IF(PE(IJ).GT.PEV) PE(IJ)=PEV
      END IF
C-----
11      CONTINUE
C-----
      ELSE
C-----
C...COMPUTE ADJUSTED P.E.T. IN [MM] USING THORNTHWAITE'S EQUATIONS
C-----
      II=0
      DO 29 J=1,12
29      II=II+(TT(J)/5)**1.51
          AA=67.5E-8*II**3-77.1E-6*II**2+0.0179*II+0.492
C-----
      DO 31 J=1,12
31      PE(J)=1.62*BB(J)*(10*TT(J)/II)**AA*10
C-----
      END IF
C-----
C-----
C...COMPUTE THE ACTUAL EVAPOTRANSPIRATION USING WATER BALANCE METHOD
C...READ ACTUAL RAINFALL DATA FROM THE BINARY FILE (RAIN.BIN)
C-----
C-----
C...COMPILE WITH THE FOLLOWING STATEMENT FOR VAX/VMS VERSION
C-----
      OPEN(UNIT=26,FILE='RAIN.BIN',STATUS='OLD',FORM='UNFORMATTED',
          ACCESS='DIRECT',RECL=4)
C-----
C...COMPILE WITH THE FOLLOWING STATEMENT FOR IBM/DOS VERSION

```



```

C-----
C      OPEN(UNIT=26,FILE='RAIN.BIN',STATUS='OLD',FORM='UNFORMATTED',
C      ACCESS='DIRECT',RECL=16)
C-----
      CNM=1000./CN-10.
C-----
C...COMPUTE DAILY RUNOFF IN INCHES
C-----
      DO 12 IJ=1,11170
        READ(26,REC=IJ) PP
        PP=PP/100.
        IF(PP.GE.(0.2*CNM)) RNF(IJ)=(PP-0.2*CNM)**2/(PP+0.8*CNM)
        IF(RNF(IJ).LT.(PP-CNM)) RNF(IJ)=0.0
12      CONTINUE
      CLOSE (UNIT=26)
C-----
C...COMPUTE AVERAGE RUNOFF IN [MM]
C-----
      SUMR=0.0
C-----
C...AVERAGING MONTHLY FOR EACH YEAR
C-----
      DO 13 JJ=1,10959
        OLDM=MONTH
        OLDY=YEAR
        IF(MOD(YEAR,4).EQ.0) THEN
          IDUR(2)=29
        ELSE
          IDUR(2)=28
        END IF
        IF(DAY.GT.IDUR(MONTH)) THEN
          DAY=DAY-IDUR(MONTH)
          MONTH=MONTH+1
        END IF
        IF(MONTH.GT.12) THEN
          MONTH=MONTH-12
          YEAR=YEAR+1
        END IF
        IF(OLDM.EQ.MONTH) THEN
          SUMR=SUMR+RNF(JJ)
        ELSE

```

```

      RRAV(OLDY-1958,OLDM)=SUMR
      SUMR=RNF(JJ)
      END IF
      DAY=DAY+1
13  CONTINUE
C-----
C...AVERAGING YEARLY
C-----
      DO 14 J=1,12
          SUMR=0.0
          DO 36 I=1,30
36      SUMR=SUMR+RRAV(I,J)
          RAV(J)=25.4*SUMR/30.
          PAV(J)=25.4*PAV(J)/100.
          AINF(J)=PAV(J)-RAV(J)
14  CONTINUE
C-----
C...COMPUTE INITIAL MOISTURE
C-----
      CS=10*(100*THF-THW)*DRZ
      DO 17 KK=1,12
17      ST(KK)=CS
C-----
      SIPET(1)=0.0
      DO 33 JJ=1,12
          DIPET(JJ)=AINF(JJ)-PE(JJ)
          IF(DIPET(JJ).LT.0) SIPET(JJ)=SIPET(JJ-1)+DIPET(JJ)
33  CONTINUE
C-----
C...CALL INTERPOLATION ROUTINE TO COMPUTE NEW STORAGE (ST)
C-----
      DO 18 JJ=1,12
          IF(SIPET(JJ).LT.0) CALL INTPOL(SIPET(JJ),ST(JJ))
          IF(DIPET(JJ-1).LT.0.AND.DIPET(JJ).GE.0) ST(JJ)=ST(JJ-1)+
              DIPET(JJ)
          IF(ST(JJ).GT.CS) ST(JJ)=CS
18  CONTINUE
C-----
C...COMPUTE MOISTURE STORAGE DIFFERENCES
C-----
      DO 19 JJ=2,12

```



```

19'      DST(JJ)=ST(JJ)-ST(JJ-1)
C-----
C...COMPUTE ACTUAL EVAPOTRANSPIRATION VALUES
C-----
      DO 34 JJ=1,12
          APE(JJ)=PE(JJ)
          IF(ST(JJ).NE.CS.OR.DST(JJ).NE.O) APE(JJ)=AINF(JJ)-DST(JJ)
          IF(APE(JJ).GT.PE(JJ)) APE(JJ)=PE(JJ)
          PERC(JJ)=AINF(JJ)-APE(JJ)-DST(JJ)
34      CONTINUE
C-----
C...COMPUTE YEARLY TOTALS
C-----
      DO 51 JJ=1,12
          SP=SP+PAV(JJ)
          SR=SR+RAV(JJ)
          SPE=SPE+PE(JJ)
          SI=SI+AINF(JJ)
          SST=SST+ST(JJ)
          SDST=SDST+DST(JJ)
          SAET=SAET+APE(JJ)
          SPERC=SPERC+PERC(JJ)
51      CONTINUE
C-----
C...TABULATE RESULTS
C-----
      WRITE(21,1018)CM,100*THF,THW,DRZ/O.3048
1018  FORMAT(/1X,'CM = ',F4.0/1X,'THF = ',F6.2,' (%)'/
      .      1X,'THW = ',F6.2,' (%)'/1X,'DRZ = ',
      .      F6.2,' (FT)'/20X,'SUMMARY OF WATER BALANCE METHOD'/
      .      23X,'(All results are in [mm])'/
      .      20X,'.....'/)
      WRITE(21,1014)
1014  FORMAT(13X,'JAN',5X,'FEB',5X,'MAR',5X,'APR',5X,'MAY',5X,
      .      'JUN',5X,'JUL',5X,'AUG'/)
      WRITE(21,10021) 'P',(PAV(K),K=1,8)
      WRITE(21,10021) 'RUNOFF',(RAV(K),K=1,8)
      WRITE(21,10021) 'I',(AINF(K),K=1,8)
      WRITE(21,10021) 'PET',(PE(K),K=1,8)
      WRITE(21,10021) 'I-PET',(DIPET(K),K=1,8)
      WRITE(21,10021) 'S(I-PET)',(SIPET(K),K=1,8)

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      WRITE(21,10021) 'ST',(ST(K),K=1,8)
      WRITE(21,10021) 'dST',(DST(K),K=1,8)
      WRITE(21,10021) 'AET',(APE(K),K=1,8)
      WRITE(21,10021) 'PERC',(PERC(K),K=1,8)
10021 FORMAT(1X,A8,8(F8.2))
      WRITE(21,10003)
10003 FORMAT(/13X,'SEP',5X,'OCT',5X,'NOV',5X,'DEC',5X,'ANNUAL TOTALS'//)
      WRITE(21,1017) 'P',(PAV(K),K=9,12),SP
      WRITE(21,1017) 'RUNOFF',(RAV(K),K=9,12),SR
      WRITE(21,1017) 'I',(AINF(K),K=9,12),SI
      WRITE(21,1017) 'PET',(PE(K),K=9,12),SPE
      WRITE(21,1016) 'I-PET',(DIPET(K),K=9,12)
      WRITE(21,1016) 'S(I-PET)',(SIPET(K),K=9,12)
      WRITE(21,1017) 'ST',(ST(K),K=9,12),SST
      WRITE(21,1017) 'dST',(DST(K),K=9,12),SDST
      WRITE(21,1017) 'AET',(APE(K),K=9,12),SAET
      WRITE(21,1017) 'PERC',(PERC(K),K=9,12),SPERC
1016  FORMAT(1X,A8,4(F8.2))
1017  FORMAT(1X,A8,4(F8.2),6X,F8.2)
C-----
C...RESETTING CALENDAR
C-----
      DAY=DIM
      MONTH=MIN
      YEAR=YIN
C-----
C...COMPUTING DAILY EVAP. RATES --- NOTE: DT CANNOT BE MORE THAN 30 DAYS
C-----
15   IF(MOD(YEAR,4).EQ.0) THEN
      IDUR(2)=29
    ELSE
      IDUR(2)=28
    END IF
    IF(DAY.GT.IDUR(MONTH)) THEN
      DAY=DAY-IDUR(MONTH)
      MONTH=MONTH+1
    END IF
    IF(MONTH.GT.12) THEN
      MONTH=MONTH-12
      YEAR=YEAR+1
    END IF

```



```

C-----
C...COMPUTE DAILY EVAPOTRANSPIRATION
C-----
      ET(JT)=APE(MONTH)/IDUR(MONTH)
C-----
      IF(IFLE.EQ.1) THEN
C-----
C...COMPUTATION OF FALLING RATE EVAPORATION
C-----
      JTM=JT-1
C-----
      IF(JT.EQ.1) THEN
        DMEAN=D(JT)
        EFR=2.*THSU(JT)*(DMEAN*DT/3.14)**0.5/DT
C-----
      ELSE
C-----
        DMEAN=(D(JT)+D(JTM))/2.
        EFR=2.*(THSU(JTM)-THSU(JT))*(DMEAN*DT/3.14)**0.5/DT
C-----
      END IF
C-----
      IF(THSU(JT).GT.THSU(JTM)) GO TO 70
      IF(THSU(JT).EQ.THS.AND.THSU(JTM).EQ.THS) GO TO 70
      IF(EFR.LT.ET(JT)) ET(JT)=EFR
C-----
      END IF
C-----
70  IF(IUN.EQ.1) ET(JT)=ET(JT)/304.8
      IF(IUN.EQ.2) ET(JT)=ET(JT)/1000.
      IF(IUN.EQ.3) ET(JT)=ET(JT)/25.4
      IF(IUN.EQ.4) ET(JT)=ET(JT)/10.
C-----
      IF(JT/INT*INT.EQ.JT) THEN
        WRITE(21,1020) JT,ET(JT),UPR,MONTH,DAY,YEAR
1020  FORMAT(/5X,'COMPUTED AVERAGE DAILY EVAPOTRANSPIRATION ',
           'FOR TIME STEP ',I4,' =',2X,E15.4,2X,A,3X,'(',I2,
           ',I2,')/ ',I4,')')
      END IF
C-----
      DAY=DAY+DT

```

RETURN

END


```

      BBB=TEMP(IJ+1)-TEMP(IJ)
      S=TEMP(IJ+1)-(ANEG(IJ+1)-SPT)*BBB/AAA
500  RETURN
      END

```



```

C-----
C-----
      SUBROUTINE PREP
C-----
C-----
C
C...THIS ROUTINE READS THE ACTUAL DAILY PRECIPITATION DATA AND COMPUTES
C...RUNOFF USING THE SCS METHOD
C
C-----
      COMMON/BLK9/P(2234),ET(2234)
      COMMON/BLK16/DZ,DT
      COMMON/BLK28/M
      COMMON/BLK29/IUNIT,JUNIT,KUNIT
      COMMON/BLK30/BELL,BOLD,BLINK,REVERS,CLEAR,HOME,NORMAL
      COMMON/BLK53/IUN
      COMMON/BLK54/CN
C-----
      CHARACTER BELL*1,CLEAR*4,NORMAL*4,BOLD*4,BLINK*4,REVERS*4,
           HOME*6,UPR*8
C-----
C...COMPILE WITH THE FOLLOWING STATEMENT FOR VAX/VMS VERSION
C-----
      OPEN(UNIT=26,FILE='RAIN.BIN',STATUS='OLD',FORM='UNFORMATTED',
           ACCESS='DIRECT',RECL=4)
C-----
C...COMPILE WITH THE FOLLOWING STATEMENT FOR IBM/DOS VERSION
C-----
C      OPEN(UNIT=26,FILE='RAIN.BIN',STATUS='OLD',FORM='UNFORMATTED',
C      ACCESS='DIRECT',RECL=16)
C-----
10  WRITE(JUNIT,100)BOLD,NORMAL
100 FORMAT(/1X,'ENTER THE SCS SOIL CURVE NUMBER ',A,'<CN>',A,
           ' : ',,$)
      READ(IUNIT,*,ERR=10) CN
      IF(IUNIT.NE.1) CALL DATA
13  IF(CN.LE.0.OR.CN.GT.100) THEN
      WRITE(JUNIT,101)BLINK,NORMAL,BELL,BELL
101  FORMAT(/5X,A,'INVALID ENTRY FOR <CN>, REENTER : ',
           A,' : ',2A,$)
      READ(IUNIT,*,ERR=13) CN

```

```
      GOTO 13
    END IF
    WRITE(KUNIT,*) CN
    CNW=1000./CN-10.
C-----
    DO 11 IJ=1,M
      SUMP=0.0
      DO 12 JJ=(IJ-1)*DT+1,IJ*DT
        READ(26,REC=JJ) PP
        PP=PP/100.
        IF(PP.GE.(0.2*CNW)) RUNF=(PP-0.2*CNW)**2/(PP+0.8*CNW)
        IF(RUNF.LT.(PP-CNW)) RUNF=0.0
        PP=PP-RUNF
        SUMP=SUMP+PP
        RUNF=0.0
12      CONTINUE
        P(IJ)=SUMP/DT
        IF(IUN.EQ.1) P(IJ)=P(IJ)/12.
        IF(IUN.EQ.2) P(IJ)=P(IJ)*0.0254
        IF(IUN.EQ.4) P(IJ)=P(IJ)*2.54
11    CONTINUE
    CLOSE (UNIT=26)
    RETURN
  END
```



```

C-----
C-----
      SUBROUTINE FLUXEQ
C-----
C-----
C...THIS SUBROUTINE COMPUTES THE APPROXIMATION TO K AND D
C...AT THE END OF EACH TIME STEP AND FORMULATES THE SYSTEM OF
C...EQUATIONS FOR SOLUTION IN MATRIX FORM FOR THE FLUX
C...BOUNDARY CONDITION
C-----
      COMMON/BLK1/N
      COMMON/BLK2/DIAG(400),SUB(400),SUP(400),R(400)
      COMMON/BLK3/THNEW(400),THOLD(400)
      COMMON/BLK4/IFL1,IFL2,AKS,THS,THF,AM,AN,AI,BE,B,THAD,AN2,AM2,
           GAMMA,ALPHA
      COMMON/BLK5/PSIR,DZER,BET,THZER
      COMMON/BLK6/AK(400),DIFF(400),AKM(400),AKP(400),DM(400),DP(400)
      COMMON/BLK7/TH(400)
      COMMON/BLK9/P(2234),ET(2234)
      COMMON/BLK10/JT,TIME(2234)
      COMMON/BLK16/DZ,DT
      COMMON/BLK24/THAV(400),TRTH(400)
      COMMON/BLK25/IT,INT
      COMMON/BLK28/M
      COMMON/BLK52/IFL9
C-----
      IF(IT.GT.0) GO TO 102
C-----
      DO 103 I=1,N
103   TRTH(I)=THNEW(I)
C-----
102   NM=N-1
      BP=B+1
C-----
      DO 101 I=1,N
101   THAV(I)=(TRTH(I)+THNEW(I))/2.
C-----
      IF(IFL1.EQ.1) GO TO 5
      IF(IFL1.EQ.2) GO TO 10
      IF(IFL1.EQ.3) GO TO 15
      IF(IFL1.EQ.4) GO TO 16

```

```

C-----
5    DO 20 I=1,N
20    AK(I)=AKS*(THAV(I)/THS)**AM
      GO TO 60
C-----
10   DO 30 I=1,N
30    AK(I)=AKS*((THAV(I)-THF)/(THS-THF))**AM
      GO TO 60
C-----
15   DO 40 I=1,N
40    AK(I)=AI*(THAV(I)**BE)
      GO TO 60
C-----
16   DO 41 I=1,N
      IF(THAV(I).GE.TH S) THAV(I)=THS-0.001
      IF(THAV(I).LE.TH F) THAV(I)=THF+0.001
      SE=(THAV(I)-THF)/(THS-THF)
41    AK(I)=AKS*SE**GAMMA*(1-(1-SE**(1/AM2))**AM2)**2
C-----
60    IF(IFL2.EQ.1) GO TO 45
      IF(IFL2.EQ.2) GO TO 50
      IF(IFL2.EQ.3) GO TO 51
C-----
45    DO 55 I=1,N
55    DIFF(I)=AK(I)*B*PSIR/THS*(THS/THAV(I))**BP
      GO TO 65
C-----
50    DO 56 I=1,N
56    DIFF(I)=DZER*EXP(BET*(THAV(I)-THZER))
      GO TO 65
C-----
51    DO 57 I=1,N
      SE=(THAV(I)-THF)/(THS-THF)
57    DIFF(I)=AK(I)/(ALPHA*(AM2-1)*(THS-THF))*(1-SE**(1/AM2))**(-AM2)*
      SE**(-1/AM2)
C-----
65    DO 70 I=2,NM
      IM=I-1
      IP=I+1
      AKM(I)=(AK(I)*DIFF(IM)+AK(IM)*DIFF(I))/(DIFF(I)+DIFF(IM))
      AKP(I)=(AK(I)*DIFF(IP)+AK(IP)*DIFF(I))/(DIFF(I)+DIFF(IP))

```



```

      DM(I)=2*(DIFF(I)*DIFF(IM))/(DIFF(I)+DIFF(IM))
      DP(I)=2*(DIFF(I)*DIFF(IP))/(DIFF(I)+DIFF(IP))
70    CONTINUE
C-----
      IF(THNEW(N).LT.THF) AKP(NM)=AK(NM)
      IF(THNEW(N).LT.THF) DP(NM)=DIFF(NM)
C-----
C...FORMULATE THE SYSTEM OF EQUATIONS FOR SOLUTION IN MATRIX FORM
C...A*TH=R
C...CALL SUB,DIAG,SUP THE THREE COEFFICIENT ARRAYS FOR THE TRIDIAGONAL
C...MATRIX (TDMA)
C-----
      SUB(1)=0.0
      DIAG(1)=DM(2)/DZ+DZ/(2.*DT)
      SUP(1)=-DM(2)/DZ
      R(1)=DZ*THOLD(1)/(2.*DT)-AKM(2)+P(JT)-ET(JT)
C-----
      DO 25 I=2,NM
      SUB(I)=-DM(I)/DZ
      DIAG(I)=(DP(I)+DM(I))/DZ+DZ/DT
25    SUP(I)=-DP(I)/DZ
C-----
      DO 26 I=2,NM
26    R(I)=DZ*THOLD(I)/DT-AKP(I)+AKM(I)
C-----
      IF(IFL9.EQ.0) THEN
        TH(N)=THS
      ELSE
        SUB(N)=-DP(NM)/DZ
        DIAG(N)=DP(NM)/DZ+DZ/(2.*DT)
        SUP(N)=0.0
        R(N)=DZ*THOLD(N)/(2.*DT)-AK(N)+AKP(NM)
        IF(THNEW(N).LT.THF) R(N)=DZ*THOLD(N)/(2.*DT)+AKP(NM)
      END IF
C-----
C...SOLVE THE TDMA
C-----
27    CALL TRDMS
      RETURN
      END

```

