

MOVEMENT OF HIGH CONCENTRATIONS OF LOW
VOLATILITY ORGANIC COMPOUNDS THROUGH THE
UNSATURATED SOIL ZONE

YEAR 3

FINAL REPORT

FOR SECOND YEAR FUNDING

(Second Year of 3-yr follow-up project)

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Preface

This project entails the development of a two-dimensional contaminant transport model for layer-heterogeneous and isotropic soils in both saturated and unsaturated conditions, accounting for immiscible phases present in the subsurface environment. The model is to be used by NJDEPE to develop regulatory clean-up levels based on an acceptable impact to groundwater for contaminants present in the unsaturated zone.

This is the final report of this project for the second year of funding. It contains a new analytical approach for the solution of the mass transport in the underlying aquifer (saturated medium), equilibrium sorption studies of dimethyl and diethyl phthalate esters, 1,2 dichlorobenzene and 1,4 dichlorobenzene on Towacco and Cohensey soils, as well as the selection of the chemical compounds to be used in the experimental studies. A brief sensitivity analysis is also included herein.

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I. Introduction

This report outlines the technical details of the modification of the IMPACT model. These modifications of the modeling effort are focused on incorporating the presence of immiscible phase organic compounds in the unsaturated zone, developing a new analytical solution for the mass transport of dilute concentrations in the underlying aquifer, and the solution of the advection-dispersion equation in two-dimensions in the unsaturated zone. The model has been updated for two-dimensional transport equation for dissolved constituents. In addition, the governing equations describing the physicochemical effects of immiscible phases have been formulated. Incorporating these equations into the IMPACT model is still in progress.

The following chapters of this report give all pertinent details of the analytical formulation and implementation of a new approach for the two-dimensional solution of the mass transport equation in saturated soils due to the impact of an unsaturated zone contamination. The existing analytical scheme implemented in the versions 3.0 and 3.1 of the IMPACT model is replaced with the new approach presented herein in version 3.2 of the model. A working copy is also submitted with this report.

II. Modification of the IMPACT Model

The following sequential steps are undertaken to update the model:

1. Develop a stable numerical scheme to solve the two-dimensional advection-dispersion equation for dissolved constituents only.
2. Modify the existing IMPACT model to incorporate the selected numerical scheme for two-dimensional transport processes for dissolved constituents.
3. Develop an analytical solution for the transport and fate of dissolved constituents in the underlying saturated zone to account for mass conservative boundary conditions.
4. Perform the necessary changes in modified two-dimensional model to incorporate the presence of immiscible phases in the unsaturated zone.

Goals stated in steps (1), (2) and (3) have already been accomplished. Step (4) that involves the incorporation of immiscible phases in the unsaturated zone is in progress.

III. The Need for Modification of the Existing Saturated Zone Transport Model (DILUTE)

The analytical solution implemented in the previous versions of the IMPACT model for the transport of dissolved constituents within the saturated zone is based on the solution given by Cleary and Ungs (1978). This solution is obtained by solving the governing advection dispersion equation analytically for a strip source of finite length, $2a$, which is assumed to be located somewhere along the groundwater table as shown in Figure (1) given below.

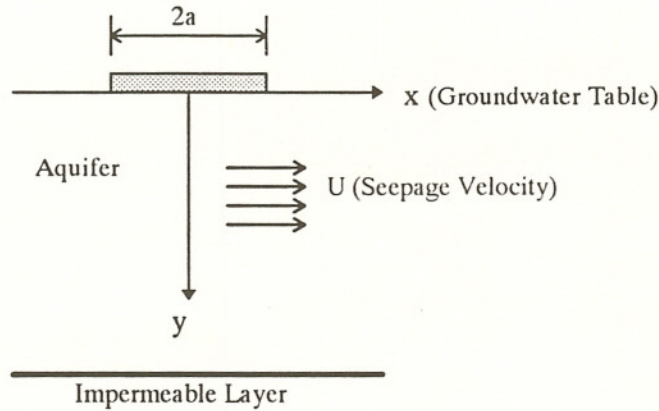


Figure 1. Schematic of a Finite-Length Strip Source

For a two-dimensional, homogeneous and isotropic, saturated medium, the equation governing solute transport can be written for steady-state flow condition as (Freeze and Cheery, 1979):

$$R_d \frac{\partial C_L}{\partial t} + U \frac{\partial C_L}{\partial x} = D_x \frac{\partial^2 C_L}{\partial x^2} + D_y \frac{\partial^2 C_L}{\partial y^2} - \lambda R_d C_L \quad (1)$$

where C_L is the liquid phase concentration, U is the average linear velocity (seepage velocity) in the longitudinal direction, D_x is the hydrodynamic dispersion coefficient in the longitudinal direction, D_y is the hydrodynamic dispersion coefficient in the transverse direction, λ is a first order degradation coefficient, x , y , and t are spatial and time variables, and R_d is the retardation coefficient which is defined as:

$$R_d = 1 + \frac{\rho_b K_d}{n} \quad (2)$$

in which ρ_b is the bulk density of the soil, K_d is the first order equilibrium partitioning coefficient between liquid and sorbed phases (adsorption coefficient), and n is the porosity of the soil.

The medium is assumed to be initially contaminant free. A strip source of length $2a$ is introduced along the x axis. If the contaminant input concentration is steady over time, the boundary and initial conditions for this system are given by Cleary and Ungs, 1978 as:

$$C_L(0, x, t) = C_0 \quad \text{for } |x| \leq a \text{ and } t \geq 0 \quad (3a)$$

$$C_L(0, x, t) = 0 \quad \text{for } |x| > a \text{ and } t \geq 0 \quad (3b)$$

$$\lim_{x \rightarrow \infty} \frac{\partial C_L}{\partial x} = 0 \quad (3c)$$

$$\lim_{y \rightarrow \infty} \frac{\partial C_L}{\partial y} = 0 \quad (3d)$$

When the input concentration is a constant with respect to time (C_0), the solution of Equation (1) takes the form (Korfiatis and Talimcioglu, 1994):

$$C_L(x, y, t) = \frac{C_0 y}{4(\pi D_y)^{1/2}} \int_0^{t/R_d} \exp \left[-\lambda R_d \tau - \frac{y^2}{4D_y \tau} \right] \tau^{-3/2} \cdot \left\{ \operatorname{erf} \left[\frac{a-x}{2(D_x \tau)^{1/2}} + \frac{U}{2} \left(\frac{\tau}{D_x} \right)^{1/2} \right] + \operatorname{erf} \left[\frac{a+x}{2(D_x \tau)^{1/2}} - \frac{U}{2} \left(\frac{\tau}{D_x} \right)^{1/2} \right] \right\} d\tau \quad (4)$$

In the pervious versions (3.0 and 3.1) of the IMPACT model, the solution of the governing mass transport equation given by Equation (4) is numerically manipulated in order to account for a time varying source instead of a step input. The details of this numerical scheme can be found in Korfiatis and Talimcioglu, 1994.

It should be noted that Equation (4) is valid for $y > 0$, i.e. undefined at the groundwater table, and for all values of x . Although accurate within the bounds dictated by Equations (3a) through (3d), the solution given by Equation (4) suffers from a boundary effect due to the condition imposed by Equation (3b). The boundary condition given by Equation (3b) forces the concentrations to be zero along the groundwater table at all times outside the domain of the strip source. This assumes an infinite mass loss through the groundwater table back to the unsaturated zone due to molecular diffusion. If the source within the strip is still active, the rate of mass loss through the groundwater table will be insignificant, given the high rate of advection within the aquifer. However, if the source has already ceased within the strip, the rate of mass loss may be dominant since the contaminant will not be contained within the aquifer at all times.

It is further stipulated that Equation (4) will describe satisfactorily concentrations very close to the free surface of an unconfined aquifer if the soil gases and pore water above the phreatic surface are uncontaminated at the onset of the event, provided that the source at the strip is still active. However, if these conditions are not satisfied, Equation (4) will underestimate the concentration distribution within the aquifer due the aforementioned boundary effect. This boundary effect is further illustrated in the Sensitivity Analysis chapter of this report. Therefore, there exists a need for a rather mass conservative formulation of the saturated zone transport by treating the groundwater table as a pseudo-impermeable boundary to the system.

IV. Modification of the Saturated Zone Transport Model (DILUTE)

IV.1 Mathematical Formulation

The governing mass transport equation for homogeneous and isotropic aquifers is given by Equation (1) which can be written with respect to normalized coefficients as:

$$\frac{\partial C_L}{\partial t} + U_r \frac{\partial C_L}{\partial x} = D_{x,r} \frac{\partial^2 C_L}{\partial x^2} + D_{y,r} \frac{\partial^2 C_L}{\partial y^2} - \lambda C_L \quad (5)$$

where $U_r = U/R_d$, $D_{x,r} = D_x/R_d$ and $D_{y,r} = D_y/R_d$.

The analytical solution of Equation (5) is given for a point source (see Figure 2) at a location along the boundary $x = \xi$, $y = 0$ with an instantaneous release of mass in the liquid phase per unit length along the source, M , as (Hunt, 1983):

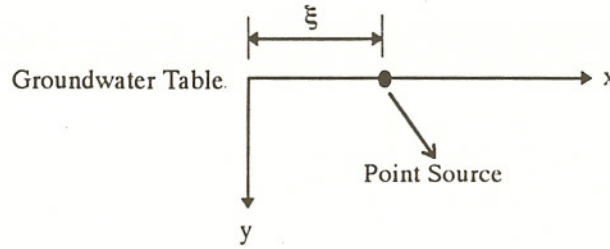


Figure 2. Schematic of a Point Source

$$C_L(x, y, t) = \frac{M}{4\pi t \sqrt{D_{x,r} D_{y,r}}} \exp \left[-\frac{(x - \xi - U_r t)^2}{4D_{x,r} t} - \frac{y^2}{4D_{y,r} t} - \lambda t \right] \quad (6)$$

If the contaminant mass in the liquid phase is released at a rate $\dot{M}$ over time, the “instantaneous” release in an infinitesimal time interval, dt , can be defined as $M = \dot{M} dt$. Then, Equation (6) becomes:

$$C_L(x, y, t) = \frac{\dot{M} dt}{4\pi t \sqrt{D_{x,r} D_{y,r}}} \exp \left[-\frac{(x - \xi - U_r t)^2}{4D_{x,r} t} - \frac{y^2}{4D_{y,r} t} - \lambda t \right] \quad (7)$$

where $\dot{M}$ is mass release rate per unit length along the source $[\text{ML}^{-1}\text{T}^{-1}]$.