```

C-----
C-----
      SUBROUTINE TRDMS
C-----
C-----
C...ALGORITHM BASED ON S.D.CONTE/C.DE BOOR,ELEMENTARY NUMERICAL
C...ANALYSIS,MC GRAW-HILL
C-----

      COMMON/BLK1/N
      COMMON/BLK2/DIAG(400),SUB(400),SUP(400),R(400)
      COMMON/BLK7/TH(400)
      COMMON/BLK52/IFL9
      DIMENSION DIAGP(400),RPR(400)

C-----
      NM=N-1
      DIAGP(1)=DIAG(1)
      RPR(1)=R(1)

C-----
      IF(IFL9.EQ.0) THEN
          NM=NM
      ELSE
          NM=N
      END IF

C-----
      DO 5 I=2,NM
          IF(DIAGP(I-1).EQ.0.) GO TO 15
          DIAGP(I)=DIAG(I)-SUB(I)/DIAGP(I-1)*SUP(I-1)
5       RPR(I)=R(I)-SUB(I)/DIAGP(I-1)*RPR(I-1)
          IF (IFL9.NE.0) TH(N)=RPR(N)/DIAGP(N)
          DO 10 I=1,NM
              K=N-I
10         TH(K)=(RPR(K)-SUP(K)*TH(K+1))/DIAGP(K)
          GO TO 20
15       WRITE(6,2000)
2000    FORMAT(/2X,'SOMETHING IS WRONG'/)
20       RETURN
      END

```



```

C-----
C-----
      SUBROUTINE CONSMO
C-----
C-----
C...THIS SUBROUTINE COMPUTES THE APPROXIMATION TO K AND D AT THE END
C...OF EACH TIME STEP , FORMULATES AND SOLVES THE EQUATIONS
C...FOR CONSTANT MOISTURE BOUNDARY CONDITION
C-----
      COMMON/BLK1/N
      COMMON/BLK2/DIAG(400),SUB(400),SUP(400),R(400)
      COMMON/BLK3/THNEW(400),THOLD(400)
      COMMON/BLK4/IFL1,IFL2,AKS,THS,THF,AM,AM,AI,BE,B,THAD,AM2,AM2,
           GAMMA,ALPHA
      COMMON/BLK5/PSIR,DZER,BET,THZER
      COMMON/BLK6/AK(400),DIFF(400),AKM(400),AKP(400),DM(400),DP(400)
      COMMON/BLK7/TH(400)
      COMMON/BLK9/P(2234),ET(2234)
      COMMON/BLK12/JK
      COMMON/BLK13/IT2
      COMMON/BLK16/DZ,DT
      COMMON/BLK24/THAV(400),TRTH(400)
      COMMON/BLK28/M
      COMMON/BLK52/IFL9
C-----
      TH(1)=THNEW(1)
C-----
      IF(IT2.GT.0) GO TO 202
      DO 200 I=1,N
200   TRTH(I)=THNEW(I)
C-----
202   NM=N-1
      BP=B+1
      NM2=N-2
      ICC=0
      JK=2
C-----
C...LOCATE THE FIRST LAYER WHICH HAS THETA BETWEEN TH_AIR - TH_SAT
C-----
      DO 120 I=2,NM
      IF(THNEW(I).EQ.TH.S.OR.THNEW(I).EQ.THAD) GO TO 120

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      IF(THNEW(I).LT.THS.AND.THNEW(I).GT.THAD) JK=I
      GO TO 110
120   CONTINUE
C-----
110   IF(ICC.EQ.0) GO TO 131
C-----
      DO 130 I=1,N
130   THNEW(I)=TH(I)
C-----
131   DO 21 I=1,N
21    THAV(I)=(TRTH(I)+THNEW(I))/2.
C-----
      IF(IFL1.EQ.1) GO TO 5
      IF(IFL1.EQ.2) GO TO 10
      IF(IFL1.EQ.3) GO TO 15
      IF(IFL1.EQ.4) GO TO 16
C-----
5     DO 20 I=1,N
20    AK(I)=AKS*(THAV(I)/THS)**AM
      GO TO 60
C-----
10    DO 30 I=1,N
30    AK(I)=AKS*((THAV(I)-THF)/(THS-THF))**AM
      GO TO 60
C-----
15    DO 40 I=1,N
40    AK(I)=AI*(THAV(I)**BE)
      GO TO 60
C-----
16    DO 41 I=1,N
      IF(THAV(I).GE.THS) THAV(I)=THS-0.001
      IF(THAV(I).LE.THF) THAV(I)=THF+0.001
      SE=(THAV(I)-THF)/(THS-THF)
41    AK(I)=AKS*SE**GAMMA*(1-(1-SE**(1/AM2))**AM2)**2
C-----
60    IF(IFL2.EQ.1) GO TO 45
      IF(IFL2.EQ.2) GO TO 50
      IF(IFL2.EQ.3) GO TO 51
C-----
45    DO 55 I=1,N
55    DIFF(I)=AK(I)*B*PSIR/THS*(THS/THAV(I))**BP

```



```

      GO TO 65
C-----
50   DO 56 I=1,N
56   DIFF(I)=DZER*EXP(BET*(THAV(I)-THZER))
      GO TO 65
C-----
51   DO 57 I=1,N
      SE=(THAV(I)-THF)/(THS-THF)
57   DIFF(I)=AK(I)/(ALPHA*(AM2-1)*(THS-THF))*(1-SE**(1/AM2))**(-AM2)*
      SE**(-1/AM2)
C-----
65   DO 70 I=2,NM
      IM=I-1
      IP=I+1
      AKM(I)=(AK(I)*DIFF(IM)+AK(IM)*DIFF(I))/(DIFF(I)+DIFF(IM))
      AKP(I)=(AK(I)*DIFF(IP)+AK(IP)*DIFF(I))/(DIFF(I)+DIFF(IP))
      DM(I)=2*(DIFF(I)*DIFF(IM))/(DIFF(I)+DIFF(IM))
70   DP(I)=2*(DIFF(I)*DIFF(IP))/(DIFF(I)+DIFF(IP))
C-----
      IF(THNEW(N).LT.THF) AKP(NM)=AK(NM)
      IF(THNEW(N).LT.THF) DP(NM)=DIFF(NM)
C-----
C...FORMULATE THE SYSTEM OF EQUATIONS FOR SOLUTION IN MATRIX FORM
C...A*TH=R
C...CALL SUB,DIAG,SUP THE THREE COEFFICIENT ARRAYS FOR THE TRIDIAGONAL
C...MATRIX (TDMA)
C-----
C...BOTTOM B.C.
C-----
      IF(IFL9.EQ.0) THEN
          TH(N)=THS
      ELSE
          SUB(N)=-DP(NM)/DZ
          DIAG(N)=DP(NM)/DZ+DZ/(2.*DT)
          SUP(N)=0.0
          R(N)=DZ*THOLD(N)/(2.*DT)-AK(N)+AKP(NM)
          IF(THNEW(N).LT.THF) R(N)=DZ*THOLD(N)/(2.*DT)+AKP(NM)
      END IF
C-----
C...ESTABLISH NEW TOP B.C. (FROM THE JKth LAYER)
C-----

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```

      SUB(JK)=0.0
      DIAG(JK)=DP(JK)/DZ+DZ/DT
      SUP(JK)=-DP(JK)/DZ
C-----
      IF(THNEW(JK-1).EQ.THS) AKM(JK)=AKS
      IF(THNEW(JK-1).EQ.THAD) AKM(JK)=0.0
C-----
      R(JK)=DZ*THOLD(JK)/DT-AKP(JK)+AKM(JK)
C-----
      IF(JK.EQ.NM) GO TO 400
      IF(JK.EQ.N) GO TO 410
C-----
C...INTERMEDIATE NODES
C-----
      DO 100 I=JK,NM2
      SUB(I+1)=-DM(I+1)/DZ
      DIAG(I+1)=DP(I+1)/DZ+DM(I+1)/DZ+DZ/DT
      SUP(I+1)=-DP(I+1)/DZ
100   R(I+1)=DZ*THOLD(I+1)/DT-AKP(I+1)+AKM(I+1)
C-----
400   CALL TRDS1
C-----
      GO TO 420
C-----
410   IF(THNEW(NM).EQ.THS) AKM(N)=AKS
      IF(THNEW(NM).EQ.THAD) AKM(N)=0.0
      IF(THNEW(N).LT.THF) AK(N)=0.0
      IF(IFL9.NE.0) TH(N)=THOLD(N)-(2.*DT)/DZ*(AK(N)-AKM(N))
      IF(TH(N).GE.THS) TH(N)=THS
      IF(TH(N).LE.THAD) TH(N)=THAD
      GO TO 150
C-----
C...CHECKING NEW SOLUTION BETWEEN JKth and Nth LAYERS
C-----
420   JKCHNG=JK
      DO 300 I=JK,N
      IF(TH(I).GE.THS) THEN
          TH(I)=THS
          JKCHNG=I
      END IF
300   CONTINUE

```



```
C-----
      JK=JKCHNG
C-----
      DO 310 I=JK,N
      IF (TH(I).LE.THAD) THEN
          TH(I)=THAD
          JKCHNG=I
      END IF
310   CONTINUE
C-----
      JK=JKCHNG
C-----
      IF (TH(JK+1).LT.THS.AND.TH(JK+1).GT.THAD) GO TO 150
C-----
      ICC=ICC+1
      GO TO 110
150   RETURN
      END
```

```

C-----
C-----
      SUBROUTINE TRDS1
C-----
C-----
C...ALGORITHM BASED ON S.D.CONTE/C.DE BOOR,ELEMENTARY NUMERICAL
C...ANALYSIS,MC GRAW-HILL
C-----
      COMMON/BLK1/N
      COMMON/BLK2/DIAG(400),SUB(400),SUP(400),R(400)
      COMMON/BLK7/TH(400)
      COMMON/BLK12/JK
      COMMON/BLK52/IFL9
      DIMENSION DIAGP(400),RPR(400)
C-----
      NM=N-1
      DIAGP(JK)=DIAG(JK)
      RPR(JK)=R(JK)
      DO 5 I=JK,NM
      IF(DIAGP(I).EQ.0.) GO TO 15
      DIAGP(I+1)=DIAG(I+1)-SUB(I+1)/DIAGP(I)*SUP(I)
5      RPR(I+1)=R(I+1)-SUB(I+1)/DIAGP(I)*RPR(I)
      IF(IFL9.NE.0) TH(N)=RPR(N)/DIAGP(N)
      NM=N-JK
      DO 10 I=1,NM
      K=N-I
10      TH(K)=(RPR(K)-SUP(K)*TH(K+1))/DIAGP(K)
      GO TO 20
15      WRITE(6,2000)
2000  FORMAT('//2X,'SOMETHING IS WRONG'/)
20      RETURN
      END

```



```

C-----
C-----
      SUBROUTINE SOLUTE
C-----
C-----
C
C   .....
C   THIS SUBROUTINE IS BASED ON HAMMING'S PREDICTOR-CORRECTOR
C   METHOD. IT SOLVES A SYSTEM OF N FIRST-ORDER DIFFERENTIAL
C   EQUATIONS, SUBJECT TO N NUMBER OF INITIAL CONDITIONS.
C   .....
C   INDEX IS A VARIABLE THAT IDENTIFIES TYPE OF THE MATERIAL.
C   INDEX=0 BIODEGRADABLE, INDEX=1 NONBIODEGRADABLE
C   AAKM= SUBSTRATE CONCENTRATION WHEN SUBSTRATE UTILIZATION
C   IS EQUAL TO ITS MAXIMUM VALUE.
C   AMU= BIOMASS SPECIFIC GROWTH RATE
C   AKK= ENDOGENOUS DEATH RATE CONSTANT
C   AKC= ZERO ORDER MONOD COEFFICIENT
C   AKL= FIRST ORDER MONOD COEFFICIENT
C   YEL= CELL YIELD GROWTH COEFFICIENT
C   TMAX= MAXIMUM SIMULATION TIME
C   YR= AN ARRAY CONTAINING VALUES OF CONCENTRATION
C   FR= AN ARRAY CONTAINING VALUES OF THE DERIVATIVES OF THE
C   EQUATIONS
C   DZ= STEP SIZE FOR DISTANCE INCREMENT
C   DT= STEP SIZE FOR TIME ENCREMENT
C-----
      COMMON/BLK1/N
      COMMON/BLK3/THNEW(400),THOLD(400)
      COMMON/BLK6/AK(400),DIFF(400),AKM(400),AKP(400),DM(400),DP(400)
      COMMON/BLK10/JT,TIME(2234)
      COMMON/BLK11/QOLD(400),QNEW(400),DISCH(400)
      COMMON/BLK16/DZ,DT
      COMMON/BLK19/BIOMI(400),CTOTAL(400),CONCI(400),H,
      TMAX,INDEX
      COMMON/BLK25/IT,INT
      COMMON/BLK26/ICOUNT
      COMMON/BLK40/TCONC(2234),BCONC(2234),BBIOM(2234),BDISCH(2234)
      COMMON/BLK42/IFL13,IMONOD,AKC,AKL
      COMMON/BLK53/IUN
      COMMON/BLK59/TTH(2,2234)
C-----

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```

      DIMENSION TE(800),YR(800),FR(800),Y(4,800),F(3,800),YOLD(800)
C-----
      JT=0
      X=0.0
      ICOUNT=0
C-----
C...DETERMINE TYPE OF THE MATERIAL TO BE CONSIDERED
C-----
      IF(INDEX.EQ.1) GO TO 14
      IF(IFL13.EQ.1) GOTO 14
      N2=2*N
      L=N2/2
      LP1=L+1
C-----
C...SET THE INITIAL VALUES
C-----
      TCONC(1)=CONCI(2)
      BCONC(1)=CONCI(N)
      BBIOM(1)=BIOMI(N)
      BDISCH(1)=QOLD(N)
      TIME(1)=X
C-----
      DO 9 I=1,L
9      YR(I)=CONCI(I)
C-----
      DO 11 J=LP1,N2
11     YR(J)=BIOMI(J-L)
C-----
      DO 2 J=1,N2
      Y(4,J)=YR(J)
2      TE(J)=0.0
C-----
35     JT=JT+1
      TIME(JT+1)=FLOAT(JT)*DT
C-----
C...CALL YGRA TO GET MOISTURE DISTRIBUTION
C-----
      ICOUNT=ICOUNT+1
C-----
      CALL YGRA
      TTH(1,JT+1)=THNEW(1)

```



```

      TTH(2,JT+1)=THNEW(2)
C-----
C...CALL RUNGE TO GET CONCENTRATION DISTRIBUTION
C-----
3      DO 1005 IJ=1,N2
1005    YOLD(IJ)=YR(IJ)
C-----
      CALL RUNGE(K,N2,YR,FR,X,H)
C-----
      DO 1000 I=1,N2
1000    IF(YR(I).LT.0.0) YR(I)=YOLD(I)
C-----
      IF(K.NE.1) GO TO 4
C-----
C...CALL BIOD TO GET DERIVATIVES OF THE EQUATIONS
C-----
      CALL BIOD(N2,YR,FR)
C-----
      GO TO 3
4      DO 80 I=1,N
      THOLD(I)=THNEW(I)
80     QOLD(I)=QNEW(I)
      TIME(JT+1)=X
      TCONC(JT+1)=YR(2)
      BCONC(JT+1)=YR(L)
      BBIOM(JT+1)=YR(N2)
      BDISCH(JT+1)=DISCH(N)
      ISUB=4-ICOUNT
      DO 5 J=1,N2
      Y(ISUB,J)=YR(J)
5      F(ISUB,J)=FR(J)
C-----
C...PRINT CALCULATED VALUES
C-----
6      IF(ICOUNT/INT*INT.NE.ICOUNT)GO TO 7
C-----
      IF(ICOUNT.LE.3) WRITE(21,220) X,'MG/L'
220    FORMAT(/20X,'CONCENTRATION DISTRIBUTION AT ',F6.0,2X,
           'DAYS ',A/)
C-----
      IF(ICOUNT.LE.3) THEN

```

```

C-----
      IF(IUM.EQ.1) WRITE(21,230) (35.314667*Y(ISUB,J),J=1,L)
      IF(IUM.EQ.2) WRITE(21,230) (Y(ISUB,J),J=1,L)
      IF(IUM.EQ.3) WRITE(21,230) (61023.744*Y(ISUB,J),J=1,L)
      IF(IUM.EQ.4) WRITE(21,230) (1E6*Y(ISUB,J),J=1,L)
230  FORMAT(8E15.4)
C-----
      END IF
C-----
      IF(ICOUNT.LE.3) WRITE(21,240) X,'MG/L'
240  FORMAT(//20X,'BIOMASS DISTRIBUTION AT ',F6.0,2X,'DAYS ',A/)
C-----
      IF(ICOUNT.LE.3) THEN
C-----
          IF(IUM.EQ.1) WRITE(21,230) (35.314667*Y(ISUB,J),J=LP1,N2)
          IF(IUM.EQ.2) WRITE(21,230) (Y(ISUB,J),J=LP1,N2)
          IF(IUM.EQ.3) WRITE(21,230) (61023.744*Y(ISUB,J),J=LP1,N2)
          IF(IUM.EQ.4) WRITE(21,230) (1E6*Y(ISUB,J),J=LP1,N2)
C-----
          END IF
C-----
          IF(ICOUNT.GT.3) WRITE(21,220) X,'MG/L'
C-----
          IF(ICOUNT.GT.3) THEN
C-----
              IF(IUM.EQ.1) WRITE(21,230) (35.314667*Y(1,J),J=1,L)
              IF(IUM.EQ.2) WRITE(21,230) (Y(1,J),J=1,L)
              IF(IUM.EQ.3) WRITE(21,230) (61023.744*Y(1,J),J=1,L)
              IF(IUM.EQ.4) WRITE(21,230) (1E6*Y(1,J),J=1,L)
C-----
              END IF
C-----
              IF(ICOUNT.GT.3) WRITE(21,240) X,'MG/L'
C-----
              IF(ICOUNT.GT.3) THEN
C-----
                  IF(IUM.EQ.1) WRITE(21,230) (35.314667*Y(1,J),J=LP1,N2)
                  IF(IUM.EQ.2) WRITE(21,230) (Y(1,J),J=LP1,N2)
                  IF(IUM.EQ.3) WRITE(21,230) (61023.744*Y(1,J),J=LP1,N2)
                  IF(IUM.EQ.4) WRITE(21,230) (1E6*Y(1,J),J=LP1,N2)
C-----

```



```

      END IF
C-----
7      IF(X.GT.TMAX-H/2.)GO TO 135
      IF(ICOUNT.LT.3) GO TO 35
C-----
C...CALL HAMMING TO GET THE NEW VALUES
C-----
8      DO 1007 IJ=1,N2
1007    YOLD(IJ)=Y(1,IJ)
C-----
      CALL HAMING(M,N2,Y,F,X,H,TE)
C-----
      DO 1008 I=1,N2
1008    IF(Y(1,I).LT.O.O) Y(1,I)=YOLD(I)
C-----
      DO 42 I=1,N2
42      YR(I)=Y(1,I)
      IF(M.EQ.2) GO TO 465
      JT=JT+1
      TIME(JT+1)=X
C-----
C...CALL YGRA TO GET MOISTURE DISTRIBUTION
C-----
      ICOUNT=ICOUNT+1
C-----
      CALL YGRA
      TTH(1,JT+1)=THNEW(1)
      TTH(2,JT+1)=THNEW(2)
C-----
465    CONTINUE
C-----
C...CALL BIOD TO GET DERIVATIVES
C-----
      CALL BIOD(N2,YR,FR)
C-----
      DO 17 K=1,N2
17      F(1,K)=FR(K)
      IF(M.EQ.1) GO TO 8
      TIME(JT+1)=X
      TCONC(JT+1)=YR(2)
      BCONEC(JT+1)=YR(L)

```

```

      BBIOM(JT+1)=YR(N2)
      BDISCH(JT+1)=DISCH(N)
      IF(M.EQ.1)GO TO 466
      DO 90 I=1,N
      THOLD(I)=THNEW(I)
90    QOLD(I)=QNEW(I)
466   GO TO 6

C-----
C...CALCULATE MOISTURE, CONCENTRATION FOR NONBIODEGRADABLE MATTER
C
C...SET INITIAL CONDITIONS FOR NONBIODEGRADABLE MATTER
C-----
14    CONTINUE
      TCONC(1)=CONCI(2)
      BCONC(1)=CONCI(N)
      BDISCH(1)=QOLD(N)
      TIME(1)=X
      DO 10 L=1,N
10    YR(L)=CONCI(L)
      DO 20 J=1,N
      Y(4,J)=YR(J)
20    TE(J)=0.0

C-----
330   JT=JT+1
      TIME(JT+1)=FLOAT(JT)*DT

C-----
C...CALL YGRA TO GET MOISTURE DISTRIBUTION
C-----
      ICOUNT=ICOUNT+1

C-----
      CALL YGRA
      TTH(1,JT+1)=THNEW(1)
      TTH(2,JT+1)=THNEW(2)

C-----
C...CALL RUNGE TO GET CONCENTRATION DISTRIBUTION
C-----
33    DO 1003 IJ=1,N
1003   YOLD(IJ)=YR(IJ)

C-----
      CALL RUNGE(K,N,YR,FR,X,H)

C-----

```



```

      DO 1001 II=1,N
1001      IF(YR(II).LT.0.0) YR(II)=YOLD(II)
C-----
      IF(K.WE.1) GO TO 44
C-----
C...CALL NBIOD TO GET DERIVATIVES
C-----
      CALL NBIOD(N,YR,FR)
C-----
      GO TO 33
44      DO 91 I=1,N
          THOLD(I)=THNEW(I)
91      QOLD(I)=QNEW(I)
          TIME(JT+1)=X
          TCONC(JT+1)=YR(2)
          BCONC(JT+1)=YR(N)
          BDISCH(JT+1)=DISCH(N)
          ISUB=4-ICOUNT
          DO 50 J=1,N
              Y(ISUB,J)=YR(J)
50      F(ISUB,J)=FR(J)
C-----
C...PRINT CALCULATED VALUES
C-----
66      IF(ICOUNT/INT*INT.WE.ICOUNT) GO TO 77
          IF(ICOUNT.LE.3) WRITE(21,220) X,'MG/L'
C-----
          IF(ICOUNT.LE.3) THEN
C-----
              IF(IUN.EQ.1) WRITE(21,230)(35.314667*Y(ISUB,J),J=1,N)
              IF(IUN.EQ.2) WRITE(21,230)(Y(ISUB,J),J=1,N)
              IF(IUN.EQ.3) WRITE(21,230)(61023.744*Y(ISUB,J),J=1,N)
              IF(IUN.EQ.4) WRITE(21,230)(1E6*Y(ISUB,J),J=1,N)
C-----
          END IF
C-----
          IF(ICOUNT.GT.3) WRITE(21,220) X,'MG/L'
C-----
          IF(ICOUNT.GT.3) THEN
C-----
              IF(IUN.EQ.1) WRITE(21,230)(35.314667*Y(1,J),J=1,N)

```

```

      IF(IUN.EQ.2) WRITE(21,230)(Y(1,J),J=1,N)
      IF(IUN.EQ.3) WRITE(21,230)(61023.744*Y(1,J),J=1,N)
      IF(IUN.EQ.4) WRITE(21,230)(1E6*Y(1,J),J=1,N)
C-----
      END IF
C-----
77   IF(X.GT.TMAX-H/2) GO TO 135
      IF(ICOUNT.LT.3) GO TO 330
C-----
C...CALL HAMMING TO GET NEW VALUES
C-----
88   DO 1004 IJ=1,N
1004   YOLD(IJ)=Y(1,IJ)
C-----
      CALL HAMING(M,N,Y,F,X,H,TE)
C-----
      DO 1002 II=1,N
1002   IF(Y(1,II).LT.0.0) Y(1,II)=YOLD(II)
C-----
      DO 45 J=1,N
45   YR(J)=Y(1,J)
      IF(M.EQ.2) GO TO 565
      JT=JT+1
      TIME(JT+1)=X
C-----
C...CALL YGRA TO GET MOISTURE DISTRIBUTION
C-----
      ICOUNT=ICOUNT+1
C-----
      CALL YGRA
      TTH(1,JT+1)=THNEW(1)
      TTH(2,JT+1)=THNEW(2)
C-----
565  CONTINUE
C-----
C...CALL NBIOD TO GET THE DERIVATIVES
C-----
      CALL NBIOD(N,YR,FR)
C-----
      DO 36 I=1,N
36   F(1,I)=FR(I)

```



```
IF(M.EQ.1) GO TO 88
TIME(JT+1)=X
TCONC(JT+1)=YR(2)
BCONC(JT+1)=YR(N)
BDISCH(JT+1)=DISCH(N)
IF(M.EQ.1)GO TO 566
DO 92 I=1,N
THOLD(I)=THNEW(I)
92 QOLD(I)=QNEW(I)
566 GO TO 66
135 CONTINUE
RETURN
END
```

```

C-----
C-----
      SUBROUTINE HAMING(M,N,Y,F,X,H,TE)
C-----
C-----
      LOGICAL PRED
      DIMENSION YPRED(110),TE(N),Y(4,N),F(3,N)
      DATA PRED/.TRUE./
      IF(.NOT.PRED)GO TO 4
      DO 1 J=1,N
1     YPRED(J)=Y(4,J)+4.*H*(2.*F(1,J)-F(2,J)+2.*F(3,J))/3.
      DO 2 J=1,N
      DO 2 K5=1,3
      K=5-K5
      Y(K,J)=Y(K-1,J)
2     IF(K.LT.4)F(K,J)=F(K-1,J)
      DO 3 J=1,N
3     Y(1,J)=YPRED(J)+112.*TE(J)/9.
      X=X+H
      PRED=.FALSE.
      M=1
      RETURN
4     DO 5 J=1,N
      Y(1,J)=(9.*Y(2,J)-Y(4,J)+3.*H*(F(1,J)+2.*F(2,J)-F(3,J)))/8.
      TE(J)=9.*(Y(1,J)-YPRED(J))/121.
5     Y(1,J)=Y(1,J)-TE(J)
      PRED=.TRUE.
      M=2
      RETURN
      END

```



```
C-----
C-----
      SUBROUTINE RUNGE(K,M,Y,F,X,H)
C-----
C-----
      DIMENSION PHI(110),SAVEY(110),Y(M),F(M)
      DATA M/0/
      M=M+1
      GO TO (1,2,3,4,5),M
1      K=1
      RETURN
2      DO 22 J=1,M
      SAVEY(J)=Y(J)
      PHI(J)=F(J)
22     Y(J)=SAVEY(J)+0.5*H*F(J)
      X=X+0.5*H
      K=1
      RETURN
3      DO 33 J=1,M
      PHI(J)=PHI(J)+2.0*F(J)
33     Y(J)=SAVEY(J)+0.5*H*F(J)
      K=1
      RETURN
4      DO 44 J=1,M
      PHI(J)=PHI(J)+2.0*F(J)
44     Y(J)=SAVEY(J)+H*F(J)
      X=X+0.5*H
      K=1
      RETURN
5      DO 55 J=1,M
55     Y(J)=SAVEY(J)+(PHI(J)+F(J))*H/6.0
      M=0
      K=0
      RETURN
      END
```

```

C-----
C-----
      SUBROUTINE BIOD(N2,V,F)
C-----
C-----
      COMMON/BLK1/N
      COMMON/BLK3/THNEW(400),THOLD(400)
      COMMON/BLK11/QOLD(400),QNEW(400),DISCH(400)
      COMMON/BLK16/DZ,DT
      COMMON/BLK18/AMU,AKK,AAKM,YEL
      COMMON/BLK50/AKD,AKPR,DDW,DDA,HENRY,POROS,ALAM,RHO
      DIMENSION V(800),F(800)
C-----
      DO 25 J=1,N
      IF(THNEW(J).GT.POROS) THNEW(J)=POROS
25  CONTINUE
      A2=HENRY*AKPR*RHO
C-----
      L=N2/2
      LP1=L+1
C-----
      DO 2 I=1,N2
      RSUB=AMU*V(L+I)*V(I)/(YEL*(AAKM+V(I)))
C-----
      A1=1./((HENRY-1)*THNEW(I)+HENRY*AKD*RHO+POROS)
      IF(I.EQ.1) GOTO 5
      A3=HENRY*QNEW(I)
      EHD1=HENRY*(ABS(QNEW(I))*ALAM+
      .      DDW*THNEW(I)**(13/3.)/POROS**2)+
      .      DDA*(POROS-THNEW(I)**(13/3.)/POROS**2
      EHD1=HENRY*(ABS(QNEW(I-1))*ALAM+
      .      DDW*THNEW(I-1)**(13/3.)/POROS**2)+
      .      DDA*(POROS-THNEW(I-1)**(13/3.)/POROS**2
      IF(I.EQ.L) GO TO 8
      IF(I.GT.L) GO TO 4
      EHD1=HENRY*(ABS(QNEW(I+1))*ALAM+
      .      DDW*THNEW(I+1)**(13/3.)/POROS**2)+
      .      DDA*(POROS-THNEW(I+1)**(13/3.)/POROS**2
C-----
C...FOR INTERMEDIATE MODES
C-----

```



```

      F(I)=A1*((EHDAP-EHDAM)*(V(I+1)-V(I-1))/(4*DZ**2)+
      .      EHDA*(V(I+1)-2*V(I)+V(I-1))/DZ**2-A2*V(I)+
      .      (THNEW(I)-THOLD(I))*V(I)/DT-A3*(V(I+1)-V(I-1))/
      .      (2*DZ)-RSUB)
      GO TO 2
C-----
C...FOR TOP B.C.
C-----
5      F(I)=A1*(-A2+(THNEW(1)-THOLD(1))/DT-RSUB)*(V(1)+V(2))/2.
      GO TO 2
C-----
C...FOR BOTTOM B.C.
C-----
8      F(I)=A1*((EHDA-EHDAM)*(V(I)-V(I-1))/DZ**2-A2*V(I)+
      .      (THNEW(I)-THOLD(I))*V(I)/DT-A3*(V(I)-V(I-1))/DZ-
      .      RSUB)
      GO TO 2
C-----
C...SOLVE FOR X EQUATION
C-----
4      J=I-L
      IF(I.EQ.LP1) GO TO 6
      IF(I.EQ.N2) GO TO 10
C-----
C...FOR INTERMEDIATE NODES
C-----
      F(I)=-QNEW(J)/THNEW(J)*(V(I+1)-V(I-1))/(2.*DZ)+AMU*V(I)*V(J)/
      .      (AAKM+V(J))-AKK*V(I)
      GO TO 2
C-----
C...FOR BOTTOM B.C.
C-----
10     F(I)=-QNEW(J)/THNEW(J)*(V(I)-V(I-1))/DZ+AMU*V(I)*V(J)/(AAKM+
      .      V(J))-AKK*V(I)
      GO TO 2
C-----
C...FOR TOP B.C.
C-----
6      F(I)=AMU*V(I)*V(J)/(AAKM+V(J))-AKK*V(I)
C-----
2      CONTINUE

```

RETURN

END


```

C-----
C-----
      SUBROUTINE NBIOD(N,V,F)
C-----
C-----

      COMMON/BLK3/THNEW(400),THOLD(400)
      COMMON/BLK11/QOLD(400),QNEW(400),DISCH(400)
      COMMON/BLK16/DZ,DT
      COMMON/BLK19/BIOMI(400),CTOTAL(400),CONCI(400),H,
      .
      .
      TMAX,INDEX
      COMMON/BLK42/IFL13,IMONOD,AKC,AKL
      COMMON/BLK50/AKD,AKPR,DDW,DDA,HENRY,POROS,ALAM,RHO
      COMMON/BLK55/IFL11
      DIMENSION V(400),F(400)
C-----

      DO 25 J=1,N
      IF(THNEW(J).GT.POROS) THNEW(J)=POROS
25  CONTINUE
      A2=HENRY*AKPR*RHO
C-----

      DO 2 I=1,N
      IF(INDEX.EQ.0) THEN
      IF(IMONOD.EQ.0) THEN
      RSUB=THNEW(I)*HENRY*AKC
      ELSE
      RSUB=THNEW(I)*HENRY*AKL*V(I)
      END IF
      ELSE
      RSUB=0.0
      END IF
      A1=1./((HENRY-1)*THNEW(I)+HENRY*AKD*RHO+POROS)
      IF(I.EQ.1) GOTO 5
      A3=HENRY*QNEW(I)
      EHDA=HENRY*(ABS(QNEW(I))*ALAM+
      .
      .
      DDW*THNEW(I)**(13/3.)/POROS**2)+
      .
      DDA*(POROS-THNEW(I))**((13/3.)/POROS**2
      EHDAM=HENRY*(ABS(QNEW(I-1))*ALAM+
      .
      .
      DDW*THNEW(I-1)**(13/3.)/POROS**2)+
      .
      DDA*(POROS-THNEW(I-1))**((13/3.)/POROS**2
      IF(I.EQ.N) GO TO 4
      EHDAP=HENRY*(ABS(QNEW(I+1))*ALAM+

```

```

      DDW*THNEW(I+1)**(13/3.)/POROS**2)+
      DDA*(POROS-THNEW(I+1))**(13/3.)/POROS**2
C-----
C...FOR INTERMEDIATE NODES
C-----
      F(I)=A1*((EHDAP-EHDAM)*(V(I+1)-V(I-1))/(4*DZ**2)+
      EHDA*(V(I+1)-2*V(I)+V(I-1))/DZ**2-A2*V(I)+
      (THNEW(I)-THOLD(I))*V(I)/DT-A3*(V(I+1)-V(I-1))/
      (2*DZ)-RSUB)
      GO TO 2
C-----
C...FOR TOP B.C.
C-----
5      IF(IFL11.EQ.0) THEN
          F(I)=0.0
      ELSE
          F(I)=A1*(-A2+(THNEW(1)-THOLD(1))/DT-RSUB)*(V(1)+V(2))/2.
      END IF
C-----
      GO TO 2
C-----
C...FOR BOTTOM B.C.
C-----
4      F(I)=A1*((EHDAP-EHDAM)*(V(I)-V(I-1))/DZ**2-A2*V(I)+
      (THNEW(I)-THOLD(I))*V(I)/DT-A3*(V(I)-V(I-1))/DZ-
      RSUB)
2      CONTINUE
      RETURN
      END

```



```

C-----
C-----
      SUBROUTINE DATA
C-----
C-----
      CHARACTER ANS*1,UNT*12,UPR*8,IRUN*1
      CHARACTER*80 TITLE,FILNM1,FILNM2,IVAR
      INTEGER DIN,MIN,YIN
C-----

      COMMON/BLK1/N
      COMMON/BLK3/THNEW(400),THOLD(400)
      COMMON/BLK4/IFL1,IFL2,AKS,THS,THF,AM,AN,AI,BE,B,THAD,AN2,AM2,
      .
      .      GAMMA,ALPHA
      COMMON/BLK5/PSIR,DZER,BET,THZER
      COMMON/BLK8/EPS
      COMMON/BLK9/P(2234),ET(2234)
      COMMON/BLK16/DZ,DT
      COMMON/BLK17/TITLE,IRUN,IC1,IFL8,IFL10,IFL12,
      .
      .      EVTR,PR,THOL
      COMMON/BLK18/AMU,AKK,AAKM,YEL
      COMMON/BLK19/BIOMI(400),CTOTAL(400),CONCI(400),H,
      .
      .      TMAX,INDEX
      COMMON/BLK20/UNT
      COMMON/BLK21/IFLE,IFLT,ID1,ID2,RR(12),ALB,TD(12),W(12),
      .
      .      SSH(12),ALI(12),DIN,MIN,YIN,TT(12),THW,DRZ
      COMMON/BLK25/IT,INT
      COMMON/BLK28/M
      COMMON/BLK41/IFL3,IFL4,IFL5,IFL6,IFL7
      COMMON/BLK42/IFL13,IMONOD,AKC,AKL
      COMMON/BLK50/AKD,AKPR,DDW,DDA,HENRY,POROS,ALAM,RHO
      COMMON/BLK51/ICUT,CONCA
      COMMON/BLK52/IFL9
      COMMON/BLK53/IUN
      COMMON/BLK54/CN
      COMMON/BLK55/IFL11
      COMMON/BLK56/AKOC,OC
C-----

1000  WRITE(6,100)
100   FORMAT(/10X,'DATA COMPLETED - ANY CHANGES? [N]: ',)$)
      READ(5,10,ERR=1000)ANS
10    FORMAT(A)

```