Furthermore, if the mass is being released along longitudinal direction over a finite length of $2a$ as depicted in Figure (1), then this release may be simulated by an infinite series of point sources distributed over the entire length $2a$. The strength of each source may be expressed as $\dot{M} = \dot{m} d\xi$ where $\dot{m}$ is the mass release rate per unit area normal to the $x - y$ plane $[\text{ML}^{-2}\text{T}^{-1}]$. Equation (7) can then be written as:

$$C_L(x, y, t) = \int_{-a}^a \frac{\dot{m} dt}{4\pi t \sqrt{D_{x,r} D_{y,r}}} \exp \left[-\frac{(x - \xi - U_r t)^2}{4D_{x,r} t} - \frac{y^2}{4D_{y,r} t} - \lambda t \right] d\xi \quad (8)$$

If the mass release is a function of time as shown in Figure (3), the above temporal distribution may be simulated by a series of “instantaneous” releases. Each release contributes to the concentration distribution with a lag time, τ . The resulting concentration distribution is therefore:

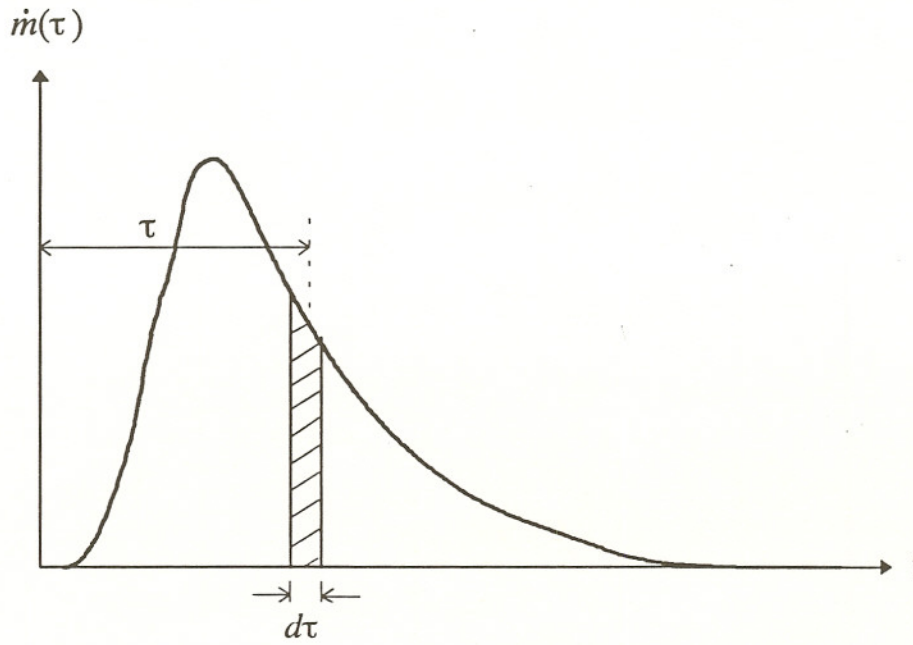


Figure 3. Schematic of a Time-Release Source

$$C_L(x, y, t) = \int_0^t \int_{-a}^a \frac{\dot{m}(\tau)}{4\pi(t-\tau)\sqrt{D_{x,r}D_{y,r}}} \exp\left[-\frac{[x-\xi-U_r(t-\tau)]^2}{4D_{x,r}(t-\tau)} - \frac{y^2}{4D_{y,r}(t-\tau)} - \lambda(t-\tau)\right] d\xi d\tau \quad (9)$$

Equation (9) may be written as

$$C_L(x, y, t) = \int_0^t \frac{\dot{m}(\tau)}{2\pi\sqrt{D_{y,r}(t-\tau)}} \exp\left[-\frac{y^2}{4D_{y,r}(t-\tau)} - \lambda(t-\tau)\right] \cdot \left\{ \int_{-a}^{+a} \frac{1}{\sqrt{4D_{x,r}(t-\tau)}} \exp\left[-\frac{[x-\xi-U_r(t-\tau)]^2}{4D_{x,r}(t-\tau)}\right] d\xi \right\} d\tau \quad (10)$$

The solution of the integral given in the curly brackets in Equation (10) can be found in terms of an error function of the form:

$$\{\dots\} = \frac{\sqrt{\pi}}{2} \left\{ \operatorname{erf} \left[\frac{x - U_r(t - \tau) + a}{\sqrt{4D_{x,r}(t - \tau)}} \right] - \operatorname{erf} \left[\frac{x - U_r(t - \tau) - a}{\sqrt{4D_{x,r}(t - \tau)}} \right] \right\} \quad (11)$$

Thus, the final solution becomes:

$$C_L(x, y, t) = \int_0^t \frac{\dot{m}(\tau)}{4\sqrt{\pi D_{y,r}(t - \tau)}} \exp \left[-\frac{y^2}{4D_{y,r}(t - \tau)} - \lambda(t - \tau) \right] \cdot \left\{ \operatorname{erf} \left[\frac{x - U_r(t - \tau) + a}{\sqrt{4D_{x,r}(t - \tau)}} \right] - \operatorname{erf} \left[\frac{x - U_r(t - \tau) - a}{\sqrt{4D_{x,r}(t - \tau)}} \right] \right\} d\tau \quad (12)$$

It should be noted that the time-varying mass release rate can explicitly be computed from the unsaturated zone solution as:

$$\dot{m}(\tau) = \bar{u} \bar{C}_L(\tau) \quad (13)$$

where $\bar{C}_L(\tau)$ is the liquid phase concentration introduced within the strip source at the groundwater table by the unsaturated zone transport, and $\bar{u}$ is the specific discharge to the groundwater table from the unsaturated zone (Darcy velocity).

IV.2 Method of Solution

Considering the temporal discretization scheme shown in Figure (4) and assuming that mass $m = \dot{m}\Delta t$ is released instantaneously at the mid-point of each rectangle, Equation (12) can be written in discretized form as:

$$C_L(x, y, t) = \sum_{j=1}^J \frac{\dot{m}_j \Delta t}{4\sqrt{\pi D_{y,r}(t - \tau_j)}} \exp \left[-\frac{y^2}{4D_{y,r}(t - \tau_j)} - \lambda(t - \tau_j) \right] \cdot \left\{ \operatorname{erf} \left[\frac{x - U_r(t - \tau_j) + a}{\sqrt{4D_{x,r}(t - \tau_j)}} \right] - \operatorname{erf} \left[\frac{x - U_r(t - \tau_j) - a}{\sqrt{4D_{x,r}(t - \tau_j)}} \right] \right\} \quad (14)$$

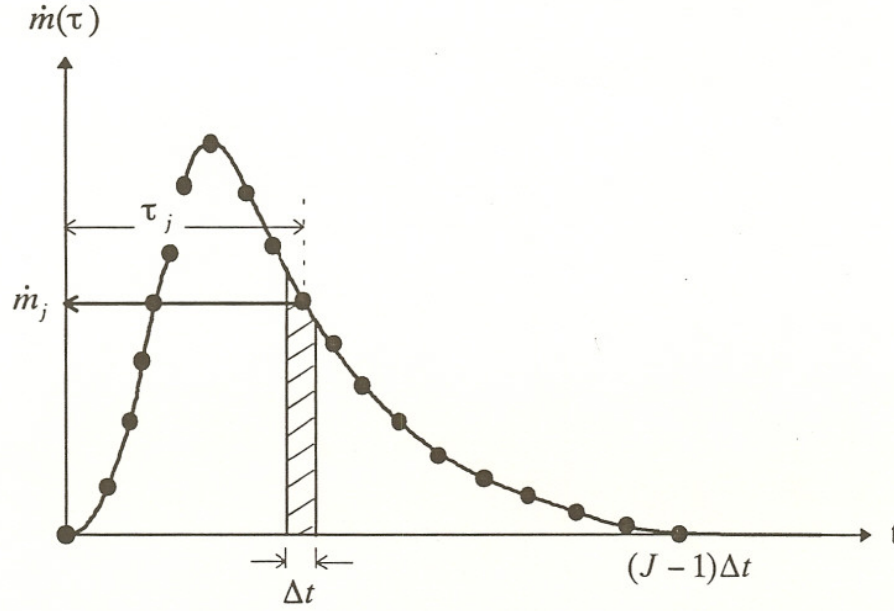


Figure 4. Temporal Discretization of Time-Release Source

where J is the total number of discrete data points, $\tau_j = (j-1)\Delta t$, and $\dot{m}_j = \bar{u}_j \bar{C}_L(\tau_j)$ in which $\bar{u}_j$ and $\bar{C}_L(\tau_j)$ are obtained from the solution of the unsaturated zone flow and transport models.

For the situation depicted in Figure (1) and in the absence of an impervious boundary, Equation (14) would be applicable. However, the presence of the impervious boundary dictates the use of an image source, which is symmetrical to the actual one, with respect to the impervious boundary. Furthermore, in order to conserve mass within the aquifer, the groundwater table is also treated as a pseudo-impermeable boundary by utilizing a second image source, which is symmetrical to the actual source with respect to the phreatic surface. Figure (5) given below shows the locations of the primary image sources utilized in this study. It should be noted that only primary image sources are used in the final formulation of the theory presented herein since a sensitivity analysis proved that the results did not change more than 1% if the secondary (complementary) image sources were used.

The solution of Equation (5), subject to $\partial C_L / \partial y = 0$ at $y = b$ where b is the total thickness of the aquifer, can then be computed as:

$$C_{imp}(x, y, t) = C_L(x, y, t) + C_L(x, 2b - y, t) \quad (15)$$

Similarly, the solution of Equation (5), subject to $\partial C_L / \partial y = 0$ at $y = 0$, can be computed as:

$$C_{gw} (x, y, t) = C_L (x, y, t) + C_L (x, 2b - y, t) \quad (16)$$

The final solution of Equation (5) is obtained by superposition of Equations (15) and (16) thus:

$$C_{actual} (x, y, t) = 2[C_L (x, y, t) + C_L (x, 2b - y, t)] \quad (17)$$

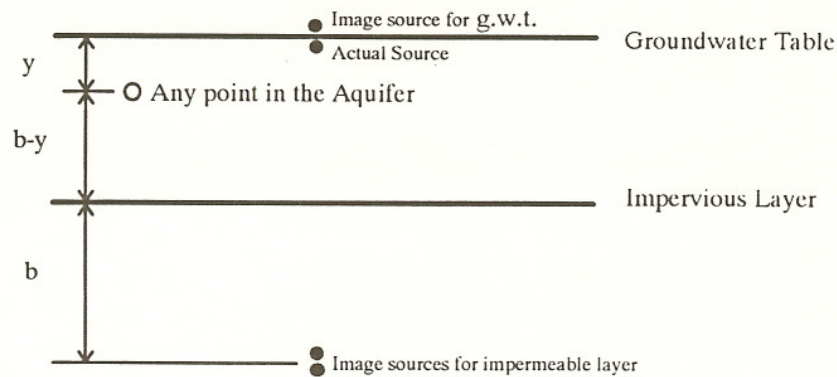


Figure 5. Schematic of Image Sources

V. Sensitivity Analysis

The old and new schemes utilized in the saturated transport model DILUTE are qualitatively compared against the results of Pickens and Lennox (1976) which are based on a finite element solution of the governing equations. It must be pointed out that direct comparisons cannot be made because many of the parameters had to be approximated from information available in their paper.

Pickens and Lennox first solved the steady-state flow problem for an approximately 50 m thick unconfined aquifer. Close observation of their results reveals that the flow field in the aquifer is approximately horizontal, especially downgradient from the input source. From their figures, it was roughly estimated that the head gradient of the flow field is 0.0122 and the length of the strip source is 160 m. The authors also provide other pertinent parameters as follows: hydraulic conductivity 0.5 m/day, porosity 0.3, and bulk density of soil 1.8 gr/cm³. Based on the above, it was estimated that the aquifer flow velocity is 0.0203 m/day. Furthermore, neglecting the molecular diffusion, the hydrodynamic dispersion coefficients are defined therein as:

$$D_L = \alpha_L U \quad (18)$$

$$D_T = \alpha_T U \quad (19)$$

where α is the soil dispersivity, and the subscripts L and T represent longitudinal and transverse directions, respectively. All subsequent runs presented in this chapter assumes no sorption, therefore the retardation coefficient R_d is equal to unity.

Figure (6) given below shows the Pickens and Lennox (1976) results for a continuous, normalized step input.