```

      IF(ANS.WE.' ' .AND.ANS.WE.'Y' .AND.ANS.WE.'y' .AND.
        . ANS.WE.'W' .AND.ANS.WE.'n') GOTO 1000
      IF(ANS.EQ.' ' .OR.ANS.EQ.'W' .OR.ANS.EQ.'n') RETURN
C-----
1001 WRITE(6,101)
101  FORMAT(/1X,'ENTER VARIABLE NAME TO BE CHANGED (RETURN TO EXIT): ',
        . $)
      READ(5,10,ERR=1001)IVAR
      IF(IVAR.EQ.' ') RETURN
      DO 11 IJ=80,1,-1
11      IF(IVAR(IJ:IJ).WE.' ') GOTO 12
12      IF(IVAR(IJ:IJ).EQ.'') GOTO 30
C-----
1002 WRITE(6,20)IVAR(1:IJ)
20  FORMAT(/1X,'ENTER THE NEW VALUE OF <' ,A,'> : ', $)
C-----
      IF(IVAR(1:IJ).EQ.'TITLE'.OR.IVAR(1:IJ).EQ.'title') THEN
          READ(5,10,ERR=1002) TITLE
          GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'IRUN'.OR.IVAR(1:IJ).EQ.'irun') THEN
          READ(5,10,ERR=1002) IRUN
          GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'IC1'.OR.IVAR(1:IJ).EQ.'ic1') THEN
          READ(5,*,ERR=1002) IC1
          GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'AKS'.OR.IVAR(1:IJ).EQ.'aks') THEN
          READ(5,*,ERR=1002) AKS
          GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'THF'.OR.IVAR(1:IJ).EQ.'thf') THEN
          READ(5,*,ERR=1002) THF
          GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'THS'.OR.IVAR(1:IJ).EQ.'ths') THEN
          READ(5,*,ERR=1002) THS
          GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'THAD'.OR.IVAR(1:IJ).EQ.'thad') THEN

```



```
      READ(5,*,ERR=1002) THAD
      GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'AM'.OR.IVAR(1:IJ).EQ.'am') THEN
      READ(5,*,ERR=1002) AM
      GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'B'.OR.IVAR(1:IJ).EQ.'b') THEN
      READ(5,*,ERR=1002) B
      GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'PSIR'.OR.IVAR(1:IJ).EQ.'psir') THEN
      READ(5,*,ERR=1002) PSIR
      GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'THOL'.OR.IVAR(1:IJ).EQ.'thol') THEN
      READ(5,*,ERR=1002) THOL
      GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'AKPR'.OR.IVAR(1:IJ).EQ.'akpr') THEN
      READ(5,*,ERR=1002) AKPR
      GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'ALAM'.OR.IVAR(1:IJ).EQ.'alam') THEN
      READ(5,*,ERR=1002) ALAM
      GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'RHO'.OR.IVAR(1:IJ).EQ.'rho') THEN
      READ(5,*,ERR=1002) RHO
      GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'OC'.OR.IVAR(1:IJ).EQ.'oc') THEN
      READ(5,*,ERR=1002) OC
      GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'AKC'.OR.IVAR(1:IJ).EQ.'akc') THEN
      READ(5,*,ERR=1002) AKC
      GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'AKL'.OR.IVAR(1:IJ).EQ.'akl') THEN
      READ(5,*,ERR=1002) AKL
```

```
GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'IFL1'.OR.IVAR(1:IJ).EQ.'ifl1') THEN
    READ(5,*,ERR=1002) IFL1
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'IFL2'.OR.IVAR(1:IJ).EQ.'ifl2') THEN
    READ(5,*,ERR=1002) IFL2
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'IFL3'.OR.IVAR(1:IJ).EQ.'ifl3') THEN
    READ(5,*,ERR=1002) IFL3
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'IFL4'.OR.IVAR(1:IJ).EQ.'ifl4') THEN
    READ(5,*,ERR=1002) IFL4
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'IFL5'.OR.IVAR(1:IJ).EQ.'ifl5') THEN
    READ(5,*,ERR=1002) IFL5
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'IFL6'.OR.IVAR(1:IJ).EQ.'ifl6') THEN
    READ(5,*,ERR=1002) IFL6
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'IFL7'.OR.IVAR(1:IJ).EQ.'ifl7') THEN
    READ(5,*,ERR=1002) IFL7
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'IFL8'.OR.IVAR(1:IJ).EQ.'ifl8') THEN
    READ(5,*,ERR=1002) IFL8
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'IFL9'.OR.IVAR(1:IJ).EQ.'ifl9') THEN
    READ(5,*,ERR=1002) IFL9
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'IFL10'.OR.IVAR(1:IJ).EQ.'ifl10') THEN
    READ(5,*,ERR=1002) IFL10
    GOTO 1001
```



```
END IF
IF (IVAR(1:IJ).EQ.'IFL11'.OR.IVAR(1:IJ).EQ.'ifl11') THEN
    READ(5,*,ERR=1002) IFL11
    GOTO 1001
END IF
IF (IVAR(1:IJ).EQ.'IFL12'.OR.IVAR(1:IJ).EQ.'ifl12') THEN
    READ(5,*,ERR=1002) IFL12
    GOTO 1001
END IF
IF (IVAR(1:IJ).EQ.'IFL13'.OR.IVAR(1:IJ).EQ.'ifl13') THEN
    READ(5,*,ERR=1002) IFL13
    GOTO 1001
END IF
IF (IVAR(1:IJ).EQ.'IMONOD'.OR.IVAR(1:IJ).EQ.'imonod') THEN
    READ(5,*,ERR=1002) IMONOD
    GOTO 1001
END IF
IF (IVAR(1:IJ).EQ.'ICUT'.OR.IVAR(1:IJ).EQ.'icut') THEN
    READ(5,*,ERR=1002) ICUT
    GOTO 1001
END IF
IF (IVAR(1:IJ).EQ.'CONCA'.OR.IVAR(1:IJ).EQ.'conca') THEN
    READ(5,*,ERR=1002) CONCA
    GOTO 1001
END IF
IF (IVAR(1:IJ).EQ.'CN'.OR.IVAR(1:IJ).EQ.'cn') THEN
    READ(5,*,ERR=1002) CN
    GOTO 1001
END IF
IF (IVAR(1:IJ).EQ.'IUN'.OR.IVAR(1:IJ).EQ.'iun') THEN
    READ(5,*,ERR=1002) IUN
    GOTO 1001
END IF
IF (IVAR(1:IJ).EQ.'DZ'.OR.IVAR(1:IJ).EQ.'dz') THEN
    READ(5,*,ERR=1002) DZ
    GOTO 1001
END IF
IF (IVAR(1:IJ).EQ.'DT'.OR.IVAR(1:IJ).EQ.'dt') THEN
    READ(5,*,ERR=1002) DT
    GOTO 1001
END IF
```

```
      IF(IVAR(1:IJ).EQ.'INT'.OR.IVAR(1:IJ).EQ.'int') THEN
        READ(5,*,ERR=1002) INT
        GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'EPS'.OR.IVAR(1:IJ).EQ.'eps') THEN
        READ(5,*,ERR=1002) EPS
        GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'N'.OR.IVAR(1:IJ).EQ.'n') THEN
        READ(5,*,ERR=1002) N
        GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'M'.OR.IVAR(1:IJ).EQ.'m') THEN
        READ(5,*,ERR=1002) M
        GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'AW'.OR.IVAR(1:IJ).EQ.'an') THEN
        READ(5,*,ERR=1002) AW
        GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'AI'.OR.IVAR(1:IJ).EQ.'ai') THEN
        READ(5,*,ERR=1002) AI
        GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'BE'.OR.IVAR(1:IJ).EQ.'be') THEN
        READ(5,*,ERR=1002) BE
        GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'GAMMA'.OR.IVAR(1:IJ).EQ.'gamma') THEN
        READ(5,*,ERR=1002) GAMMA
        GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'AW2'.OR.IVAR(1:IJ).EQ.'an2') THEN
        READ(5,*,ERR=1002) AW2
        GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'ALPHA'.OR.IVAR(1:IJ).EQ.'alpha') THEN
        READ(5,*,ERR=1002) ALPHA
        GOTO 1001
      END IF
      IF(IVAR(1:IJ).EQ.'DZER'.OR.IVAR(1:IJ).EQ.'dzer') THEN
```



```
      READ(5,*,ERR=1002) DZER
      GOTO 1001

END IF

IF(IVAR(1:IJ).EQ.'BET'.OR.IVAR(1:IJ).EQ.'bet') THEN
      READ(5,*,ERR=1002) BET
      GOTO 1001

END IF

IF(IVAR(1:IJ).EQ.'THZER'.OR.IVAR(1:IJ).EQ.'thzer') THEN
      READ(5,*,ERR=1002) THZER
      GOTO 1001

END IF

IF(IVAR(1:IJ).EQ.'PR'.OR.IVAR(1:IJ).EQ.'pr') THEN
      READ(5,*,ERR=1002) PR
      GOTO 1001

END IF

IF(IVAR(1:IJ).EQ.'EVTR'.OR.IVAR(1:IJ).EQ.'evtr') THEN
      READ(5,*,ERR=1002) EVTR
      GOTO 1001

END IF

IF(IVAR(1:IJ).EQ.'INDEX'.OR.IVAR(1:IJ).EQ.'index') THEN
      READ(5,*,ERR=1002) INDEX
      GOTO 1001

END IF

IF(IVAR(1:IJ).EQ.'UNT'.OR.IVAR(1:IJ).EQ.'unt') THEN
      READ(5,10,ERR=1002) UNT
      GOTO 1001

END IF

IF(IVAR(1:IJ).EQ.'AKOC'.OR.IVAR(1:IJ).EQ.'akoc') THEN
      READ(5,*,ERR=1002) AKOC
      GOTO 1001

END IF

IF(IVAR(1:IJ).EQ.'DDW'.OR.IVAR(1:IJ).EQ.'ddw') THEN
      READ(5,*,ERR=1002) DDW
      GOTO 1001

END IF

IF(IVAR(1:IJ).EQ.'DDA'.OR.IVAR(1:IJ).EQ.'dda') THEN
      READ(5,*,ERR=1002) DDA
      GOTO 1001

END IF

IF(IVAR(1:IJ).EQ.'HENRY'.OR.IVAR(1:IJ).EQ.'henry') THEN
      READ(5,*,ERR=1002) HENRY
```

```
GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'AMU'.OR.IVAR(1:IJ).EQ.'amu') THEN
    READ(5,*,ERR=1002) AMU
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'AKK'.OR.IVAR(1:IJ).EQ.'akk') THEN
    READ(5,*,ERR=1002) AKK
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'AAKM'.OR.IVAR(1:IJ).EQ.'aakm') THEN
    READ(5,*,ERR=1002) AAKM
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'YEL'.OR.IVAR(1:IJ).EQ.'yel') THEN
    READ(5,*,ERR=1002) YEL
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'IFLE'.OR.IVAR(1:IJ).EQ.'ifle') THEN
    READ(5,*,ERR=1002) IFLE
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'ID1'.OR.IVAR(1:IJ).EQ.'id1') THEN
    READ(5,*,ERR=1002) ID1
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'ID2'.OR.IVAR(1:IJ).EQ.'id2') THEN
    READ(5,*,ERR=1002) ID2
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'ALB'.OR.IVAR(1:IJ).EQ.'alb') THEN
    READ(5,*,ERR=1002) ALB
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'IFLT'.OR.IVAR(1:IJ).EQ.'iflt') THEN
    READ(5,*,ERR=1002) IFLT
    GOTO 1001
END IF
IF(IVAR(1:IJ).EQ.'DIN'.OR.IVAR(1:IJ).EQ.'din') THEN
    READ(5,*,ERR=1002) DIN
    GOTO 1001
```



```

      END IF
      IF (IVAR(1:IJ).EQ.'MIN'.OR.IVAR(1:IJ).EQ.'min') THEN
        READ(5,*,ERR=1002) MIN
        GOTO 1001
      END IF
      IF (IVAR(1:IJ).EQ.'YIN'.OR.IVAR(1:IJ).EQ.'yin') THEN
        READ(5,*,ERR=1002) YIN
        GOTO 1001
      END IF
      IF (IVAR(1:IJ).EQ.'THW'.OR.IVAR(1:IJ).EQ.'thw') THEN
        READ(5,*,ERR=1002) THW
        GOTO 1001
      END IF
      IF (IVAR(1:IJ).EQ.'DRZ'.OR.IVAR(1:IJ).EQ.'drz') THEN
        READ(5,*,ERR=1002) DRZ
        GOTO 1001
      END IF
      GOTO 1001
C-----
30  OPEN(UNIT=24,STATUS='SCRATCH')
    DO 13 JJ=IJ,1,-1
      IF (IVAR(JJ:JJ).EQ.'(') THEN
        WRITE(24,21) IVAR(JJ+1:IJ-1)
21  FORMAT(1X,A)
        REWIND(UNIT=24)
        READ(24,*) MMM
        CLOSE(UNIT=24)
        GOTO 14
      END IF
13  CONTINUE
C-----
14  WRITE(6,22) IVAR(1:JJ-1),MMM
22  FORMAT(/1X,'ENTER THE NEW VALUE OF <',A,'(',I3,')> : ', $)
C-----
      IF (IVAR(1:JJ-1).EQ.'THOLD'.OR.IVAR(1:JJ-1).EQ.'thold') THEN
        READ(5,*,ERR=14) THOLD(MMM)
        GOTO 1001
      END IF
      IF (IVAR(1:JJ-1).EQ.'P'.OR.IVAR(1:JJ-1).EQ.'p') THEN
        READ(5,*,ERR=14) P(MMM)
        GOTO 1001

```

```
      END IF
      IF(IVAR(1:JJ-1).EQ.'ET'.OR.IVAR(1:JJ-1).EQ.'et') THEN
        READ(5,*,ERR=14) ET(MMM)
        GOTO 1001
      END IF
      IF(IVAR(1:JJ-1).EQ.'CTOTAL'.OR.IVAR(1:JJ-1).EQ.'ctotal') THEN
        READ(5,*,ERR=14) CTOTAL(MMM)
        GOTO 1001
      END IF
      IF(IVAR(1:JJ-1).EQ.'BIOMI'.OR.IVAR(1:JJ-1).EQ.'biomi') THEN
        READ(5,*,ERR=14) BIOMI(MMM)
        GOTO 1001
      END IF
      IF(IVAR(1:JJ-1).EQ.'RR'.OR.IVAR(1:JJ-1).EQ.'rr') THEN
        READ(5,*,ERR=14) RR(MMM)
        GOTO 1001
      END IF
      IF(IVAR(1:JJ-1).EQ.'TD'.OR.IVAR(1:JJ-1).EQ.'td') THEN
        READ(5,*,ERR=14) TD(MMM)
        GOTO 1001
      END IF
      IF(IVAR(1:JJ-1).EQ.'W'.OR.IVAR(1:JJ-1).EQ.'w') THEN
        READ(5,*,ERR=14) W(MMM)
        GOTO 1001
      END IF
      IF(IVAR(1:JJ-1).EQ.'SSH'.OR.IVAR(1:JJ-1).EQ.'ssh') THEN
        READ(5,*,ERR=14) SSH(MMM)
        GOTO 1001
      END IF
      IF(IVAR(1:JJ-1).EQ.'ALI'.OR.IVAR(1:JJ-1).EQ.'ali') THEN
        READ(5,*,ERR=14) ALI(MMM)
        GOTO 1001
      END IF
      IF(IVAR(1:JJ-1).EQ.'TT'.OR.IVAR(1:JJ-1).EQ.'tt') THEN
        READ(5,*,ERR=14) TT(MMM)
        GOTO 1001
      END IF
      GOTO 1001
    END
```


Appendix C

Literature Review on Adsorption and Desorption

Within the last quarter of a century, there has developed an increased interest, in both the private and public sector, regarding the chemical compounds that are being introduced into the environment. Of specific interest are those organic chemicals being commonly found in surface and subsurface waters, which due to their physicochemical and toxicological properties might prove to be detrimental. In conjunction with this interest, the need for definitive knowledge of the behavior and fate of known or potential pollutants became paramount, thus promoting a substantial amount of scientific research.

The impact of having an organic chemical introduced into the environment is contingent on a variety of physical, chemical, and biological processes.(2) While attempting to study the fate and distribution of organic pollutants, it became evident that the inherent properties of organic compounds could be used to characterize their environmental interactions. During the last 10 to 15 years, the partition coefficient has become one of the most important parameters to be investigated.(25) Ideally, determination of the partition coefficient requires measurement of the equilibrium ratio for the concentration of a single component (contaminant) dissolved in nonpolar and polar layers. The partition coefficient for an organic/aqueous system can be considered as a measure of the relative affinity of the solute for the two immiscible liquids, as an index of comparative solubility in the two liquids, and therefore as a parameter of the relative degree of partitioning between one phase and the other.(26) Although the polar phase is nearly always water, the nonpolar phase to be used may often be arbitrary(i.e. chloroform, hexane, octanol, etc.). (35)

Established in numerous experiments, the partitioning system found to be most suitable, and therefore chosen as the reference system for characterizing the interactions between chemical substances and biological systems has been n-octanol /water [Kow]. (45,57,112) By definition, Kow expresses the equilibrium concentration ratio of an organic chemical partitioned between an organic liquid (e.g., n-octanol) and water and can be equated to the partitioning of any organic chemical between itself and water.(16) Partitioning of organic solutes between a soil organic phase and water may also be treated in a manner similar to that between an organic solvent phase and water.(19) Additionally, it has generally been assumed that the mechanism leading to the uptake of organic pollutants by organisms (bioconcentration) is analogous to the partitioning between an organic phase and water. (20) In this manner, the partition coefficient has gained popular application for correlations involving water solubility, soil sorption, bioconcentration factors, and other chemical, biochemical, and toxic effects of a given chemical. (54,80)

Many investigators have lamented a lack in the data base for measured partition coefficients (1,10), but as has been aptly stated in a paper by Leo, A. et al.(62), "the task of making a complete listing is nearly impossible". Since Leo's compilation is still currently one of the most referenced pieces of literature regarding partition coefficients, the validity of this statement would seem irrefutable. When also considering that the partition coefficients pertaining to soil sorption may include organic carbon (Koc), organic matter (Kom), or soil/sediment (Kp), the complexity of organizing a logical tabulation of published partitioning values becomes further apparent. Nevertheless, it is the desire of this current undertaking to accrue a list of partitioning coefficients for the following twelve organic chemicals:

- Benzene
- Benzo(a)pyrene
- Bis(2-ethylhexyl)phthalate
- Chlorobenzene
- 1,1 - Dichloroethylene
- Ethylbenzene
- 4 - Methylphenol
- Naphthalene
- Tetrachloroethylene
- 1,1,1 - Trichloroethane
- Trichloroethylene
- Toluene

As a supplement to the attached tables of partitioning values, the following set of descriptions hope to impart better insight into the origins of these cited values. The five common analytical techniques used for developing partition coefficients are as follows:

1. Shake-Flask (Batch) - This direct method of measurement is the most traditional, and has been adopted in the Organization for Economic Cooperation and Development (OECD) Test Guideline 107 as the standard procedure for determining partitioning coefficients.(25,30,45,54) This technique involves mixing a solution containing the chemical of interest with a known solvent (i.e. n-octanol), allowing the mixture to reach equilibrium, and then separating the two liquid phases (water and solvent) for quantitative analysis.

2. Generator Column - In order to avoid the emulsion problems associated with the shake-flask method, this direct method of measurement was adapted from standard liquid chromatography column design. An inert solid support medium (silanized Chromosorb W, diatomaceous silica, or glass beads) is first coated with an unsaturated octanol-water solution of the solute of interest by drawing it through the column. The solute is then eluted with octanol-saturated water and finally the effluent is collected and analyzed chromatographically. (25,86)