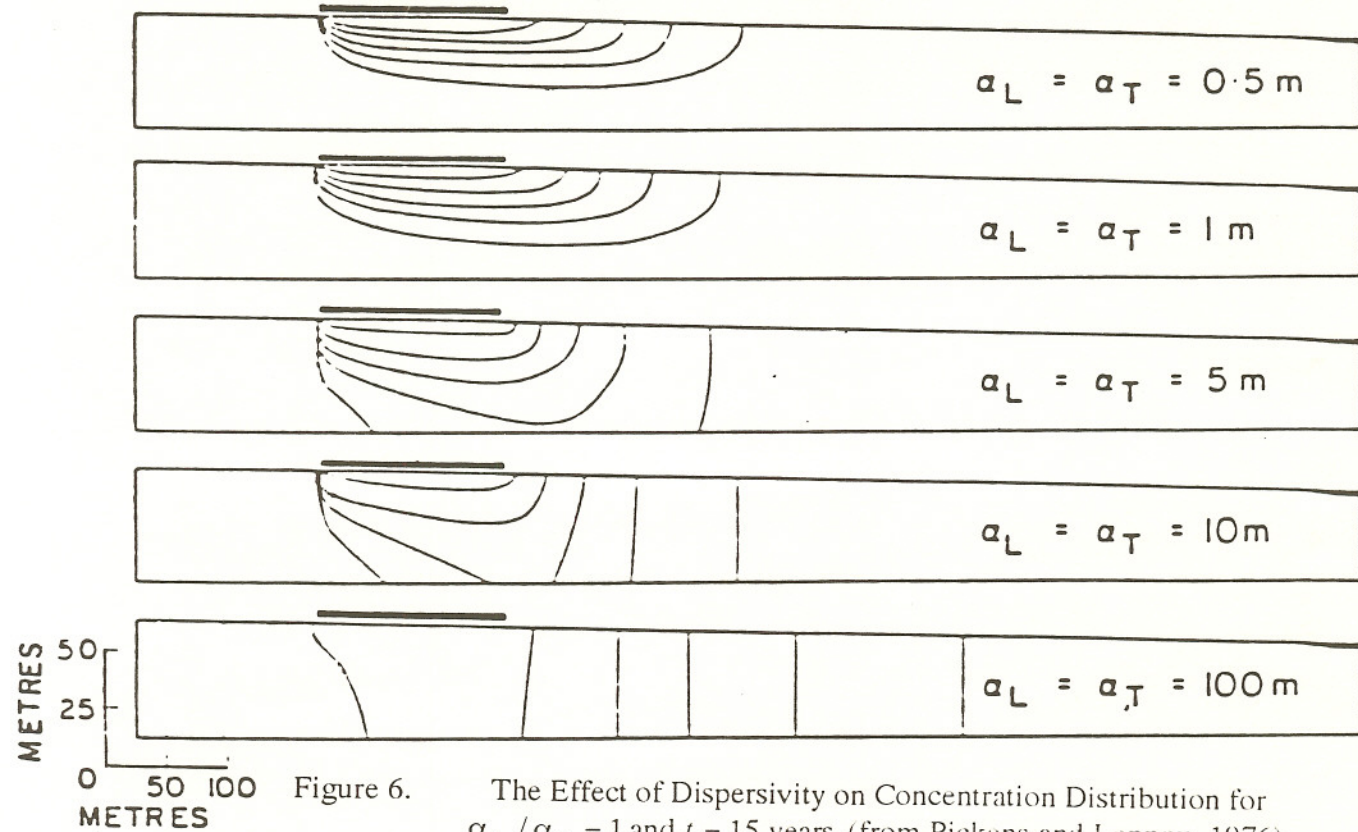


Figure 6.

The Effect of Dispersivity on Concentration Distribution for $\alpha_L / \alpha_T = 1$ and $t = 15$ years (from Pickens and Lennox, 1976).

Figure (7) given below shows the results obtained from previous and new versions of the DILUTE model executed for the same scenario used by Pickens and Lennox (1976) for $\alpha_L = \alpha_T = 1$ m. A close observation of the results shown in Figure (7) reveals that the agreement between the two schemes is very good, except for the boundary effect observed in the old scheme. The boundary effect which was discussed previously is apparent in isoconcentration lines shown in Figure (7). They tend to close back to the source since the concentrations are forced to be zero at the groundwater table outside the strip source. If, however, the contour lines continued instead of closing back to the source, one would observe the exact same behavior shown in the results of the new scheme.

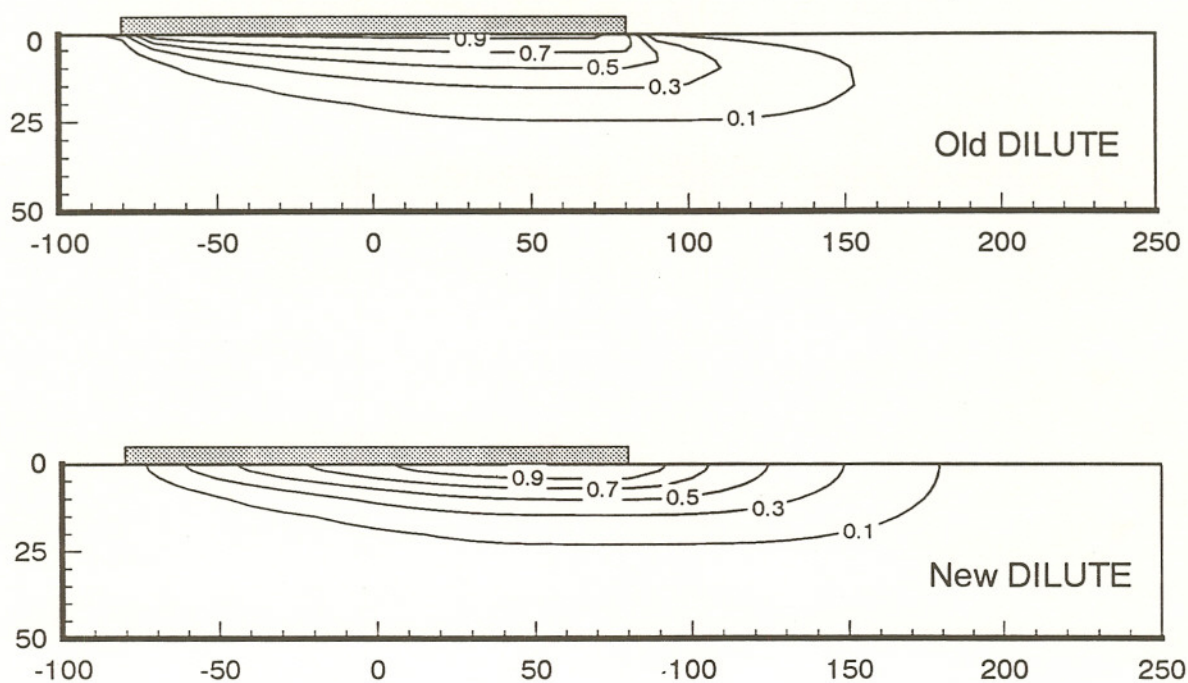


Figure 7. The Effect of Dispersivity on Concentration Distribution for $\alpha_L = \alpha_T = 1$ m and $t = 15$ years

Similarly, Figure (8) shows the results obtained from previous and new versions of the DILUTE model executed for $\alpha_L = \alpha_T = 10$ m. As was the case in Figure (7), the results of both schemes are in agreement except for the aforementioned boundary effect. It should be noted however, that the source for these runs was assumed to be continuous for the total duration of simulation (15 years). As discussed earlier, the rate of mass loss due to the boundary effect is negligible as long as there is contaminant replenishment in the system.

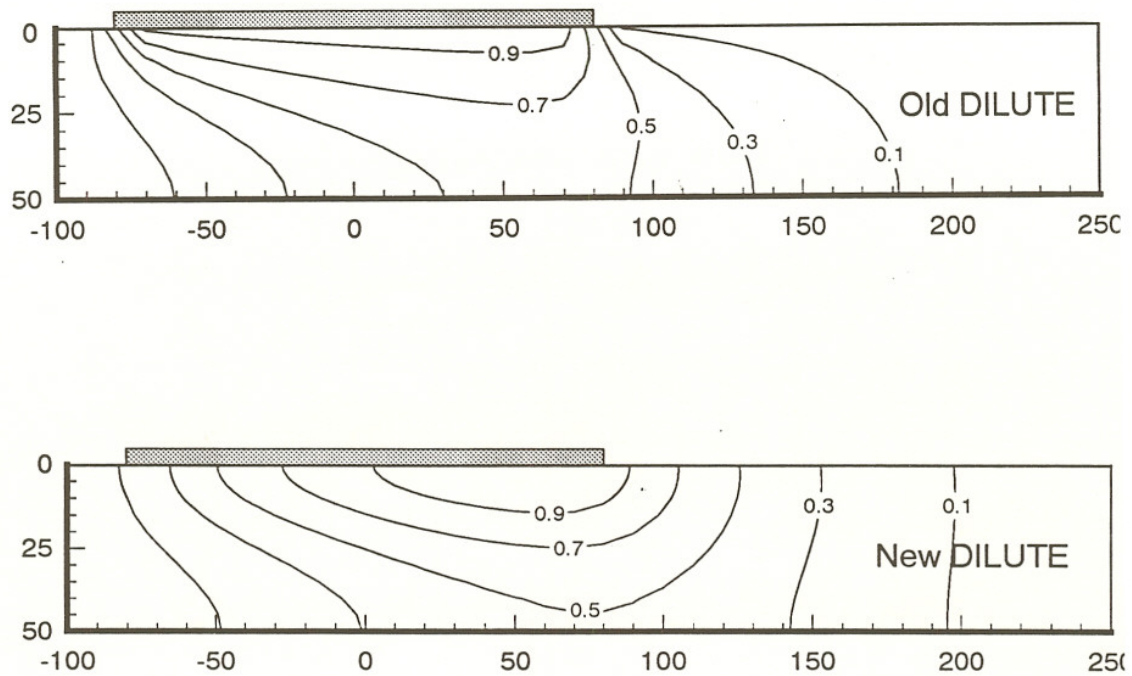


Figure 8. The Effect of Dispersivity on Concentration Distribution for
 $\alpha_L = \alpha_T = 10$ m and $t = 15$ years

Pickens and Lennox also performed a simulation for variable input concentration by using a time-variable source as shown in Figure (9) given below. The results obtained by the finite element model for the time-varying source are shown in Figure (10).

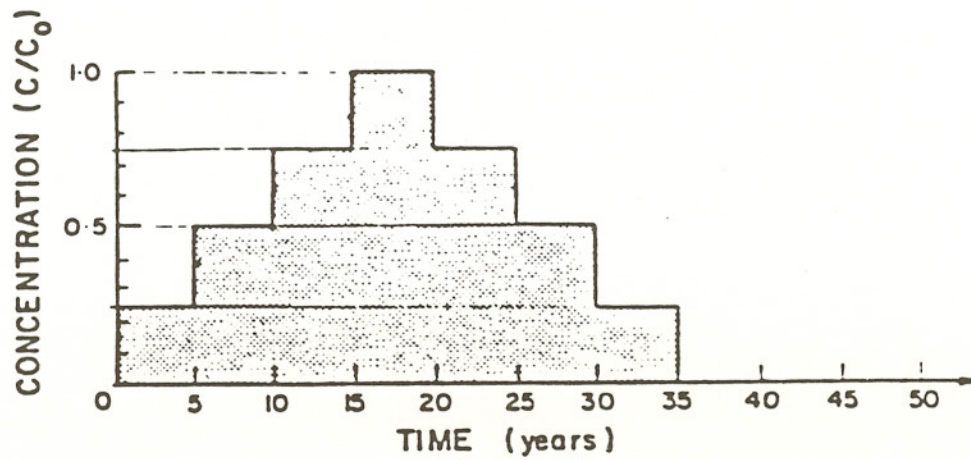


Figure 9. A Variable Input Concentration History (from Pickens and Lennox, 1976)

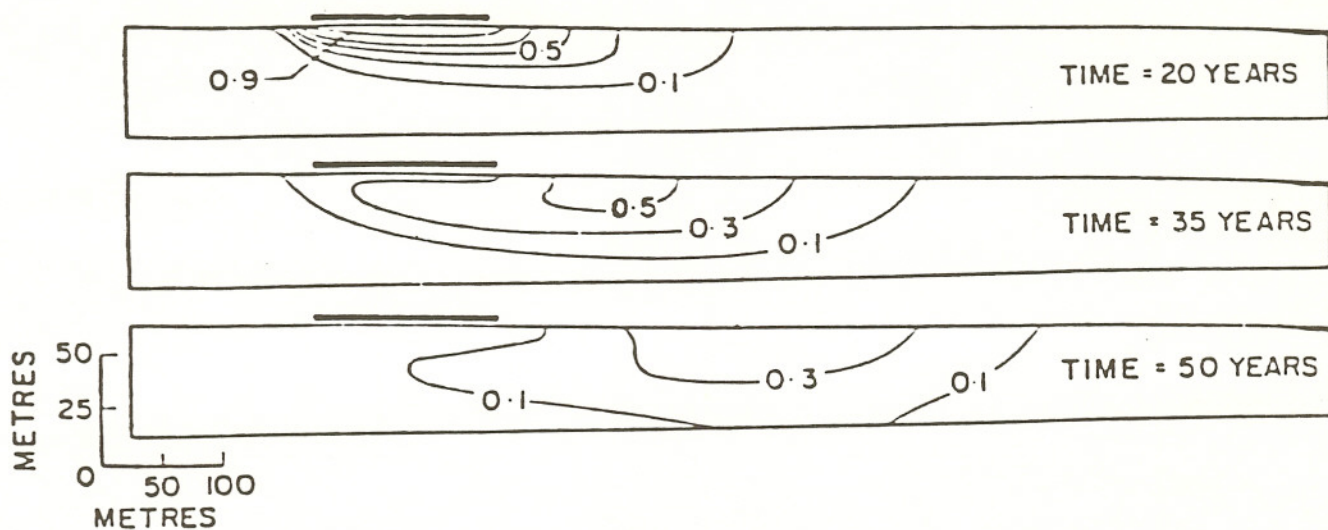


Figure 10. Concentration Distributions for Variable Concentration Distribution Shown in Figure (9) and $\alpha_L = 10$ m and $\alpha_T = 0.5$ m (from Pickens and Lennox, 1976).

For the scenario depicted in Figure (9), the results obtained with the present model as well as the previous one are shown in Figures (11) through (13).

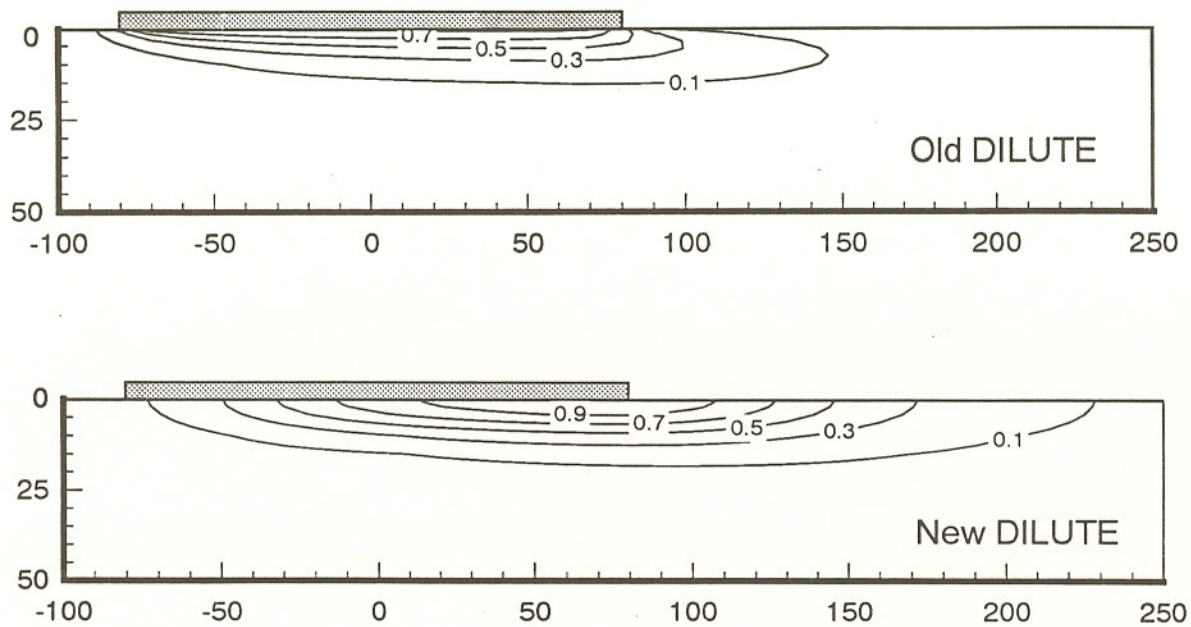


Figure 11. Concentration Distributions for $\alpha_L = 10$ m and $\alpha_T = 0.5$ m, $t = 20$ years .

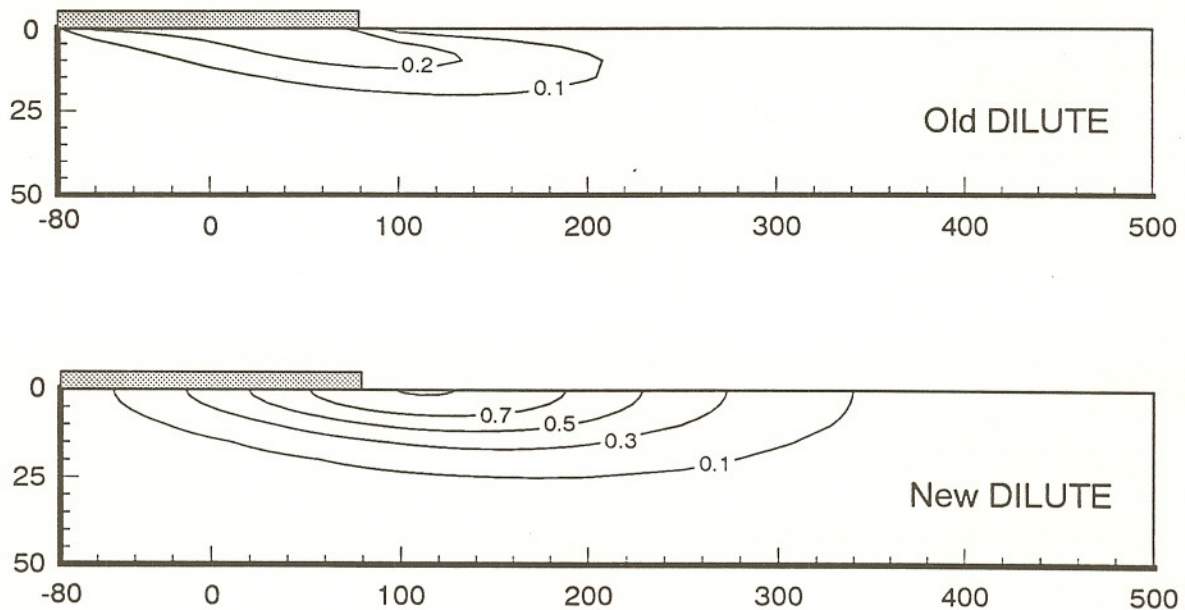


Figure 12. Concentration Distributions for $\alpha_L = 10$ m and $\alpha_T = 0.5$ m, $t = 35$ years .

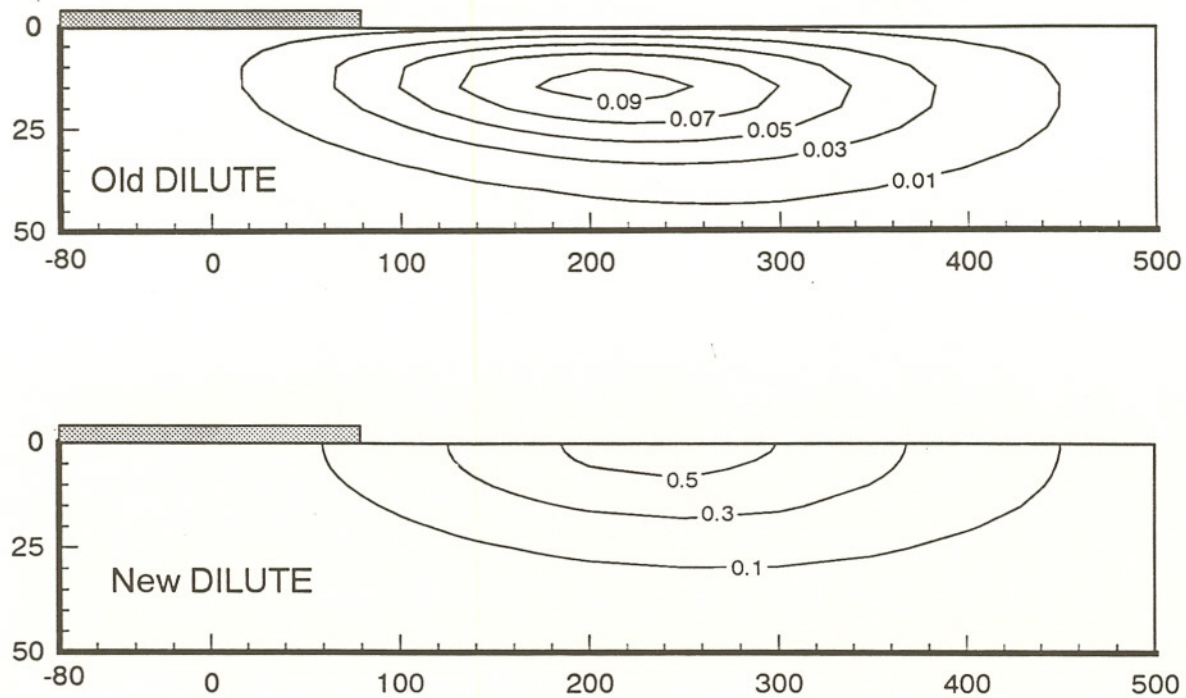


Figure 13. Concentration Distributions for $\alpha_L = 10$ m and $\alpha_T = 0.5$ m, $t = 50$ years .

The results presented in Figure (11) show the same trend observed in Figures (7) and (8). Since the source at the strip is still active at $t = 20$ years (see Figure 9), the rate of mass loss through the phreatic surface due to the aforementioned boundary effect is negligible in the results of the old scheme. However, the boundary effect is more prominent for the results presented in Figure (12) for $t = 35$ years which is the source cessation time. Figure (13) shows a great magnitude of mass loss (reduced concentrations) for the simulations performed for $t = 50$ years. It should be noted, however, that despite the boundary effect observed in the old DILUTE model, both schemes approximate the plume delineation with the same accuracy.