3. Chromatography - Unlike the direct generator column method, these types of chromatographic methods are indirect. The method is based on developing a retention time for the solute of interest via reverse-phase high performance liquid chromatography, or similar chromatographic method, then correlating it to the octanol-water partitioning coefficient. The correlation involves a solute retention volume or a chromatographic capacity factor (86), which has been determined by passing a reverse-phase aqueous mobile phase through a column packed with a given stationary phase. (42) The stationary phase has been chemically bonded to an inorganic support prior to the experiment. (9)

4. Modeling - As an alternative to direct measurement, octanol-water partitioning coefficients may also be determined by applying mathematical models. By using other physico-chemical characteristics such as aqueous solubility, charge density, Henry's Law constants etc., for the solutes of interest, the partition coefficient is predicted via mathematical formulas or correlations. Other popular estimation methods use structural aspects of the chemical constituent such as molecular connectivity indices (MCI's), substitution constants, activity coefficients, or fragment constants. (2,62,84,87)

SUMMARY

In interpreting the findings of this compilation for a specific compound, a quick visual assessment of the tabulations may offer a better evaluation than that which could be expressed verbally. The partitioning value thought by investigators to be most representative for a specific chemical is often made self-evident in the literature (references) column of the tables. While not consistent for all of the organic chemicals, for those chemicals where a plethora of data has been accumulated or referenced (i.e. benzene, toluene, etc.) the above statement may be taken as an axiom. For better clarification, all the octanol-water partition coefficients for the organic chemicals surveyed have been organized into a series of frequency histograms. Due to error, precision, or bias of either an analytical, experimental, or mathematical nature, there tends to be an extensive scatter of values in addition to the possibility of having more than one dominant partitioning coefficient for a particular compound.

Since partitioning behavior of a substance is very closely related to adsorption isotherm characteristics, an additional and insightful aspect of any partitioning coefficient evaluation is the methodology incorporated into the experimental design. More precisely, and especially for soil sorption, it is of interest whether the batch or column studies performed were also conducted as desorption investigations. Unfortunately, there is only

limited information and literature pertaining to adsorption/desorption work. Currently in this compilation there were only four publications which refer to, or contain desorption experimentation. While Karickhoff, S.W. et al., 1979. and Uchrin, C.G. and Mangels, G., 1987. both describe the desorption procedure within the materials and methods section, only the second article applied to the actual compounds under investigation. In the case of Rogers, R.D. et al., 1980. and Schwarzenbach, R.P. and Westall, J., 1981. neither of these publications offer too much insight as to methodology on the desorption aspects of the experiment.

Results for soil sorption coefficients, specifically organic carbon (Koc), have been statistically tabulated as follows:

<u>Compound</u>	<u>Log Koc</u>
Benzene	1.95
Benzo(a)pyrene	6.26
Bis(2-ethylhexyl)-phthalate	7.44*
Chlorobenzene	2.43
1,1-Dichloroethylene	1.66*
Ethylbenzene	2.58
4-Methylphenol	1.76*
Napthalene	3.08
Tetrachloroethylene	2.39
Toluene	2.28
1,1,1-Trichloroethane	2.03
Trichloroethylene	2.01

* From Kow and Karickhoff, et al. (1979)

$K_d = K_{oc} * f_{oc}$ is the organic carbon mass fraction of the soil (%)

K_d in the units [ml-liq/g-soil]

At present, use irreversible desorption coefficient equal to zero (totally reversible-hyperconservation)

Consistent for all the chemicals investigated, regarding the various data sources cited was the continual referencing of several primary publications or authors. Due to their prominence, the following references encountered in this present compilation are felt to merit specific notation :

Chiou, ., 1981. Partition coefficient and water solubility in environmental chemistry. In Hazard assessment of chemicals (edited by Saxena J. and Fisher, F.), Academic Press, New York.

Hansch, C., and Leo, A.J., 1979. Substituent constants for correlation analysis in chemistry and biology. John Wiley & Sons, New York.

Kenega, E.E., and Goring, C.A.I., 1980. Relationship between water solubility, soil sorption octanol-water partitioning, and bioconcentration of chemicals in biota. In J.C. Eaton (ed.) Aquatic toxicology ASTM STP 707. American Society for Testing and Materials, Philadelphia, PA.

Leo, A., Hansch, C. and Elkins, D., 1971. Partition coefficients and their uses. Chemical Reviews, 71(6), pp. 525.

OECD Guideline for testing of chemicals 107, partition coefficient (n-octanol/water) - flask shaking method, OECD, Paris, 1981.

Pomona College Medicinal Chemistry Project, 1982. Log P and parameter database : A tool for the quantitative prediction of bioactivity. Hansch, C. and Leo, A., Comtex Scientific Corporation, New York.

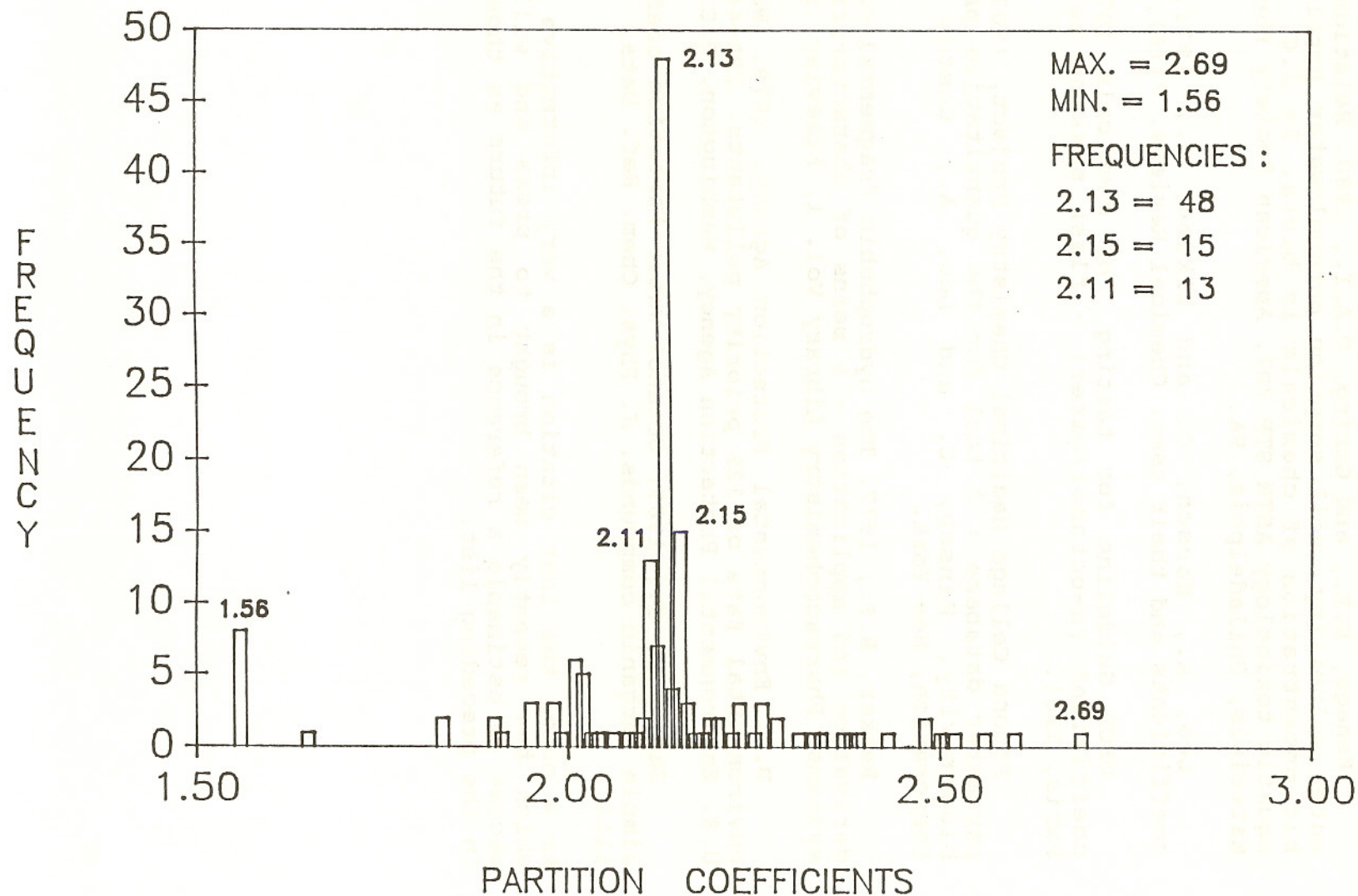
Rekker, R.F., 1977. The hydrophobic fragmental constant, its derivation and application - A means of characterizing membrane systems, Pharmacochemistry Library Vol. 1, Elsevier, Amsterdam.

U.S. Environmental Protection Agency. 1979. Water-related environmental fate of 129 priority pollutants. EPA-440/4-79-029. U.S. Environmental Protection Agency, Washington, D.C.

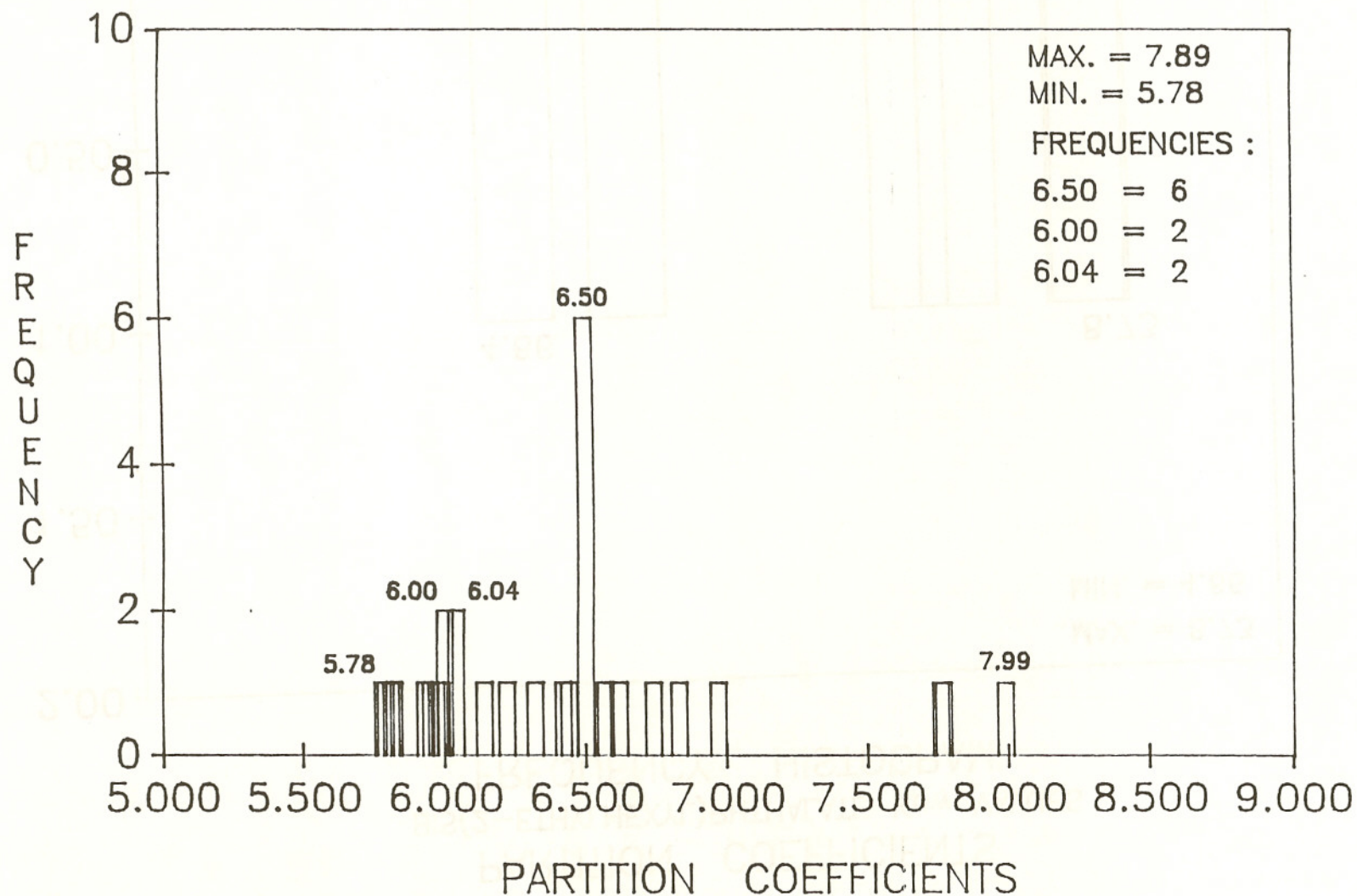
Sangster, J., 1989. Octanol-water Partition coefficients of simple organic compounds. J. Phys. Chem. Ref. Data, 18(3), pp. 1111.

As a note, the last citation is a very informative compilation which has recently been brought to press and will assuredly become as estimable a reference in the future as those contained in the preceding list.

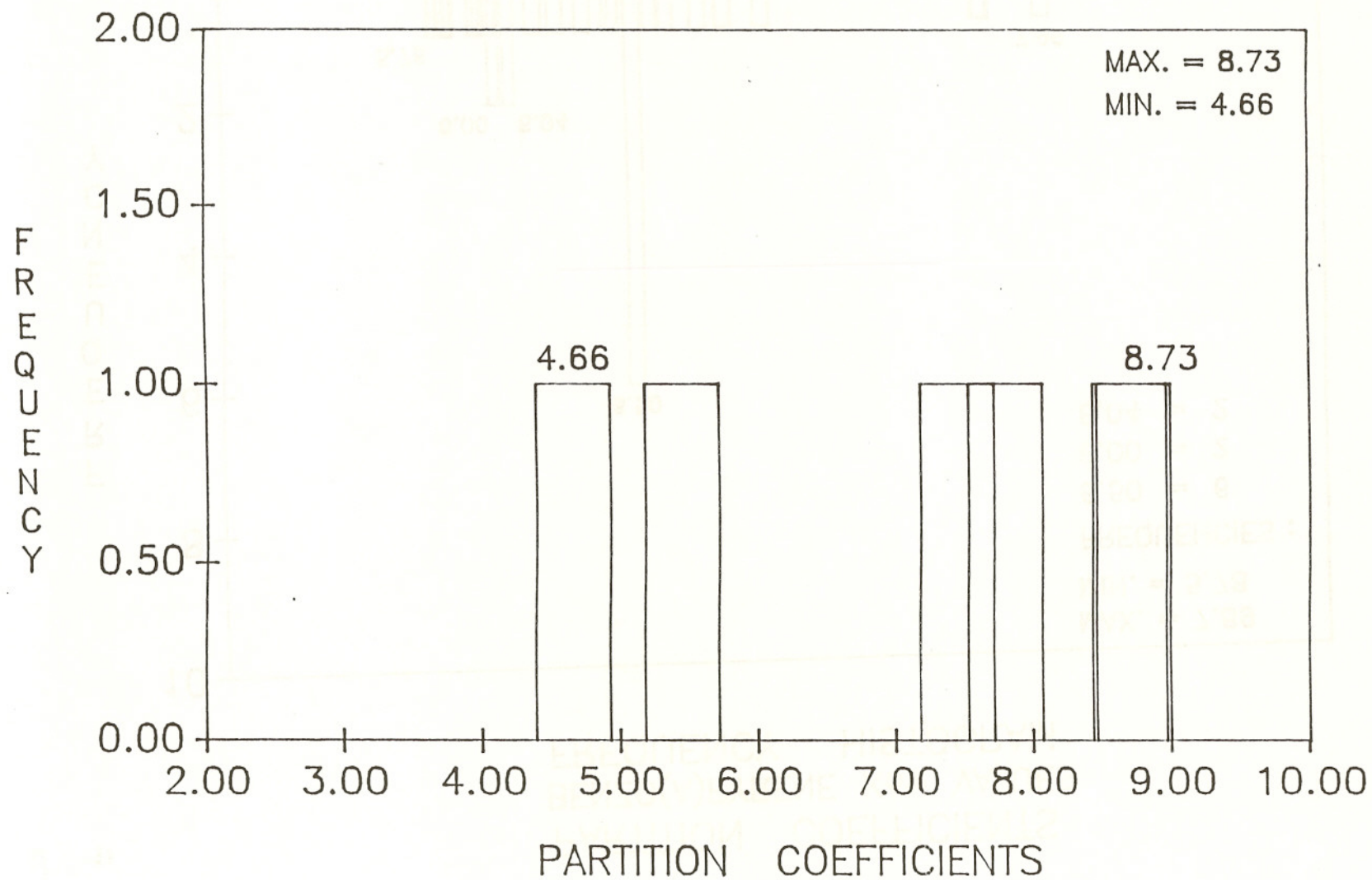
PARTITION COEFFICIENTS BENZENE K_{OW} VALUES FREQUENCY HISTORGRAM