VI. Source Code of New DILUTE Subroutine

The old DILUTE subroutine was replaced with the following in IMPACT v3.2.


```

C-----
C-----
SUBROUTINE DILUTE(CD)
C-----
C-----
C
C...THIS IS A TWO-DIMENSIONAL SATURATED TRANSPORT MODEL WHICH TAKES
C...THE CONCENTRATION HISTORY OBSERVED AT THE GROUNDWATER TABLE AS INPUT
C...INTO THE UNDERLYING AQUIFER IN TERMS OF MASS FLUXES AT G.W.T.
C-----
C-----
C...OPEN AND READ FILE WITH RESPECT TO THE RUN NUMBER SUPPLIED IN IMPACT
C-----
      INTEGER XDIM,ZDIM,TDIM
      PARAMETER(ZDIM=201,XDIM=51,TDIM=2235,NLAY=4)
C-----
      COMMON/BLK15/UDT,UTHO,UAKE,UDZ,UDIS
      COMMON/BLK29/IUNIT,JUNIT,KUNIT
      COMMON/BLK30/BELL,BLINK
      COMMON/BLK32/REVERS,NORMAL
      COMMON/BLK33/BOLD
      COMMON/BLK40/IUN
      COMMON/BLK44/FTIME
      COMMON/BLK47/NUMX,NUMY,NUMT,BAQ
      COMMON/BLK48/XX,YY,SIMT(100),TAU,IK
      COMMON/BLK49/DSX,DSY,VX,A
      COMMON/BLK50/ALAMDA,RD
      COMMON/BLK51/XL(100),YL(100)
C-----
      DIMENSION TIM(TDIM),CONC(TDIM),FLUX(TDIM),CD(20,20,100)
      CHARACTER*8 UDT,UTHO,UDZ,UAKE,UDIS
      CHARACTER BELL*1,BLINK*4,NORMAL*4,BOLD*4,REVERS*4
      LOGICAL FTIME
C-----
C...READ DATA FROM THE FILE AND DETERMINE NUMBER OF TIME VALUES
C-----
      REWIND(UNIT=30)
      III=1
10      READ(30,*,END=111) TIM(III),CONC(III),FLUX(III)
      III=III+1
      GOTO 10
C-----
111      NTIME=III-1
      JTIME=NTIME-1
      DTT=(TIM(NTIME)-TIM(1))/JTIME
C-----
C...READ AQUIFER PROPERTIES, LOCATION AND THE TIME VALUE IN QUESTION
C-----
      IF(FTIME) THEN
C-----
101      WRITE(JUNIT,104)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,BOLD,
      .      NORMAL,REVERS,NORMAL
104      FORMAT(/1X,A,'ENTER',A,/,5X,'NUMBER OF X LOCATIONS IN THE ',
      .      'AQUIFER [MAX 20]',T55,A,'<NUMX>',A,/,5X,
      .      'NUMBER OF Y LOCATIONS IN THE AQUIFER [MAX 20]',T55,
      .      A,'<NUMY>',A,/,5X,'NUMBER OF SIMULATION ',
      .      'TIMES [MAX 100]',T55,A,'<NUMT>',A,/,1X,A,
      .      'RESPECTIVELY',A,' : ',A,$)
      READ(IUNIT,*,ERR=101) NUMX,NUMY,NUMT
      IF(IUNIT.NE.1) CALL DATA
109      IF(NUMX.LT.1.OR.NUMX.GT.20) THEN
      .      WRITE(JUNIT,115)BLINK,NORMAL,BELL,BELL
115      .      FORMAT(/5X,A,'INVALID ENTRY FOR <NUMX>, REENTER',
      .      A,' : ',2A,$)
      .      READ(IUNIT,*,ERR=109) NUMX
      .      GOTO 109
      .      END IF
116      IF(NUMY.LT.1.OR.NUMY.GT.20) THEN
      .      WRITE(JUNIT,117)BLINK,NORMAL,BELL,BELL
117      .      FORMAT(/5X,A,'INVALID ENTRY FOR <NUMY>, REENTER',
      .      A,' : ',2A,$)
      .      READ(IUNIT,*,ERR=116) NUMY
      .      GOTO 116
      .      END IF
118      IF(NUMT.LT.1.OR.NUMT.GT.100) THEN
      .      WRITE(JUNIT,119)BLINK,NORMAL,BELL,BELL
119      .      FORMAT(/5X,A,'INVALID ENTRY FOR <NUMT>, REENTER',
      .      A,' : ',2A,$)
      .      READ(IUNIT,*,ERR=118) NUMT
      .      GOTO 118
      .      END IF
      WRITE(KUNIT,*)NUMX,NUMY,NUMT
C-----
      DO 14 I=1,NUMX
103      WRITE(JUNIT,105)BOLD,I,NORMAL
105      FORMAT(/1X,A,'ENTER X VALUE',2X,A,'<XL(',I3,')>',A,' : ',A,$)
      READ(IUNIT,*,ERR=103)XL(I)
      IF(IUNIT.NE.1) CALL DATA

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        WRITE(KUNIT,*)XL(I)
14      CONTINUE
C-----
      DO 15 I=1,NUMY
150     WRITE(JUNIT,106)BOLD,I,NORMAL
106     FORMAT(/1X,'ENTER Y VALUE',2X,A,'<YL('',I3,'')>',A,' : ', $)
        READ(IUNIT,*,ERR=150)YL(I)
        IF(IUNIT.NE.1) CALL DATA
        WRITE(KUNIT,*)YL(I)
15      CONTINUE
C-----
      DO 16 I=1,NUMT
120     WRITE(JUNIT,102)BOLD,I,NORMAL
102     FORMAT(/1X,'ENTER TIME VALUE',2X,A,'<SIMT('',I3,'')>',A,
        .       ' : ', $)
        READ(IUNIT,*,ERR=120)SIMT(I)
        IF(IUNIT.NE.1) CALL DATA
        WRITE(KUNIT,*)SIMT(I)
16      CONTINUE
C-----
130     WRITE(JUNIT,107)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,BOLD,
        .       NORMAL,BOLD,NORMAL,REVERS,NORMAL
107     FORMAT(/1X,A,'ENTER',A//5X,'LONGITUDINAL DISPERSION ',
        .       'COEFFICIENT',T45,A,'<DSX>',A/5X,'TRANSVERSE ',
        .       'DISPERSION COEFFICIENT',T45,A,'<DSY>',A/5X,
        .       'AQUIFER VELOCITY',T45,A,'<VX>',A/5X,
        .       'HALF-LENGTH OF THE STRIP SOURCE',T45,
        .       A,'<A>',A//1X,A,'RESPECTIVELY',A,' : ', $)
        READ(IUNIT,*,ERR=130)DSX,DSY,VX,A
        IF(IUNIT.NE.1) CALL DATA
        WRITE(KUNIT,*)DSX,DSY,VX,A
C-----
140     WRITE(JUNIT,108)REVERS,NORMAL,BOLD,NORMAL,BOLD,NORMAL,BOLD,
        .       NORMAL,REVERS,NORMAL
108     FORMAT(/1X,A,'ENTER',A//5X,'FIRST ORDER DECAY COEFFICIENT',
        .       T45,A,'<ALAMDA>',A/5X,'RETARDATION COEFFICIENT',T45,
        .       A,'<RD>',A/5X,'AQUIFER THICKNESS',T45,A,'<BAQ>',A//
        .       1X,A,'RESPECTIVELY',A,' : ', $)
        READ(IUNIT,*,ERR=140)ALAMDA,RD,BAQ
        IF(IUNIT.NE.1) CALL DATA
121     IF(RD.LT.1.0) THEN
        .       WRITE(JUNIT,122)BLINK,NORMAL,BELL,BELL
122     .       FORMAT(/5X,A,'<RD> MUST BE >= 1, REENTER',
        .       A,' : ',2A,$)
        .       READ(IUNIT,*,ERR=121)RD
        .       GOTO 121
        .       END IF
        WRITE(KUNIT,*)ALAMDA,RD,BAQ
C-----
C...WRITE INPUT PARAMETERS
C-----
        WRITE(21,610) VX,UAKS,DSX,UDIS,DSY,UDIS,A,UDZ,BAQ,UDZ
        WRITE(6,610) VX,UAKS,DSX,UDIS,DSY,UDIS,A,UDZ,BAQ,UDZ
610     FORMAT(/2X,37H*SATURATED ZONE TRANSPORT PARAMETERS*,//
        .       43H AQUIFER VELOCITY----- =,F10.4,
        .       1X,A/
        .       43H LONGITUDINAL DISPERSION COEFFICIENT----- =,F10.4,
        .       1X,A/
        .       43H TRANSVERSE DISPERSION COEFFICIENT----- =,F10.4,
        .       1X,A/
        .       43H HALF LENGTH SOURCE----- =,F10.4
        .       1X,A/
        .       43H AQUIFER THICKNESS----- =,F10.4,
        .       1X,A//)
        WRITE(21,620) ALAMDA,RD
        WRITE(6,620) ALAMDA,RD
620     FORMAT(/
        .       43H FIRST ORDER DECAY COEFFICIENT----- =,
        .       F10.4,1X,'1/DAY' /
        .       43H RETARDATION FACTOR----- =,
        .       F10.4//)
        WRITE(21,630) NUMX,NUMY,NUMT
        WRITE(6,630) NUMX,NUMY,NUMT
630     FORMAT(/1X,42HTOTAL NUMBER OF X POSITIONS----- =,I5/
        .       43H TOTAL NUMBER OF Y POSITIONS----- =,I5/
        .       43H TOTAL NUMBER OF SIMULATIONS----- =,I5//)
C-----
      END IF
C-----
C...OPEN OUTPUT FILE
C-----
      OPEN(UNIT=31,FILE='AQCON.DAT',STATUS='UNKNOWN')
      REWIND(UNIT=31)
C-----
C...START COMPUTING AQUIFER CONCENTRATIONS FOR EACH SIMULATION TIME
C-----
      DO 222 IK=1,NUMT
C-----
C...INITIALIZE NORMALIZED CONCENTRATION MATRIX

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C-----
      DO 30 KK=1,NUMX
      DO 20 JJ=1,NUMY
      CD(KK,JJ,IK)=0.0
20  CONTINUE
30  CONTINUE
C-----
C...DETERMINE NUMBER OF STEPS REQUIRED FOR SLICING --- NTIML
C-----
      IF(SIMT(IK).GT.TIM(NTIME)) THEN
      NTIML=NTIME
      ELSE
      DO 11 JJ=1,NTIME
      IF(SIMT(IK).GT.TIM(JJ)) THEN
      NTIML=JJ
      ELSE
      GOTO 12
      END IF
11  CONTINUE
      END IF
12  CONTINUE
      WRITE(6,110) BOLD,NTIML,SIMT(IK),NORMAL
110  FORMAT(/1X,A,'TOTAL OF ',I4,' TIME RELEASES WILL BE USED ',
      .      'FOR TIME = ',F8.0,' DAYS!',A/)
C-----
C...BEGIN SLICING AND CALL 2-D TRANSPORT MODEL -- REPEAT NTIML TIMES
C-----
      DO 13 IJ=1,NTIML
      FM=CONC(IJ)*FLUX(IJ)*DTT
      WRITE(6,112)IJ
112  FORMAT(/10X,'ITERATING FOR SLICE # : ',I4//)
      TAU=(IJ-1)*DTT
C-----
C...CALL TRANSPORT MODEL FOR THE REAL + IMAGE SOURCES AT G.W.T.
C-----
      DO 50 J=1,NUMX
      XX=XL(J)
      DO 40 K=1,NUMY
      YY=YL(K)
      CD(J,K,IK)=CD(J,K,IK)+2*FCT(FM)
      WRITE(6,113)J,K
113  FORMAT('+', 'COMPUTING CONCENTRATION AT ',
      .      'THE NODE (',I3,',',I3,' ) FOR THE ',
      .      'ACTUAL SOURCE')
40  CONTINUE
50  CONTINUE
C-----
C...CALL TRANSPORT MODEL FOR THE IMAGE SOURCES ACROSS IMPERMEABLE LAYER
C-----
      DO 70 J=1,NUMX
      XX=XL(J)
      DO 80 K=1,NUMY
      YY=2*BAQ-YL(K)
      CD(J,K,IK)=CD(J,K,IK)+2*FCT(FM)
      WRITE(6,114)J,K
114  FORMAT('+', 'COMPUTING CONCENTRATION AT ',
      .      'THE NODE (',I3,',',I3,' ) FOR THE ',
      .      'IMAGE SOURCES')
80  CONTINUE
70  CONTINUE
13  CONTINUE
C-----
C...PRINT RESULTS INTO THE FILE 'AQCON.DAT'
C-----
      WRITE(21,777)SIMT(IK),UDZ,UDZ
      WRITE(31,777)SIMT(IK),UDZ,UDZ
777  FORMAT(/10X,'FOR TIME = ',F8.0,' DAYS'
      .      //6X,'X',1X,A,'Y',1X,A,'CONCENTRATION (ppm)')
      DO 60 J=1,NUMX
      DO 60 K=1,NUMY
      IF(CD(J,K,IK).LT.0) CD(J,K,IK)=0.0
      IF(IUN.EQ.1) THEN
      WRITE(21,666) XL(J),YL(K),35.314667*CD(J,K,IK)
      WRITE(31,666) XL(J),YL(K),35.314667*CD(J,K,IK)
      ELSE
      IF(IUN.EQ.2) THEN
      WRITE(21,666) XL(J),YL(K),CD(J,K,IK)
      WRITE(31,666) XL(J),YL(K),CD(J,K,IK)
      ELSE
      IF(IUN.EQ.3) THEN
      WRITE(21,666) XL(J),YL(K),61023.744*CD(J,K,IK)
      WRITE(31,666) XL(J),YL(K),61023.744*CD(J,K,IK)
      ELSE
      IF(IUN.EQ.4) THEN
      WRITE(21,666) XL(J),YL(K),1E6*CD(J,K,IK)
      WRITE(21,666) XL(J),YL(K),1E6*CD(J,K,IK)
      END IF
      END IF
      END IF

```



```

      END IF
666  FORMAT(F10.2,1X,F10.2,1X,F12.6)
60   CONTINUE
222  CONTINUE
C-----
      CLOSE(UNIT=31)
      RETURN
      END
C-----
C-----
      FUNCTION FCT(FM)
C-----
C-----
C...INTEGRAND
C-----
      COMMON/BLK48/XX,YY,SIMT(100),TAU,IK
      COMMON/BLK49/DSX,DSY,VX,A
      COMMON/BLK50/ALAMDA,RD
C-----
      PI=4.*ATAN(1.)
      AA=FM/(4*SQRT(PI*DSY/RD*(SIMT(IK)-TAU)))
      AB=-YY**2/(4*DSY/RD*(SIMT(IK)-TAU))-ALAMDA*(SIMT(IK)-TAU)
      AAA=AA*EXP(AB)
      BB=(XX-VX/RD*(SIMT(IK)-TAU)+A)/SQRT(4*DSX/RD*(SIMT(IK)-TAU))
      CC=(XX-VX/RD*(SIMT(IK)-TAU)-A)/SQRT(4*DSX/RD*(SIMT(IK)-TAU))
      BBB=ERF(BB)-ERF(CC)
      FCT=AAA*BBB
      RETURN
      END
C-----
C-----
      FUNCTION ERF(X)
C-----
C-----
C...ERROR FUNCTION APPROXIMATION
C-----
      DIMENSION D(101)
C-----
      IF(X.GE.4) THEN
        ERF=1.0
        GOTO 10
      ELSE
        IF(X.LE.-4) THEN
          ERF=-1.0
          GOTO 10
        END IF
      END IF
C-----
      ERF=0
      N=100
      N1=N+1
      PI=4*ATAN(1.)
      C=2./SQRT(PI)
      H=X/N
      DO 130 I=1,N1
        Y=(I-1)*H
130    D(I)=EXP(-Y*Y)
      E1=0.0
      DO 140 I=3,N1,2
140    E1=E1+(D(I-2)+4.*D(I-1)+D(I))*(H/3.)
      ERF=C*E1
10    RETURN
      END

```

VII. Sample Run

The following is the sample run submitted with the working copy of the IMPACT model. All pertinent values of the model input parameters are given in the proceeding output.

SAMPLE RUN: Sandy Loam Contaminated with Benzene (21 x 11 f
RUN NO : 1

THIS IS A SIMULATION FOR BOTH MOISTURE AND SOLUTE TRANSPORT

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

.....

FLAG1 = 1	FLAG2 = 1	FLAG3 = 0	FLAG4 = 2
FLAG5 = 1	FLAG6 = 1	FLAG7 = 1	FLAG8 = 1
FLAG9 = 1	FLAG10 = 0	FLAG11 = 0	FLAG12 = 0

HYDRAULIC PROPERTIES AND SIMULATION PARAMETERS

.....

SOIL 1

SATURATED HYDRAULIC CONDUCTIVITY =	9.8300	FT/DAY
FIELD CAPACITY MOISTURE CONTENT =	0.1000	FT3/FT3
SATURATION MOISTURE CONTENT =	0.4400	FT3/FT3
AIR-DRY MOISTURE CONTENT =	0.0500	FT3/FT3
COEFFICIENT <AM> =	12.8000	
COEFFICIENT =	4.9000	
SATURATION SUCTION HEAD =	0.7200	FT
LATERAL DISTANCE INCREMENT =	1.0000	FT
VERTICAL DISTANCE INCREMENT =	1.0000	FT
TIME INCREMENT =	2.0000	DAYS

*** OUTPUT PRINTED EVERY 200 TIME INCREMENTS ***

EPSILON =	0.001000
NUMBER OF COLUMNS =	11
NUMBER OF ROWS =	21
NUMBER OF TIME STEPS =	2000

INITIAL MOISTURE CONTENT (FT3/FT3)

.....

0.2000 CONSTANT FOR ALL NODES

INFILTRATION RATE (FT/DAY)

.....

0.0554	0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0104	0.0004	0.0185
0.0075	0.0000	0.0012	0.0042	0.0008	0.0000	0.0029	0.0213	0.0000	0.0085
0.0208	0.0058	0.0171	0.0000	0.0004	0.0000	0.0021	0.0000	0.0000	0.0000
0.0008	0.0050	0.0584	0.0000	0.0042	0.0404	0.0021	0.0021	0.0000	0.0075
0.0000	0.0000	0.0167	0.0008	0.0267	0.0213	0.0008	0.0004	0.0000	0.0094
0.0150	0.0000	0.0000	0.0000	0.0042	0.0000	0.0000	0.0021	0.0283	0.0038
0.0096	0.0025	0.0000	0.0146	0.0000	0.0000	0.0221	0.0000	0.0004	0.0012
0.0108	0.0000	0.0000	0.0000	0.0000	0.0000	0.0587	0.0000	0.0142	0.0000
0.0000	0.0217	0.0000	0.0000	0.0008	0.0063	0.0300	0.0133	0.0004	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0125	0.0004	0.0417	0.0000	0.0125
0.0175	0.0137	0.0054	0.0000	0.0000	0.0000	0.0000	0.0000	0.0532	0.0522
0.0892	0.0000	0.0000	0.0000	0.0038	0.0000	0.0012	0.0063	0.0000	0.0000

0.0183	0.1054	0.0029	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0067	0.0167	0.0000	0.0000	0.0171
0.0362	0.0004	0.0071	0.0138	0.0000	0.0000	0.0000	0.0175	0.0533	0.0067
0.0000	0.0046	0.0017	0.0012	0.0317	0.0296	0.0000	0.0000	0.0313	0.0000
0.0154	0.0000	0.0000	0.0401	0.0083	0.0029	0.0017	0.0000	0.0000	0.0362
0.0279	0.0000	0.0397	0.0033	0.0000	0.0025	0.0000	0.0183	0.0000	0.0017
0.0321	0.0117	0.0000	0.0262	0.0000	0.0000	0.0000	0.0004	0.0446	0.0150
0.0000	0.0088	0.0000	0.0000	0.0000	0.0050	0.0162	0.0000	0.0000	0.0000
0.0375	0.0000	0.0012	0.0385	0.0121	0.0000	0.0283	0.0063	0.0000	0.0000
0.0425	0.0000	0.0046	0.0483	0.0050	0.0004	0.0000	0.0000	0.0000	0.0000
0.0167	0.0000	0.0000	0.0113	0.0000	0.0017	0.0000	0.0392	0.0000	0.0626
0.0304	0.0012	0.0038	0.0012	0.0000	0.0000	0.0067	0.0000	0.0000	0.0000
0.0200	0.0021	0.0000	0.0354	0.0000	0.0000	0.0075	0.0350	0.0142	0.0012
0.0008	0.0138	0.0000	0.0096	0.0417	0.0000	0.0000	0.0100	0.0021	0.0004
0.0000	0.0000	0.0000	0.0000	0.0213	0.0150	0.0042	0.0004	0.0000	0.0000
0.0012	0.0000	0.0021	0.0237	0.0408	0.0000	0.0000	0.0000	0.0000	0.0000
0.0501	0.0000	0.0008	0.0021	0.0000	0.0000	0.0408	0.0000	0.0829	0.0000
0.0017	0.0042	0.0083	0.0133	0.0000	0.0000	0.0000	0.0000	0.0769	0.0371
0.0000	0.0000	0.0000	0.0079	0.0258	0.0000	0.0008	0.0000	0.0150	0.0435
0.0732	0.0000	0.0000	0.0490	0.0321	0.0000	0.0000	0.0000	0.0117	0.0204
0.0000	0.0000	0.0012	0.0000	0.0000	0.0000	0.0000	0.0075	0.0108	0.0651
0.0000	0.0054	0.0004	0.0133	0.0042	0.0308	0.0000	0.0117	0.0000	0.0397
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0000	0.0000	0.0162
0.0004	0.0000	0.0000	0.0000	0.0000	0.0714	0.0000	0.0096	0.0000	0.0050
0.0426	0.0000	0.0008	0.0000	0.0267	0.0358	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0129	0.0088	0.0267	0.0341	0.0017	0.0029	0.0162	0.0000
0.0000	0.0000	0.0929	0.0000	0.0000	0.0000	0.0000	0.0038	0.0038	0.0096
0.0000	0.0121	0.0025	0.0288	0.0021	0.0117	0.0012	0.0100	0.0300	0.0033
0.0000	0.0447	0.0012	0.0033	0.0167	0.0012	0.0588	0.0000	0.0096	0.0000
0.0133	0.0000	0.0000	0.0000	0.0000	0.0441	0.0346	0.0004	0.0444	0.0246
0.0000	0.0121	0.0271	0.0033	0.0237	0.0083	0.0138	0.0000	0.0250	0.0213
0.0067	0.0104	0.0158	0.0125	0.0012	0.0225	0.0296	0.0104	0.0441	0.0004
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000
0.0000	0.0000	0.0083	0.0607	0.0004	0.0938	0.0000	0.0300	0.0000	0.0000
0.0325	0.0572	0.0308	0.0000	0.0000	0.0000	0.0008	0.0058	0.0000	0.0000
0.0000	0.0525	0.0258	0.0008	0.0573	0.0000	0.0000	0.0000	0.0012	0.0000
0.0000	0.0000	0.0000	0.0162	0.0196	0.0000	0.0133	0.0117	0.0000	0.0000
0.0000	0.0000	0.0088	0.0250	0.0000	0.0000	0.0000	0.0000	0.0370	0.0004
0.0000	0.0000	0.0029	0.0000	0.0012	0.0000	0.0104	0.0000	0.0000	0.0012
0.0113	0.0004	0.0000	0.0012	0.0154	0.0237	0.0000	0.0254	0.0000	0.0313
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0042	0.0100	0.0150	0.0000
0.0079	0.0514	0.0004	0.0283	0.0233	0.0000	0.0108	0.0000	0.0004	0.0000
0.0595	0.0108	0.0000	0.0000	0.0000	0.0117	0.0000	0.0004	0.0029	0.0025
0.0096	0.0012	0.0021	0.0000	0.0129	0.0008	0.0000	0.0196	0.0008	0.0000
0.0225	0.0046	0.0092	0.0038	0.0100	0.0250	0.0566	0.0108	0.0000	0.0000
0.0096	0.0008	0.0012	0.0791	0.0000	0.0000	0.0000	0.0167	0.0000	0.0000
0.0000	0.0000	0.0133	0.0506	0.0000	0.0004	0.0346	0.0162	0.0088	0.0054
0.0058	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0192	0.0204	0.0021
0.0000	0.0033	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0325
0.0000	0.0000	0.0000	0.0025	0.0000	0.0250	0.0004	0.0000	0.0000	0.0425
0.0004	0.0000	0.0063	0.0054	0.0058	0.0346	0.0412	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000	0.0292	0.0067	0.0577
0.0000	0.0008	0.0000	0.0000	0.0000	0.0004	0.0000	0.0187	0.0503	0.0008
0.0000	0.0346	0.0283	0.0012	0.0121	0.0000	0.0000	0.0587	0.0283	0.0000
0.0113	0.0271	0.0000	0.0000	0.0008	0.0000	0.0017	0.0321	0.0050	0.0000
0.0000	0.0000	0.0535	0.0042	0.0000	0.0000	0.0850	0.0042	0.0100	0.0029
0.0000	0.0000	0.0000	0.0000	0.0000	0.0012	0.0117	0.0092	0.0008	0.0138
0.0008	0.0321	0.0000	0.0000	0.0653	0.0000	0.0008	0.0000	0.0250	0.0004
0.0500	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0433	0.0017	0.0117
0.0000	0.0004	0.0000	0.0000	0.0000	0.0271	0.0000	0.0050	0.0000	0.0104
0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0204	0.0000	0.0000	0.0083
0.0154	0.0138	0.0000	0.0275	0.0000	0.0042	0.0146	0.0008	0.0000	0.0004
0.0004	0.0383	0.0004	0.0000	0.0000	0.0283	0.0000	0.0050	0.0017	0.0000
0.0283	0.0100	0.0472	0.0000	0.0000	0.0250	0.0004	0.0117	0.0088	0.0208
0.0000	0.0000	0.0088	0.0012	0.0000	0.0000	0.0012	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0012	0.0000	0.0038	0.0000	0.0000	0.0000
0.0329	0.0000	0.0000	0.0000	0.0050	0.0167	0.0008	0.0162	0.0000	0.0258
0.0171	0.0000	0.0000	0.0017	0.0138	0.0000	0.0000	0.0275	0.0163	0.0038
0.0038	0.0012	0.0092	0.0088	0.0000	0.0004	0.0000	0.0000	0.0000	0.0063
0.0067	0.0012	0.0000	0.0000	0.0158	0.0000	0.0000	0.0213	0.0000	0.0000
0.0518	0.0008	0.0000	0.0000	0.0000	0.0017	0.0346	0.0004	0.0004	0.0000
0.0000	0.0092	0.0075	0.0000	0.0000	0.0121	0.0162	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0062	0.0100	0.0000	0.0000	0.0250	0.0058	0.0071
0.0283	0.0012	0.0000	0.0000	0.0000	0.0000	0.0694	0.0000	0.0021	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