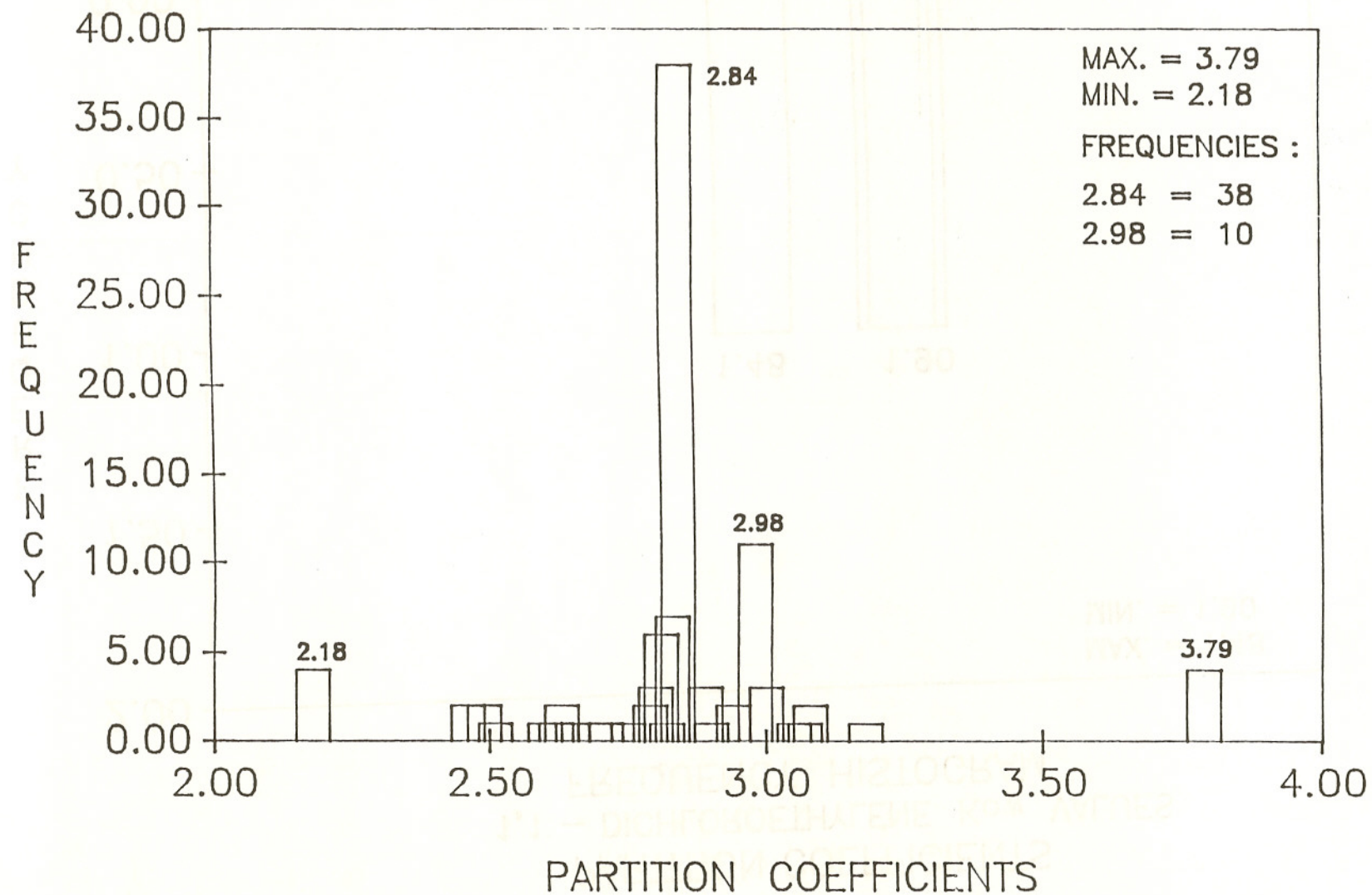
PARTITION COEFFICIENTS BENZO(A)PYRENE K_{ow} VALUES FREQUENCY HISTOGRAM



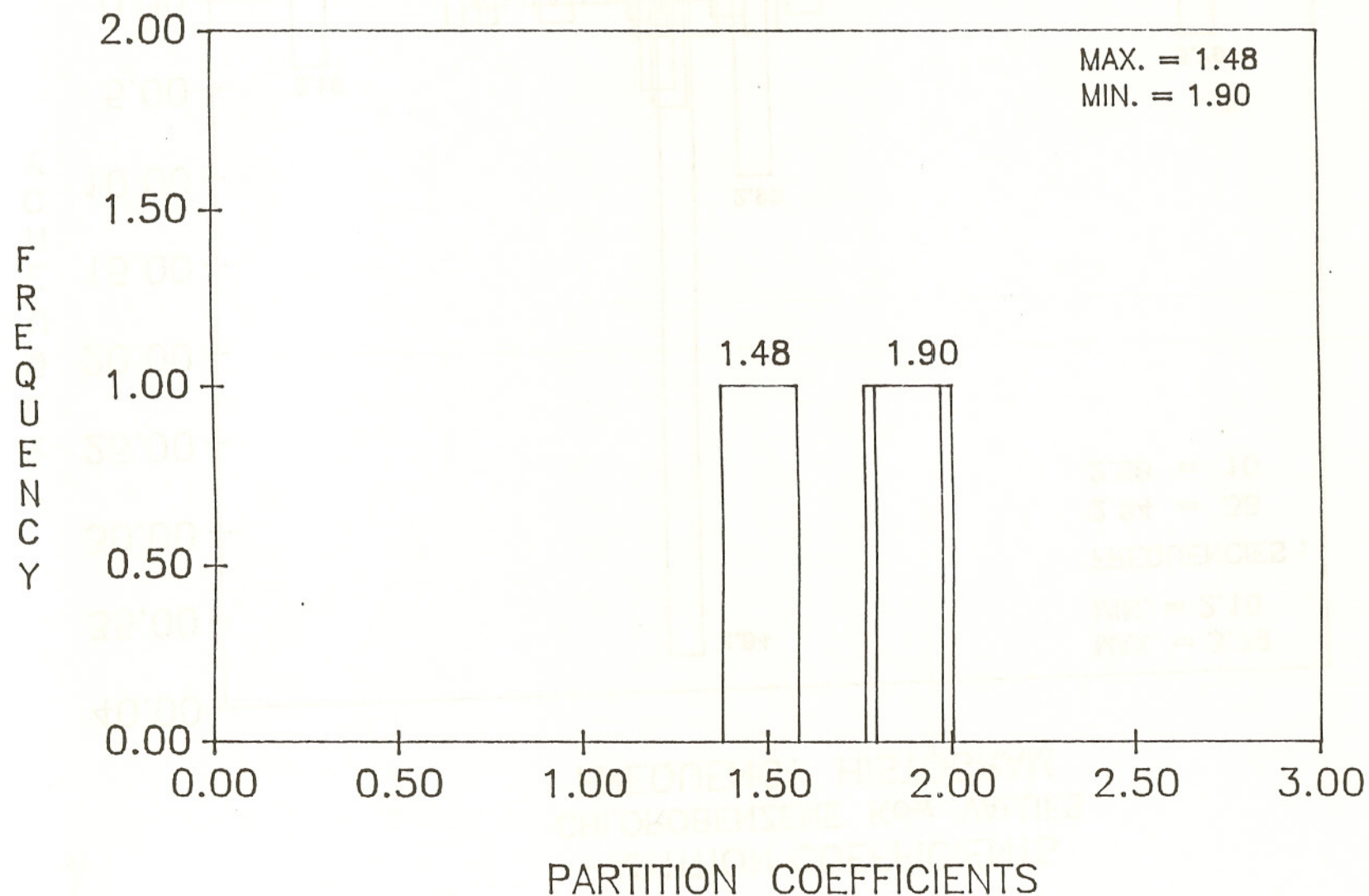
PARTITION COEFFICIENTS
BIS(2-ETHYLHEXYL)PHTHALATE K_{ow} VALUES
FREQUENCY HISTOGRAM



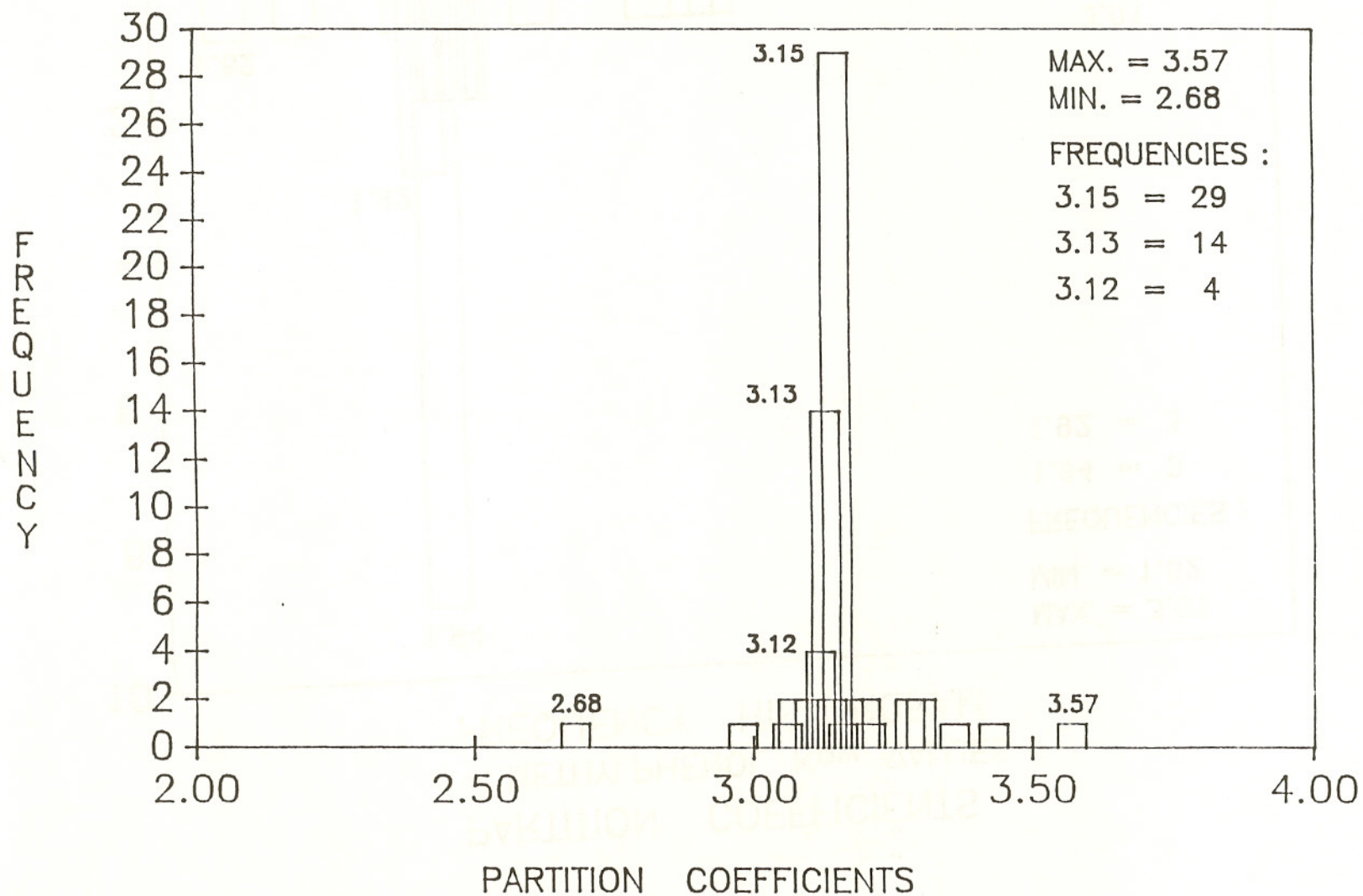
PARTITION COEFFICIENTS CHLOROBENZENE K_{ow} VALUES FREQUENCY HISTOGRAM



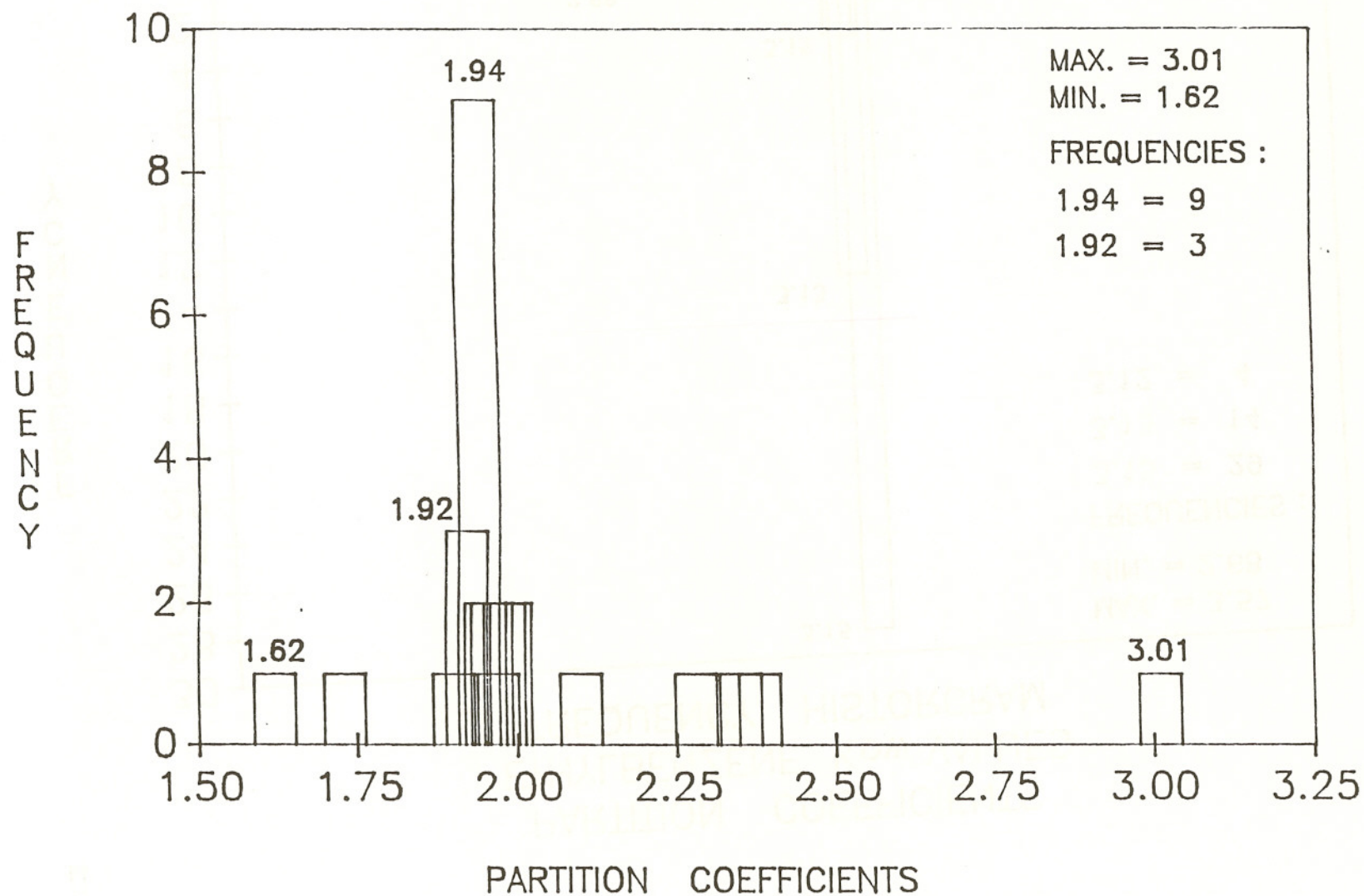
PARTITION COEFFICIENTS
1,1 - DICHLOROETHYLENE K_{ow} VALUES
FREQUENCY HISTOGRAM



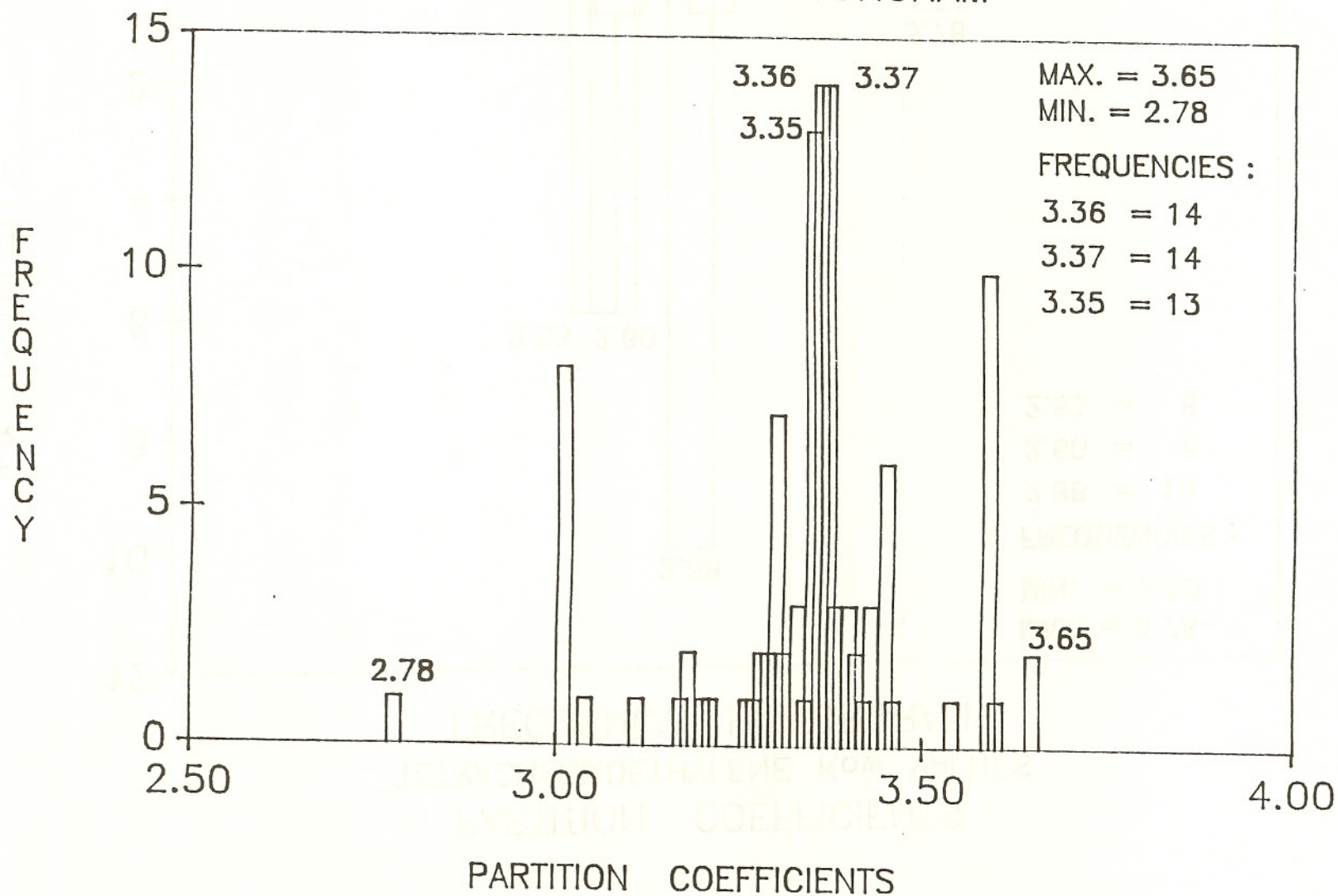
PARTITION COEFFICIENTS ETHYLBENZENE K_{ow} VALUES FREQUENCY HISTORGRAM



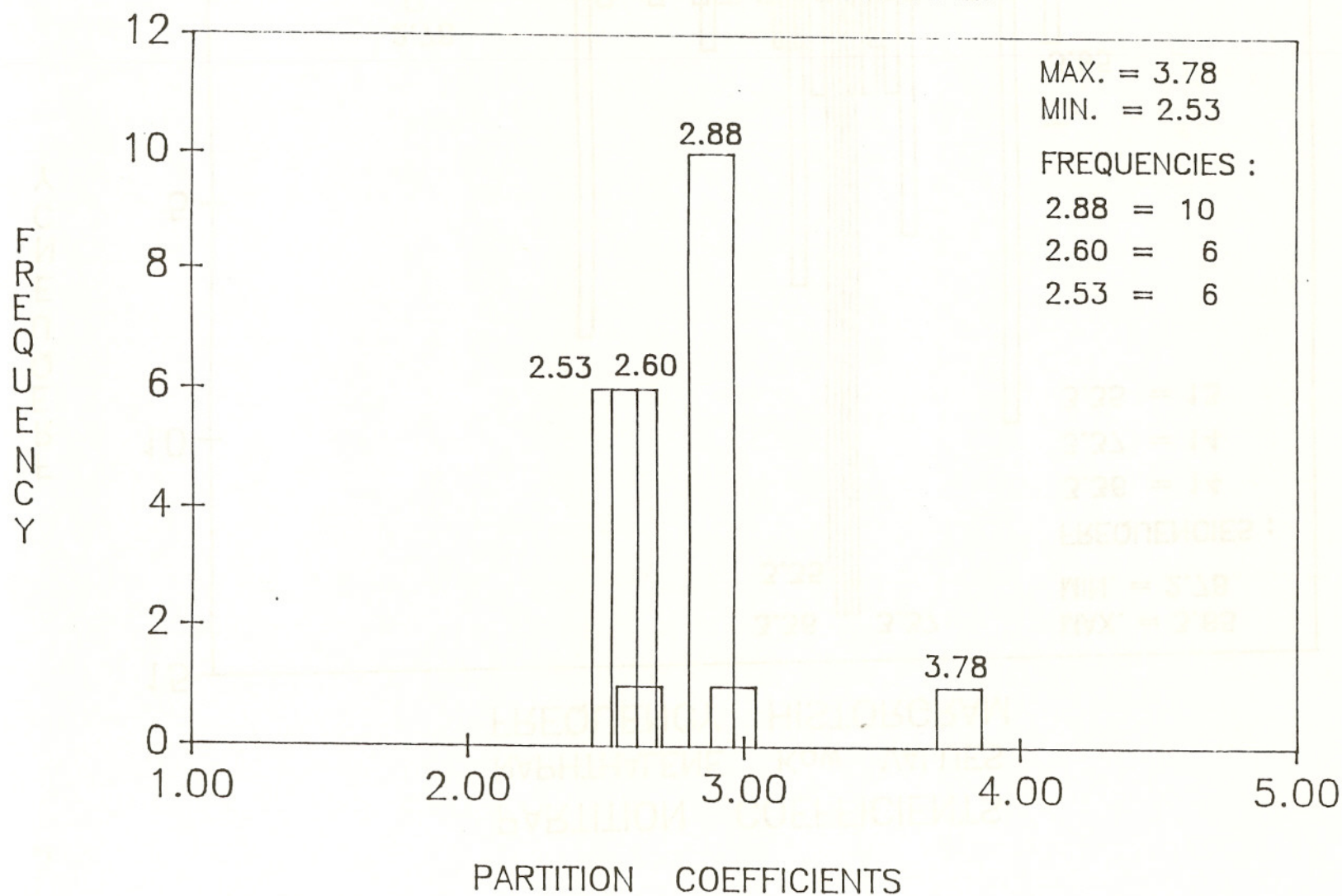
PARTITION COEFFICIENTS 4 - METHYLPHENOL K_{ow} VALUES FREQUENCY HISTORGRAM



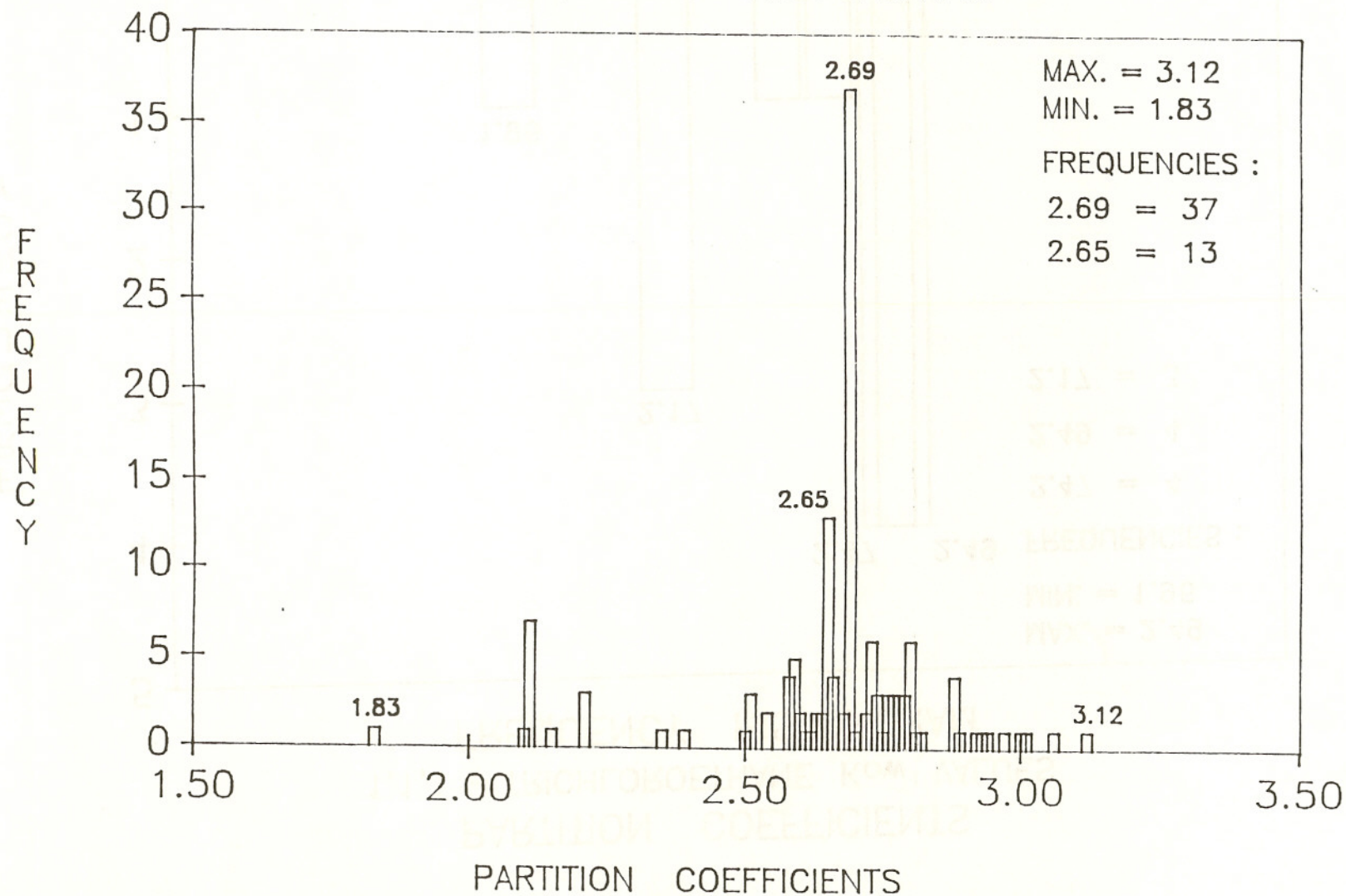
PARTITION COEFFICIENTS NAPHTHALENE K_{ow} VALUES FREQUENCY HISTORGRAM



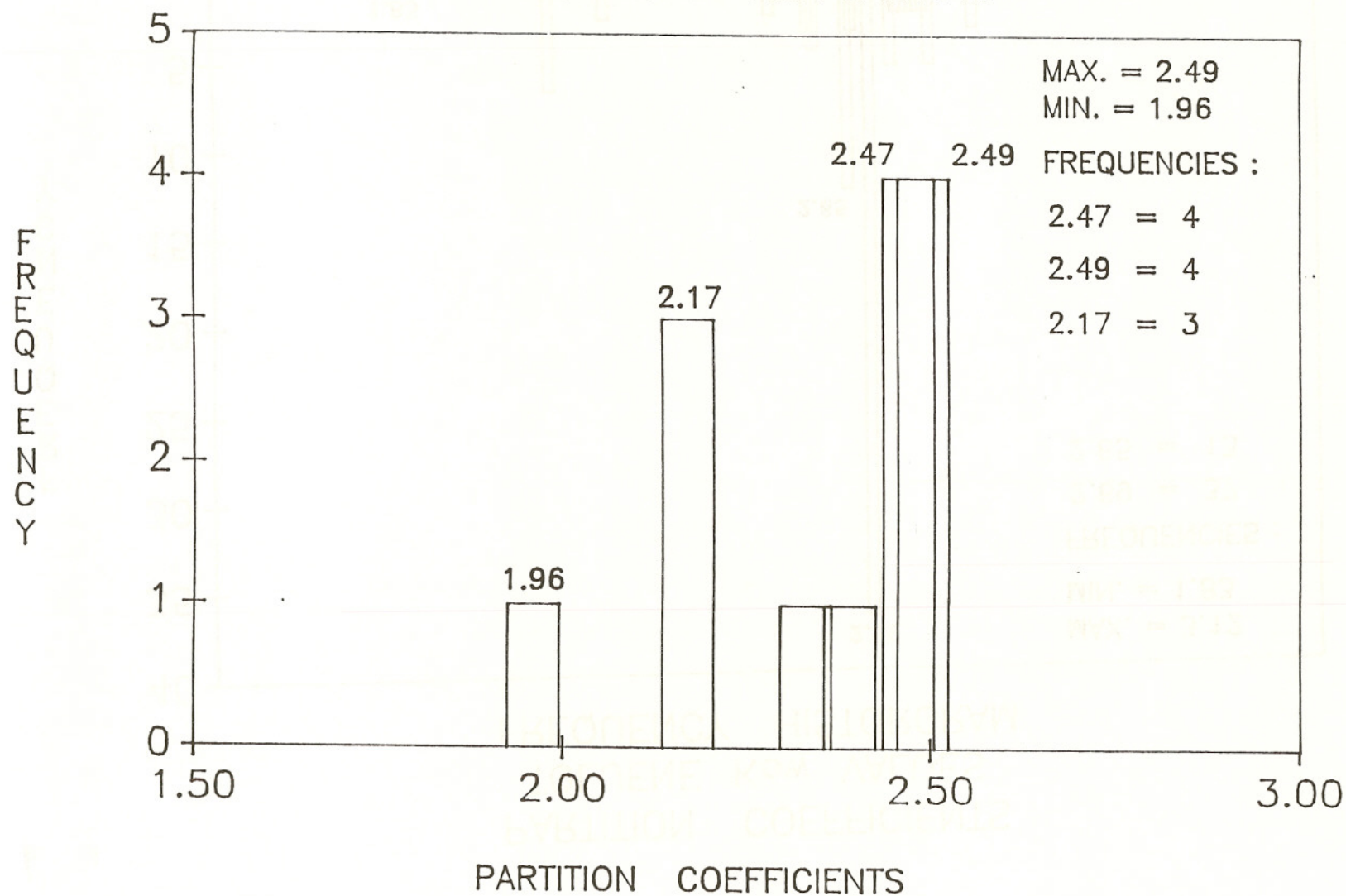
PARTITION COEFFICIENTS TETRACHLOROETHYLENE K_{ow} VALUES FREQUENCY HISTORGRAM



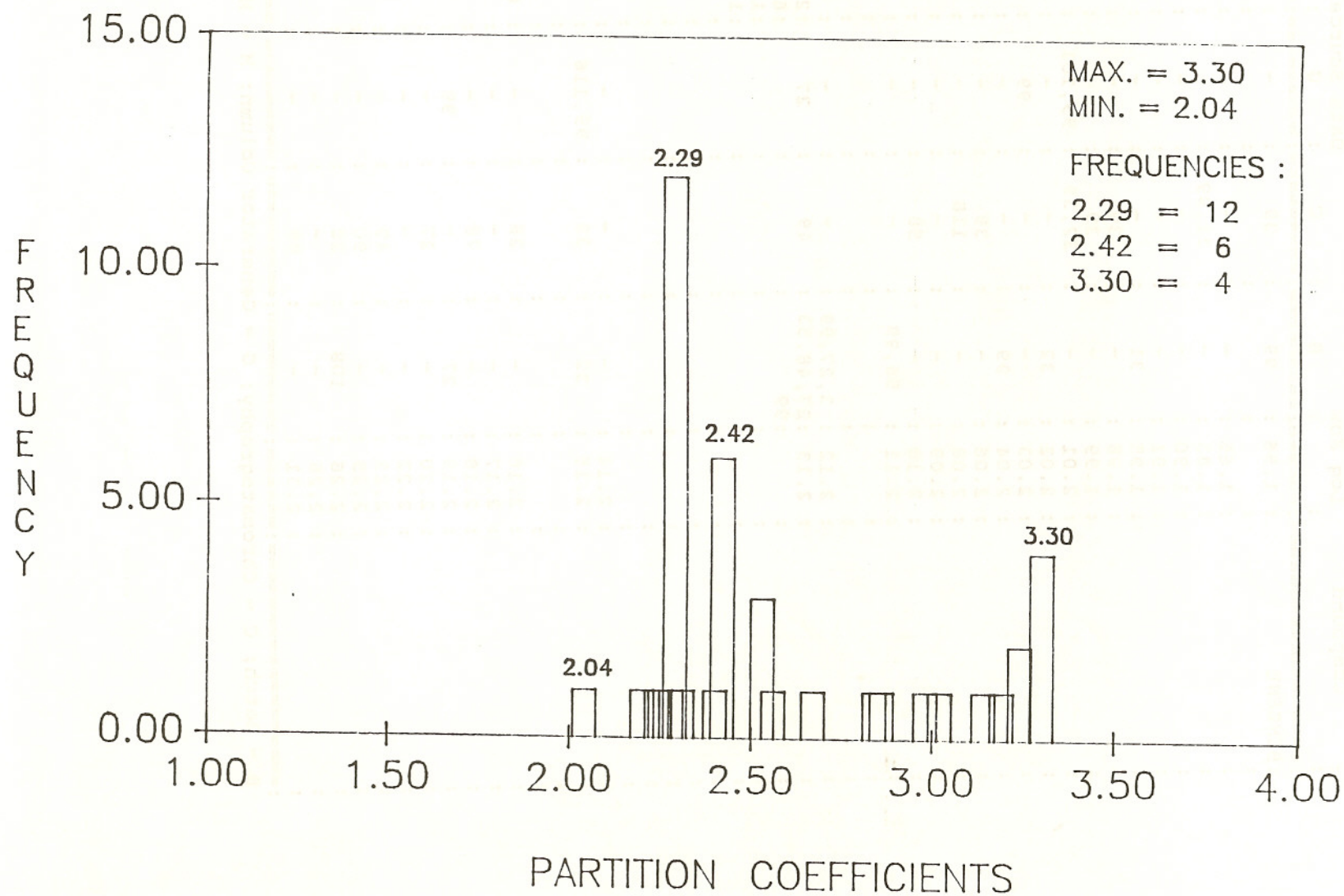
PARTITION COEFFICIENTS TOLUENE K_{ow} VALUES FREQUENCY HISTORGRAM



PARTITION COEFFICIENTS 1,1,1 - TRICHLOROETHANE K_{ow} VALUES FREQUENCY HISTORGRAM



PARTITION COEFFICIENTS TRICHLOROETHYLENE K_{ow} VALUES FREQUENCY HISTOGRAM



PARTITION COEFFICIENTS FOR SEVERAL ORGANIC CHEMICALS

Table 1
Octanol-Water (Log Kow)

Compound	Log Kow	Data Sources				
		B	C	G	M	L
BENZENE	1.56	99	39	-	-	5,63,67,92
						98,111
	1.65	-	-	-	92	-
	1.83	-	31,99	-	-	-
	1.90	-	-	-	70,99	-
	1.91	-	-	-	4	-
	1.95	31	-	-	-	86,127
	1.98	-	39	-	99,101	-
	1.99	-	39	-	-	-
	2.01	-	32,39	99,101	-	46,122
	2.02	32	-	-	63,95	64,113
	2.03	-	-	99	-	-
	2.04	99	-	-	-	-
	2.06	-	39	-	-	-
	2.08	-	118	-	-	-
	2.09	-	-	-	30	-
	2.10	-	58	-	-	88
	2.11	56,99	-	-	95	24,28,41,42
						44,51,57,69
						90,103
	2.12	3,27,99	-	-	107	1,16,52
	2.13	27,48,53	49	27	28,30,49	4,11,17,19
		99			61,62,75	20,21,22,28
					107,132	31,34,35,41
					133	58,66,67
						71,78,79,80
						82,84,87,96
						100,107,111
						120,121,123
						125,129,130
	2.14	-	-	-	30	15,55,61
	2.15	32	39	99,116	1,107	13,28,63,67
						98,109,117
						118,127
	2.16	-	26	-	63,107	-
	2.17	-	-	-	82	-
	2.18	-	78	-	-	-
	2.19	27	-	99	-	-
	2.20	-	27	-	-	107
	2.22	-	-	-	111	-
	2.23	-	49	-	13	107
	2.25	-	90	-	-	-
	2.26	108	28	-	13	-
	2.28	-	-	-	30,47	-
	2.31	-	99	-	-	-

B = Batch; C = Chromatography; G = Generator Column; M = Model; L = Literature

PARTITION COEFFICIENTS FOR SEVERAL ORGANIC CHEMICALS

Table 2
Octanol-Water (Log Kow)

Compound	Log Kow	Data Sources				
		B	C	G	M	L
BENZENE (Cont.)	2.33	-	-	-	22	-
	2.34	-	-	-	61	-
	2.37	-	-	-	66	-
	2.38	-	32	-	-	-
	2.39	-	123	-	-	-
	2.43	-	-	-	69	-
	2.48	-	31,109	-	-	-
	2.50	-	-	-	30	-
	2.52	-	-	-	30	-
	2.56	-	-	-	30	-
	2.60	-	-	-	69	-
	2.69	-	32	-	-	-
BENZO(A) PYRENE	5.78	-	-	-	73	-
	5.79	-	-	-	4	-
	5.81	-	-	-	-	73
	5.82	-	-	-	73	-
	5.93	-	-	-	73	-
	5.95	-	-	-	-	31
	5.97	-	-	-	-	4
	5.98	-	73	-	-	-
	5.99	-	-	-	73	-
	6.00	-	73	-	-	29
	6.04	-	-	-	-	91,96
	6.14	-	-	-	-	73
	6.22	-	-	-	73	-
	6.32	-	-	-	73	-
	6.42	-	90	-	-	-
	6.44	-	-	-	95	-
	6.50	9	-	-	-	65,73,90, 126,130
	6.56	-	-	-	73	-
	6.57	-	-	-	-	73
	6.62	-	-	-	73	-
	6.74	-	-	100	-	-
	6.83	-	-	100	-	-
	6.97	-	-	-	47	-
	7.76	-	-	100	-	-
	7.77	-	-	100	-	-
	7.99	-	-	100	-	-
BIS(2-ETHYLHEXYL)-	4.66	-	-	-	-	27
PHTHALATE	5.45	-	-	-	-	27
	7.45	27	-	-	-	-

B = Batch; C = Chromatography; G = Generator Column; M = Model; L = Literature

PARTITION COEFFICIENTS FOR SEVERAL ORGANIC CHEMICALS

Table 3
Octanol-Water (Log Kow)

Compound	Log Kow	Data Sources				
		B	C	G	M	L
BIS(2-ETHYLHEXYL)-	7.80	-	-	-	-	27
PHTHALATE (Cont.)	8.70	-	-	-	-	86
	8.73	-	-	-	-	96
CHLOROBENZENE	2.18	-	38,39	-	-	52,98
	2.46	27,99	-	-	-	-
	2.49	-	-	-	12	46
	2.51	-	-	-	4	-
	2.60	99	-	-	-	-
	2.62	-	-	-	-	10
	2.63	-	-	-	70,99	-
	2.65	-	-	-	-	13
	2.69	-	-	-	111	-
	2.71	-	-	-	-	103
	2.75	-	99	-	-	-
	2.79	-	39	-	66	-
	2.80	124	58	-	-	59
	2.81	-	26,39	99	47,61,62	-
	2.82	-	-	-	30	-
	2.83	-	27,99	-	132,133	74,119,127
	2.84	48,53,99	22,38,39,77,116	-	28,30,61	4,15,17,19,20,21,28,34,55,58,66,67,68,69,70,77,78,79,80,86,96,10,106,111,112,117,122,129
	2.89	-	-	-	13,27,69	-
	2.90	27	-	-	-	-
	2.94	-	78	-	30	-
	2.98	-	-	27,30,74,99,112,128	75	28,43,52,120
	3.00	-	28,99	-	30	-
	3.05	-	-	-	69	-
	3.07	-	-	-	30	-
	3.08	-	-	-	13,99	-
	3.18	-	-	-	30	-
	3.79	-	-	-	-	24,52,72,98
1,1 - DICHLORO-ETHYLENE	1.48	-	-	-	-	96
	1.87	-	-	-	-	42
	1.90	-	-	-	-	5

B = Batch; C = Chromatography; G = Generator Column; M = Model; L = Literature

PARTITION COEFFICIENTS FOR SEVERAL ORGANIC CHEMICALS

Table 4
Octanol-Water (Log Kow)

Compound	Log Kow	Data Sources				
		B	C	G	M	L
ETHYLBENZENE	2.68	-	-	-	4	-
	2.98	-	-	-	82	-
	3.06	-	-	-	63	-
	3.07	-	31,99	-	-	-
	3.10	-	-	-	70,99	-
	3.12	-	26,99	-	47,63	-
	3.13	-	-	99,101,112,128	49,75,107,133	22,64,100,113,120,125
	3.14	-	-	-	99,101	-
	3.15	31,48,53,99	-	-	-	4,11,13,19,20,21,35,49,51,58,66,67,70,78,79,82,84,86,96,105,106,112,117,122,130
	3.16	-	78	-	-	-
	3.17	-	49	-	-	107
	3.20	-	58	-	107	-
	3.21	-	-	-	107	-
	3.28	-	-	-	13,99	-
	3.30	-	49	-	-	107
	3.36	-	-	-	-	31
	3.43	-	-	-	66	-
	3.57	-	31	-	-	-
4 - METHYLPHENOL	1.62	-	-	-	46	-
	1.73	-	-	-	13	-
	1.90	-	58	-	-	-
	1.92	-	38,39	-	-	67
	1.94	-	-	-	14	13,43,46,58,67,79,80,123
	1.95	-	-	-	-	50,117
	1.96	-	112	-	-	78
	1.97	-	78	-	-	-
	1.98	-	38,39	-	-	-
	1.99	-	38,39	-	-	-
	2.10	-	-	-	-	67
	2.28	-	-	-	-	67
	2.35	-	-	-	-	67
	2.38	-	-	-	13	-
	3.01	-	-	-	-	78

B = Batch; C = Chromatography; G = Generator Column; M = Model; L = Literature

PARTITION COEFFICIENTS FOR SEVERAL ORGANIC CHEMICALS

Table 5
Octanol-Water (Log Kow)

Compound	Log Kow	Data Sources				
		B	C	G	M	L
NAPHTHALENE	2.78	-	-	-	92	-
	3.01	32,99	31,38,39	-	-	67,92
	3.04	-	-	-	4	-
	3.11	56	-	-	-	-
	3.17	-	123	-	-	-
	3.18	-	26	-	63	-
	3.20	-	32	-	-	-
	3.21	-	-	-	47	-
	3.26	-	90	-	-	-
	3.27	-	-	-	-	86
	3.28	31,99	-	-	-	-
	3.29	-	-	-	28	31
	3.30	99	-	-	70,94	4,13,41,76
	3.31	32	-	-	-	113
	3.33	-	-	-	76	64,114
	3.34	-	39	-	13	-
	3.35	9,99	32	128	75,131, 132,133	28,74,120, 121,125
	3.36	8,99	28	-	-	15,19,44,51 57,66,69,90 95,103,126
	3.37	99	-	-	-	16,34,40,41 46,55,67,70 71,82,94,96 123
	3.38	-	22	-	63	16
	3.40	99,124	-	-	69	-
	3.41	-	-	-	-	50,123
	3.42	-	-	-	82	-
	3.43	-	31,32,38	-	-	-
	3.45	32,99,108	38	-	-	28,67
	3.46	-	78	-	-	-
	3.54	-	-	-	69	-
	3.59	86	35,36	-	-	24,28,58,72 78,79,80
	3.60	-	59	-	-	-
	3.65	-	-	-	13,99	-
TETRACHLOROETHYLENE	2.53	3	-	-	-	1,25,57,69 98
	2.60	103	-	-	111	17,34,70,134
	2.61	-	-	-	-	120
	2.88	-	-	-	65	24,52,66,72 77,84,96,98 111