0.0067	0.0000	0.0200	0.0063	0.0025	0.1032	0.0075	0.0038	0.0000	0.0000
0.0000	0.0000	0.0004	0.0279	0.0000	0.0000	0.0529	0.0017	0.0012	0.0000
0.0000	0.0346	0.0000	0.0092	0.0025	0.0000	0.0038	0.0000	0.0271	0.0017
0.0021	0.0000	0.0000	0.0162	0.0000	0.0008	0.0058	0.0513	0.0033	0.0456
0.0000	0.0000	0.0554	0.0025	0.0000	0.0217	0.0029	0.0000	0.0071	0.0000
0.0000	0.0258	0.0033	0.0112	0.0008	0.0046	0.0138	0.0279	0.0025	0.0000
0.0000	0.0000	0.0113	0.0000	0.0121	0.0017	0.0021	0.0213	0.0117	0.0000
0.0004	0.0000	0.0000	0.0171	0.0000	0.0046	0.0233	0.0004	0.0000	0.0133
0.0000	0.0607	0.0262	0.0000	0.0000	0.0458	0.0000	0.0138	0.0258	0.0029
0.0000	0.0004	0.0383	0.0033	0.0000	0.0000	0.0000	0.0000	0.0000	0.0113
0.0100	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0033
0.0250	0.0071	0.0229	0.0000	0.0000	0.0000	0.0473	0.0000	0.0104	0.0108
0.0004	0.0000	0.0000	0.0000	0.0008	0.0004	0.0000	0.0607	0.0262	0.0000
0.0453	0.0029	0.0000	0.0000	0.0192	0.0012	0.0004	0.0000	0.0333	0.0000
0.0004	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0158	0.0000
0.0042	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012	0.0000	0.0000	0.0000
0.0067	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0096	0.0362
0.0279	0.0088	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0204	0.0063
0.0012	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0025	0.0000	0.0000
0.0000	0.0000	0.0000	0.0017	0.0213	0.0046	0.0000	0.0393	0.0100	0.0071
0.0000	0.0058	0.0604	0.0129	0.0000	0.0004	0.0346	0.0004	0.0012	0.0012
0.0133	0.0012	0.0004	0.0362	0.0004	0.0008	0.0133	0.0000	0.0000	0.0283
0.0325	0.0000	0.0000	0.0162	0.0000	0.0000	0.0000	0.0271	0.0017	0.0000
0.0000	0.0042	0.0000	0.0000	0.0490	0.0125	0.0142	0.0054	0.0025	0.0000
0.0000	0.0000	0.0017	0.0300	0.0000	0.0000	0.0000	0.0329	0.0000	0.0000
0.0000	0.0000	0.0100	0.0175	0.0083	0.0121	0.0071	0.0000	0.0075	0.0217
0.0000	0.0079	0.0000	0.0000	0.0075	0.0167	0.0017	0.0000	0.0325	0.0042
0.0000	0.0000	0.0075	0.0292	0.0012	0.0000	0.0221	0.0000	0.0038	0.0113
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0017	0.0025
0.0096	0.0158	0.0183	0.0000	0.0000	0.0021	0.0000	0.0000	0.0067	0.0046
0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0033	0.0050	0.0012	0.0000
0.0042	0.0262	0.0000	0.0004	0.0171	0.0167	0.0000	0.0004	0.0000	0.0008
0.0000	0.0000	0.0313	0.0058	0.0033	0.0329	0.0162	0.0000	0.0054	0.0000
0.0029	0.0000	0.0146	0.0012	0.0054	0.0000	0.0000	0.0242	0.0000	0.0000
0.0000	0.0000	0.0000	0.0117	0.0000	0.0000	0.0008	0.0000	0.0000	0.0527
0.0000	0.0000	0.0167	0.0000	0.0000	0.0538	0.0033	0.0025	0.0088	0.0008
0.0000	0.0000	0.0008	0.0063	0.0000	0.0000	0.0000	0.0000	0.0021	0.0000
0.0000	0.0096	0.0000	0.0008	0.0042	0.0088	0.0012	0.0000	0.0204	0.0021
0.0004	0.0121	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0117	0.0296
0.0004	0.0000	0.0000	0.0000	0.0000	0.0354	0.0000	0.0000	0.0000	0.0233
0.0000	0.0208	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0217
0.0000	0.0054	0.0033	0.0208	0.0121	0.0012	0.0000	0.0000	0.0000	0.0012
0.0687	0.0183	0.0000	0.0008	0.0000	0.0233	0.0113	0.0362	0.0083	0.0021
0.0071	0.0000	0.0000	0.0112	0.0029	0.0000	0.0000	0.0004	0.0021	0.0125
0.0000	0.0000	0.0000	0.0000	0.0008	0.0021	0.0004	0.0000	0.0000	0.0042
0.0000	0.0000	0.0000	0.0108	0.0104	0.0275	0.0138	0.0237	0.0413	0.0021
0.0000	0.0000	0.0146	0.0000	0.0033	0.0000	0.0004	0.0793	0.0000	0.0104
0.0054	0.0100	0.0470	0.0000	0.0000	0.0000	0.0000	0.0058	0.0079	0.0000
0.0017	0.0000	0.0012	0.0000	0.0000	0.0000	0.0000	0.0021	0.0017	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0187	0.0000
0.0000	0.0017	0.0071	0.0096	0.0000	0.0012	0.0000	0.0000	0.0000	0.0321
0.0029	0.0308	0.0529	0.0000	0.0000	0.0021	0.0000	0.0000	0.0000	0.0033
0.0000	0.0275	0.0000	0.0000	0.0000	0.0000	0.0640	0.0058	0.0000	0.0025
0.1172	0.0004	0.0000	0.0050	0.0150	0.0354	0.0000	0.0008	0.0000	0.0008
0.0000	0.0000	0.0083	0.0017	0.0853	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0449	0.0054	0.0071	0.0000	0.0088	0.0038	0.0000	0.0000	0.0083
0.0000	0.0000	0.0029	0.0113	0.0350	0.0000	0.0000	0.0008	0.0017	0.0000
0.0012	0.0117	0.0058	0.0000	0.0000	0.0242	0.0000	0.0279	0.0000	0.0500
0.0008	0.0000	0.0000	0.0008	0.0104	0.0000	0.0000	0.0021	0.0000	0.0000
0.0017	0.0000	0.0000	0.0000	0.0288	0.0021	0.0021	0.0113	0.0000	0.0652
0.0000	0.0067	0.0008	0.0000	0.0000	0.0071	0.0063	0.0213	0.0000	0.0000
0.0046	0.0000	0.0213	0.1019	0.0000	0.0004	0.0050	0.0175	0.0233	0.0000
0.0117	0.0337	0.0000	0.0000	0.0233	0.0000	0.0000	0.0000	0.0192	0.0008
0.0017	0.0000	0.0000	0.0075	0.0229	0.0000	0.0046	0.0100	0.0125	0.0389
0.0000	0.0100	0.0042	0.0292	0.0390	0.0000	0.0346	0.0029	0.0033	0.0000
0.0008	0.0000	0.0000	0.0071	0.0000	0.0175	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0038	0.0000	0.0714	0.0000	0.0271	0.0125	0.0000
0.0000	0.0217	0.0629	0.0296	0.0000	0.0008	0.1019	0.0008	0.0108	0.0192
0.0000	0.0033	0.0208	0.0313	0.0000	0.0129	0.0058	0.0000	0.0399	0.0393
0.0000	0.0233	0.0000	0.0029	0.0000	0.0000	0.0063	0.0017	0.0046	0.0525
0.0557	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012	0.0104	0.0000	0.0000
0.0054	0.0000	0.0117	0.0000	0.0004	0.0000	0.0271	0.0000	0.0000	0.0000
0.0000	0.0000	0.0506	0.0000	0.0004	0.0000	0.0267	0.0000	0.0000	0.0393
0.0000	0.0000	0.0000	0.0233	0.0017	0.0000	0.0000	0.0000	0.0025	0.0008
0.0033	0.0125	0.0004	0.0050	0.0254	0.0125	0.0000	0.0104	0.0000	0.0557
0.0000	0.0037	0.0088	0.0581	0.0000	0.0000	0.0000	0.0000	0.0117	0.0012

0.0075	0.0304	0.0000	0.0133	0.0021	0.0008	0.0113	0.0017	0.0000	0.0000
0.0401	0.0000	0.0000	0.0000	0.0071	0.0000	0.0000	0.0033	0.0038	0.0296
0.0000	0.0000	0.0000	0.0017	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0254	0.0000	0.0000	0.0000	0.0029	0.0058	0.0648
0.0000	0.0449	0.0079	0.0000	0.0150	0.0000	0.0000	0.0000	0.0000	0.0033
0.0017	0.0038	0.0012	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000
0.0595	0.0008	0.0021	0.0150	0.0000	0.0058	0.0000	0.0000	0.0000	0.0354
0.0000	0.0113	0.0012	0.0075	0.0017	0.0229	0.0000	0.0221	0.1014	0.0029
0.0075	0.0000	0.0000	0.0000	0.0000	0.0650	0.0008	0.0071	0.0509	0.0067
0.0000	0.0242	0.0100	0.0000	0.0000	0.0025	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0283	0.0000	0.0000	0.0459	0.0000	0.0000	0.0000
0.0246	0.0067	0.0000	0.0000	0.0146	0.0000	0.0000	0.0246	0.0000	0.0012
0.0192	0.0063	0.0033	0.0000	0.0000	0.0000	0.0419	0.0000	0.0154	0.0000
0.0453	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0017	0.0000	0.0333	0.0000	0.0000	0.0000	0.0000	0.0000	0.0337
0.0000	0.0000	0.0142	0.0000	0.0012	0.0000	0.0000	0.0012	0.0000	0.0366
0.0478	0.0300	0.0000	0.0021	0.0406	0.0008	0.0000	0.0054	0.0008	0.0071
0.0092	0.0163	0.0687	0.0017	0.0000	0.0000	0.0000	0.0208	0.0100	0.0000
0.0004	0.0179	0.0175	0.0000	0.0108	0.0000	0.0054	0.0000	0.0000	0.0067
0.0004	0.0000	0.0000	0.0000	0.0000	0.0021	0.0000	0.0083	0.0179	0.0000
0.0054	0.0204	0.0029	0.0158	0.0000	0.0000	0.0553	0.0000	0.0000	0.0000
0.0000	0.0133	0.0000	0.0208	0.0000	0.0004	0.0046	0.0092	0.0000	0.0108
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0071	0.0541	0.0486	0.0000
0.0075	0.0000	0.0029	0.0187	0.0000	0.0000	0.0125	0.0000	0.0004	0.0183
0.0421	0.0000	0.0457	0.0038	0.0000	0.0008	0.0000	0.0033	0.0000	0.0021
0.0667	0.0008	0.0000	0.0004	0.0000	0.0021	0.0370	0.0000	0.0000	0.0000
0.0000	0.0000	0.0071	0.0079	0.0017	0.0000	0.0150	0.0000	0.0175	0.0358
0.0000	0.0033	0.0000	0.0063	0.0108	0.0000	0.0000	0.0000	0.0021	0.0000
0.0237	0.0217	0.0275	0.0050	0.0000	0.0242	0.0200	0.0046	0.0250	0.0050
0.0821	0.0490	0.0021	0.0071	0.0292	0.0000	0.0008	0.0117	0.0000	0.0288
0.0079	0.0054	0.0000	0.0000	0.0000	0.0017	0.0000	0.0000	0.0008	0.1667
0.0129	0.0079	0.0000	0.0000	0.0000	0.0000	0.0208	0.0000	0.0000	0.0000
0.0000	0.0183	0.0000	0.0288	0.0121	0.0000	0.0100	0.0000	0.0004	0.0033
0.0000	0.0000	0.0054	0.0129	0.0000	0.0000	0.0000	0.0000	0.0000	0.0225
0.0354	0.0187	0.0096	0.0000	0.0063	0.0058	0.0000	0.0142	0.0033	0.0000
0.0000	0.0000	0.0000	0.0025	0.0000	0.0000	0.0083	0.0325	0.0538	0.0000

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PRINTOUT FREQUENCY          = 200
NATURE OF THE SUBSTRATE     = BENZENE
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FUGACITY COEFFICIENT	=	0.8300E+02	ML/GR
LONGITUDINAL SOIL DISPERSIVITY	=	0.2000	FT
TRANSVERSE SOIL DISPERSIVITY	=	0.0200	FT
FIRST ORDER ADSORPTION COEFFICIENT	=	0.4150E+00	ML/GR
FIRST ORDER DESORPTION COEFFICIENT	=	0.0000E+00	ML/GR 1/DAY
BULK WATER DIFFUSION COEFFICIENT	=	0.6950E-04	M2/DAY
BULK AIR DIFFUSION COEFFICIENT	=	0.8310E+00	M2/DAY
HENRY'S CONSTANT	=	0.2330	
SOIL BULK DENSITY	=	0.1500E+01	GR/CM3