	2.96	-	-	-	66	-
	3.78	-	-	-	-	69

B = Batch; C = Chromatography; G = Generator Column; M = Model; L = Literature

PARTITION COEFFICIENTS FOR SEVERAL ORGANIC CHEMICALS

Table 6
Octanol-Water (Log Kow)

Compound	Log Kow	Data Sources				
		B	C	G	M	L
TOLUENE	1.83	-	-	-	92	-
	2.10	-	-	-	-	40
	2.11	99	38,39	-	-	63,67,92,98
	2.15	-	-	-	-	127
	2.21	3,99	-	-	-	1
	2.35	-	118	-	-	-
	2.39	-	-	-	4	-
	2.50	-	-	-	-	127
	2.51	-	31	-	70,99	-
	2.54	-	-	-	63,82	-
	2.58	29	-	-	-	10,83,122
	2.59	-	26	-	47,61,62,63	-
	2.60	-	-	-	30,49	-
	2.61	99	-	-	-	-
	2.62	-	78	-	-	-
	2.63	-	-	-	-	11,100
	2.64	-	-	-	45,101	-
	2.65	32	49,101	30,99,112,128	75,107	27,28,107,113
	2.66	-	39	-	99,107,121	-
	2.68	99	83	-	-	-
	2.69	48,99	22,38,39	-	107,111	15,17,19,21,27,34,35,41,51,58,61,66,67,69,70,77,78,79,80,84,86,90,96,102,103,112,118,121,127,130
	2.70	-	58	-	-	-
	2.72	-	38,39	-	-	-
	2.73	99	-	-	107	4,28,67,82
	2.74	-	-	-	-	16,46,50
	2.75	-	-	-	30	-
	2.76	108	-	-	1,99	-
	2.77	-	49,99	-	-	107
	2.78	-	10	-	-	27,107
	2.79	27	-	-	10,28	-
	2.80	99	38,39	-	-	31,63,67
	2.81	-	-	-	30	-
	2.82	-	-	-	107	-
	2.88	-	32	-	45,99	28
	2.89	-	90	-	-	-
	2.92	-	-	-	66	-
	2.93	-	-	-	30	-

B = Batch; C = Chromatography; G = Generator Column; M = Model; L = Literature

PARTITION COEFFICIENTS FOR SEVERAL ORGANIC CHEMICALS

Table 7
Octanol-Water (Log Kow)

Compound	Log Kow	Data Sources				
		B	C	G	M	L
TOLUENE (Cont.)	2.94	-	99	-	61	-
	2.97	-	-	-	69	-
	3.00	-	28	-	-	-
	3.01	-	-	-	30	-
	3.06	-	31	-	-	-
	3.12	-	-	-	69	-
1,1,1 -TRICHLORO-ETHANE	1.96	-	-	-	4	-
	2.17	-	-	-	-	84,86,96
	2.33	-	-	-	111	-
	2.39	-	-	-	66	-
	2.47	3	-	-	-	25,52,57
	2.49	-	-	-	62	4,66,111
TRICHLOROETHYLENE	2.04	-	-	-	111	-
	2.20	-	-	-	66	31
	2.24	-	-	-	-	49
	2.25	-	-	-	-	49
	2.28	-	-	-	49	-
	2.29	-	-	-	-	43,46,51,56
						84,86,9
						102,111,122
						134
	2.31	-	-	-	-	5
	2.40	-	58	-	-	-
	2.42	3,31	-	-	-	1,58,69,51
	2.53	-	-	112	75	52
	2.56	-	49	-	-	-
	2.67	-	49	-	-	-
	2.84	-	31	-	-	-
	2.86	-	-	-	69	-
	2.98	-	-	-	-	5
	3.02	-	-	-	69	-
	3.14	49	-	-	-	-
	3.19	-	-	-	-	49
	3.24	-	-	-	-	41,42
	3.30	-	-	-	-	25,41,42,98

B = Batch; C = Chromatography; G = Generator Column; M = Model; L = Literature

PARTITION COEFFICIENTS FOR SEVERAL ORGANIC CHEMICALS

Table 8
Organic-Carbon (Log K_{oc})

Compound	Log K _{oc}	Data Sources				
		B	C	G	M	L
BENZENE	1.58	-	-	104	-	-
	1.63	-	-	104	-	-
	1.72	-	-	-	57	-
	1.73	-	-	104	-	-
	1.78	57	-	-	-	-
	1.82	-	-	-	57	-
	1.90	-	-	-	103	-
	1.91	-	-	-	-	51
	1.92	-	-	-	-	44, 54, 63, 103
	1.93	-	-	-	63	93
	1.95	-	-	-	63	-
	1.96	93	-	-	-	-
	1.98	-	-	-	-	103
	2.00	93	-	-	-	-
	2.01	-	-	-	103	-
	2.09	115	-	-	-	-
	2.16	115	-	-	-	-
	2.31	115	-	-	-	-
	2.53	115	-	-	-	-
	2.73	115	-	-	-	-
	3.01	115	-	-	-	-
BENZO(A) PYRENE	6.26	-	-	-	63	-
CHLOROBENZENE	2.18	-	-	-	-	54
	2.37	105	-	-	-	106
	2.39	105	-	-	-	106
	2.41	-	-	-	-	2
	2.44	-	-	-	2, 103	-
	2.50	-	-	-	-	103
	2.59	-	-	-	-	103
	2.73	-	-	-	12	-
ETHYLBENZENE	2.38	-	51	-	-	-
	2.41	-	-	-	-	51
	2.75	105	-	-	-	106
	2.78	105	-	-	-	106

B = Batch; C = Chromatography; G = Generator Column; M = Model; L = Literature

PARTITION COEFFICIENTS FOR SEVERAL ORGANIC CHEMICALS

Table 9
Organic-Carbon (Log K_{oc})

Compound	Log K _{oc}	Data Sources				
		B	C	G	M	L
NAPHTHALENE	2.91	-	-	-	103	-
	2.94	57	-	-	-	-
	2.96	-	-	-	-	51
	2.97	-	-	-	57	-
	2.98	-	-	-	57	-
	3.00	110	-	-	57	-
	3.04	-	-	-	-	51
	3.11	56	-	-	-	2, 23, 44, 51
						54, 63, 64
	3.15	-	-	-	-	103
	3.18	-	-	-	63	-
	3.27	-	-	-	2	-
	3.25	-	-	-	23	-
	3.52	-	-	-	-	23
	3.89	-	-	-	23	-
TETRACHLOROETHYLENE	2.14	-	-	-	57	-
	2.32	-	-	-	-	103
	2.35	-	-	-	57	-
	2.36	-	-	-	103	-
	2.39	-	-	-	-	103
	2.54	-	-	-	57	-
	2.56	-	-	-	-	57
	2.57	-	-	-	57	-
	2.89	-	-	-	57	-
TOLUENE	1.74	-	-	104	-	-
	1.89	36	-	-	-	-
	1.93	-	-	-	36	-
	1.98	-	-	104	-	-
	2.13	-	-	104	-	-
	2.18	37	-	-	-	-
	2.21	37	-	-	-	-
	2.28	36	-	-	-	-
	2.43	-	-	-	36	-
	2.49	-	-	-	36	-
	2.74	115	-	-	-	-
	2.87	115	-	-	-	-
	2.92	115	-	-	-	-
	3.33	115	-	-	-	-
	3.41	115	-	-	-	-

B = Batch; C = Chromatography; G = Generator Column; M = Model; L = Literature

PARTITION COEFFICIENTS FOR SEVERAL ORGANIC CHEMICALS

Table 10
Organic-Carbon (Log K_{oc})

Compound	Log K _{oc}	Data Sources				
		B	C	G	M	L
1,1,1 -TRICHLORO-ETHANE	1.70	-	-	-	2	-
	1.78	-	-	104	-	-
	1.80	-	-	104	-	-
	2.02	-	-	-	57	-
	2.03	-	-	104	-	-
	2.04	-	-	-	57	-
	2.08	-	-	-	57	-
	2.11	-	51	-	-	-
	2.25	-	-	-	-	57
	2.26	-	-	-	-	2
TRICHLOROETHYLENE	1.66	-	-	-	36	-
	1.76	36	-	-	-	-
	1.84	-	-	-	2	-
	1.86	-	-	104	-	-
	1.98	-	-	104	-	-
	2.00	-	-	-	-	2
	2.02	-	-	-	-	51
	2.03	37	-	-	-	-
	2.09	37	-	-	36	-
	2.14	-	-	-	36	-
	2.15	-	-	104	-	-
	2.20	36	-	-	-	-

B = Batch; C = Chromatography; G = Generator Column; M = Model; L = Literature

PARTITION COEFFICIENTS FOR SEVERAL ORGANIC CHEMICALS

Table 11
Soil-Organic Matter (Log Kom)

Compound	Log Kom	Data Sources				
		B	C	G	M	L
BENZENE	1.04	7	-	-	-	-
	1.26	20	-	-	-	6,97
	1.89	7	-	-	-	-
	1.92	-	-	-	-	97
	2.00	6	-	-	-	-
	2.09	-	-	-	97	-
	2.45	6	-	-	-	-
	2.50	6	-	-	-	-
BENZO(A) PYRENE	2.53	7	-	-	-	-
	2.38	74	-	-	-	-
CHLOROBENZENE	1.19	8	-	-	-	-
	1.33	8	-	-	-	-
	1.68	20	-	-	-	-
	2.10	-	-	-	-	97
	2.32	-	-	-	97	-
ETHYLBENZENE	1.98	20	-	-	-	97
	2.61	-	-	-	97	-
NAPHTHALENE	2.38	-	-	-	8	-
	3.11	-	-	-	-	97
	3.18	-	-	-	97	-
TETRACHLOROETHYLENE	2.32	-	-	-	18	-
TOLUENE	1.12	-	-	-	-	98
	1.74	-	-	-	-	98
	1.90	-	-	-	-	98
	2.32	-	-	-	98	-
	2.85	-	-	-	-	98
1,1,1 -TRICHLORO-ETHANE	1.55	-	-	-	97	-
	2.02	-	-	-	18	97
TRICHLOROETHYLENE	1.28	-	-	-	-	98
	1.70	6	-	-	-	-
	1.72	-	-	-	-	6
	1.97	-	-	-	-	98
	2.19	-	-	-	-	98
	2.30	6	-	-	-	-
	3.16	-	-	-	-	98

B = Batch; C = Chromatography; G = Generator Column; M = Model; L = Literature

PARTITION COEFFICIENTS FOR SEVERAL ORGANIC CHEMICALS

Table 12
Sediment-Water (Log Kp)

Compound	Log Kp	Data Sources				
		B	C	G	M	L
BENZENE	0.02	-	-	-	125	-
	0.23	-	-	-	-	102
	0.29	-	-	104	-	-
	1.80	-	-	-	-	60
	1.92	-	-	-	89	-
BENZO(A) PYRENE	1.26	110	-	-	-	-
	1.84	110	-	-	-	-
CHLOROBENZENE	1.46	59	-	-	-	-
	1.68	59	-	-	-	-
	2.10	-	-	-	-	60
	2.40	-	-	-	89	-
ETHYLBENZENE	1.01	-	-	-	125	-
	1.98	-	-	-	-	60
NAPHTHALENE	1.36	110	-	-	-	-
	1.51	110	-	-	-	-
	1.53	-	-	-	125	-
	2.63	-	-	-	-	60
	3.11	-	-	-	89	-
TETRACHLOROETHYLENE	0.65	-	-	104	-	-
	2.10	-	-	-	-	60
TOLUENE	0.32	-	-	104	-	-
	1.84	-	-	-	-	60
1,1,1 -TRICHLORO-ETHANE	0.60	-	-	104	-	-
	2.30	-	-	-	79	-
TRICHLOROETHYLENE	0.30	-	-	-	-	102
	0.32	-	-	104	-	-
	0.72	-	-	104	-	-

B = Batch; C = Chromatography; G = Generator Column; M = Model; L = Literature

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