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***** RESULTS *****

MONTHLY MEAN TEMPERATURES (F)

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

CN = 72.
 THF = 10.00 (%)
 THW = 7.00 (%)
 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

COMPUTED AVERAGE DAILY EVAPOTRANSPIRATION FOR TIME STEP 200 = 0.4111E-04 FT/DAY (2/ 3/1960)

CONCENTRATION DISTRIBUTION AT 400. DAYS MG/L

0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00					
0.2050E-01	0.2102E-01	0.2240E-01	0.2410E-01	0.2547E-01	0.2600E-01	0.2547E-01	0.2410E-01
0.2240E-01	0.2102E-01	0.2050E-01					
0.5665E-01	0.5810E-01	0.6192E-01	0.6664E-01	0.7046E-01	0.7192E-01	0.7046E-01	0.6664E-01
0.6192E-01	0.5810E-01	0.5665E-01					
0.1094E+00	0.1122E+00	0.1197E+00	0.1288E+00	0.1362E+00	0.1390E+00	0.1362E+00	0.1288E+00
0.1197E+00	0.1122E+00	0.1094E+00					
0.1744E+00	0.1789E+00	0.1907E+00	0.2053E+00	0.2171E+00	0.2217E+00	0.2171E+00	0.2053E+00
0.1907E+00	0.1789E+00	0.1744E+00					
0.2437E+00	0.2500E+00	0.2665E+00	0.2869E+00	0.3034E+00	0.3097E+00	0.3034E+00	0.2869E+00
0.2665E+00	0.2500E+00	0.2437E+00					
0.3077E+00	0.3156E+00	0.3364E+00	0.3620E+00	0.3827E+00	0.3907E+00	0.3827E+00	0.3620E+00
0.3364E+00	0.3156E+00	0.3077E+00					
0.3563E+00	0.3654E+00	0.3892E+00	0.4187E+00	0.4425E+00	0.4517E+00	0.4425E+00	0.4187E+00
0.3892E+00	0.3654E+00	0.3563E+00					
0.3812E+00	0.3908E+00	0.4161E+00	0.4473E+00	0.4726E+00	0.4823E+00	0.4726E+00	0.4473E+00
0.4161E+00	0.3908E+00	0.3812E+00					

0.3784E+00	0.3879E+00	0.4127E+00	0.4434E+00	0.4682E+00	0.4777E+00	0.4682E+00	0.4434E+00
0.4127E+00	0.3879E+00	0.3784E+00					
0.3495E+00	0.3581E+00	0.3807E+00	0.4087E+00	0.4313E+00	0.4399E+00	0.4313E+00	0.4087E+00
0.3807E+00	0.3581E+00	0.3495E+00					
0.3008E+00	0.3081E+00	0.3273E+00	0.3510E+00	0.3702E+00	0.3775E+00	0.3702E+00	0.3510E+00
0.3273E+00	0.3081E+00	0.3008E+00					
0.2416E+00	0.2474E+00	0.2626E+00	0.2814E+00	0.2966E+00	0.3024E+00	0.2966E+00	0.2814E+00
0.2626E+00	0.2474E+00	0.2416E+00					
0.1815E+00	0.1858E+00	0.1970E+00	0.2109E+00	0.2222E+00	0.2265E+00	0.2222E+00	0.2109E+00
0.1970E+00	0.1858E+00	0.1815E+00					
0.1277E+00	0.1307E+00	0.1385E+00	0.1481E+00	0.1559E+00	0.1588E+00	0.1559E+00	0.1481E+00
0.1385E+00	0.1307E+00	0.1277E+00					
0.8429E-01	0.8622E-01	0.9128E-01	0.9753E-01	0.1026E+00	0.1045E+00	0.1026E+00	0.9753E-01
0.9128E-01	0.8622E-01	0.8429E-01					
0.5225E-01	0.5343E-01	0.5652E-01	0.6034E-01	0.6343E-01	0.6461E-01	0.6343E-01	0.6034E-01
0.5652E-01	0.5343E-01	0.5225E-01					
0.3038E-01	0.3106E-01	0.3283E-01	0.3502E-01	0.3679E-01	0.3746E-01	0.3679E-01	0.3502E-01
0.3283E-01	0.3106E-01	0.3038E-01					
0.1636E-01	0.1672E-01	0.1766E-01	0.1882E-01	0.1976E-01	0.2012E-01	0.1976E-01	0.1882E-01
0.1766E-01	0.1672E-01	0.1636E-01					
0.7550E-02	0.7714E-02	0.8145E-02	0.8676E-02	0.9106E-02	0.9271E-02	0.9106E-02	0.8676E-02
0.8145E-02	0.7714E-02	0.7550E-02					
0.1309E-02	0.1337E-02	0.1410E-02	0.1500E-02	0.1573E-02	0.1601E-02	0.1573E-02	0.1500E-02
0.1410E-02	0.1337E-02	0.1309E-02					

COMPUTED AVERAGE DAILY EVAPOTRANSPIRATION FOR TIME STEP 400 = 0.1588E-02 FT/DAY (3/ 9/1961)

CONCENTRATION DISTRIBUTION AT 800. DAYS MG/L

0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00					
0.1069E-01	0.1069E-01	0.1079E-01	0.1092E-01	0.1102E-01	0.1106E-01	0.1102E-01	0.1092E-01
0.1079E-01	0.1069E-01	0.1065E-01					
0.3112E-01	0.3123E-01	0.3153E-01	0.3189E-01	0.3219E-01	0.3230E-01	0.3219E-01	0.3189E-01
0.3153E-01	0.3123E-01	0.3112E-01					
0.6113E-01	0.6135E-01	0.6194E-01	0.6267E-01	0.6326E-01	0.6348E-01	0.6326E-01	0.6267E-01
0.6194E-01	0.6135E-01	0.6113E-01					
0.9919E-01	0.9956E-01	0.1005E+00	0.1017E+00	0.1027E+00	0.1031E+00	0.1027E+00	0.1017E+00
0.1005E+00	0.9956E-01	0.9919E-01					
0.1429E+00	0.1434E+00	0.1448E+00	0.1466E+00	0.1480E+00	0.1485E+00	0.1480E+00	0.1466E+00
0.1448E+00	0.1434E+00	0.1429E+00					
0.1891E+00	0.1898E+00	0.1917E+00	0.1940E+00	0.1958E+00	0.1965E+00	0.1958E+00	0.1940E+00
0.1917E+00	0.1898E+00	0.1891E+00					
0.2338E+00	0.2347E+00	0.2370E+00	0.2399E+00	0.2422E+00	0.2431E+00	0.2422E+00	0.2399E+00
0.2370E+00	0.2347E+00	0.2338E+00					
0.2730E+00	0.2740E+00	0.2767E+00	0.2801E+00	0.2828E+00	0.2838E+00	0.2828E+00	0.2801E+00
0.2767E+00	0.2740E+00	0.2730E+00					
0.3025E+00	0.3037E+00	0.3067E+00	0.3104E+00	0.3134E+00	0.3146E+00	0.3134E+00	0.3104E+00
0.3067E+00	0.3037E+00	0.3025E+00					
0.3194E+00	0.3206E+00	0.3238E+00	0.3277E+00	0.3309E+00	0.3321E+00	0.3309E+00	0.3277E+00
0.3238E+00	0.3206E+00	0.3194E+00					
0.3219E+00	0.3231E+00	0.3263E+00	0.3303E+00	0.3335E+00	0.3347E+00	0.3335E+00	0.3303E+00
0.3263E+00	0.3231E+00	0.3219E+00					
0.3102E+00	0.3114E+00	0.3144E+00	0.3182E+00	0.3213E+00	0.3225E+00	0.3213E+00	0.3182E+00
0.3144E+00	0.3114E+00	0.3102E+00					
0.2861E+00	0.2872E+00	0.2900E+00	0.2935E+00	0.2963E+00	0.2974E+00	0.2963E+00	0.2935E+00
0.2900E+00	0.2872E+00	0.2861E+00					
0.2528E+00	0.2538E+00	0.2563E+00	0.2593E+00	0.2618E+00	0.2628E+00	0.2618E+00	0.2593E+00
0.2563E+00	0.2538E+00	0.2528E+00					
0.2141E+00	0.2149E+00	0.2170E+00	0.2196E+00	0.2217E+00	0.2225E+00	0.2217E+00	0.2196E+00
0.2170E+00	0.2149E+00	0.2141E+00					
0.1737E+00	0.1743E+00	0.1760E+00	0.1781E+00	0.1798E+00	0.1804E+00	0.1798E+00	0.1781E+00
0.1760E+00	0.1743E+00	0.1737E+00					
0.1345E+00	0.1350E+00	0.1363E+00	0.1379E+00	0.1392E+00	0.1397E+00	0.1392E+00	0.1379E+00
0.1363E+00	0.1350E+00	0.1345E+00					
0.9851E-01	0.9887E-01	0.9981E-01	0.1010E+00	0.1019E+00	0.1023E+00	0.1019E+00	0.1010E+00
0.9981E-01	0.9887E-01	0.9851E-01					
0.6607E-01	0.6630E-01	0.6693E-01	0.6771E-01	0.6833E-01	0.6857E-01	0.6833E-01	0.6771E-01
0.6693E-01	0.6630E-01	0.6607E-01					
0.3602E-01	0.3615E-01	0.3649E-01	0.3691E-01	0.3724E-01	0.3737E-01	0.3724E-01	0.3691E-01
0.3649E-01	0.3615E-01	0.3602E-01					

COMPUTED AVERAGE DAILY EVAPOTRANSPIRATION FOR TIME STEP 600 = 0.4989E-02 FT/DAY (4/13/1962)

CONCENTRATION DISTRIBUTION AT 1200. DAYS MG/L

0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00					
0.5780E-02	0.5783E-02	0.5792E-02	0.5803E-02	0.5812E-02	0.5816E-02	0.5812E-02	0.5803E-02
0.5792E-02	0.5783E-02	0.5780E-02					
0.1669E-01	0.1670E-01	0.1672E-01	0.1676E-01	0.1678E-01	0.1679E-01	0.1678E-01	0.1676E-01
0.1672E-01	0.1670E-01	0.1669E-01					
0.3284E-01	0.3286E-01	0.3291E-01	0.3298E-01	0.3303E-01	0.3305E-01	0.3303E-01	0.3298E-01
0.3291E-01	0.3286E-01	0.3284E-01					
0.5401E-01	0.5405E-01	0.5414E-01	0.5424E-01	0.5433E-01	0.5436E-01	0.5433E-01	0.5424E-01
0.5414E-01	0.5405E-01	0.5401E-01					
0.7977E-01	0.7982E-01	0.7995E-01	0.8011E-01	0.8024E-01	0.8029E-01	0.8024E-01	0.8011E-01
0.7995E-01	0.7982E-01	0.7977E-01					
0.1093E+00	0.1094E+00	0.1096E+00	0.1098E+00	0.1100E+00	0.1100E+00	0.1100E+00	0.1098E+00
0.1096E+00	0.1094E+00	0.1093E+00					
0.1413E+00	0.1414E+00	0.1417E+00	0.1419E+00	0.1422E+00	0.1423E+00	0.1422E+00	0.1419E+00
0.1417E+00	0.1414E+00	0.1413E+00					
0.1740E+00	0.1742E+00	0.1745E+00	0.1748E+00	0.1751E+00	0.1752E+00	0.1751E+00	0.1748E+00
0.1745E+00	0.1742E+00	0.1740E+00					
0.2053E+00	0.2054E+00	0.2058E+00	0.2062E+00	0.2066E+00	0.2067E+00	0.2066E+00	0.2062E+00
0.2058E+00	0.2054E+00	0.2053E+00					
0.2328E+00	0.2329E+00	0.2334E+00	0.2339E+00	0.2343E+00	0.2344E+00	0.2343E+00	0.2339E+00
0.2334E+00	0.2329E+00	0.2328E+00					
0.2544E+00	0.2545E+00	0.2550E+00	0.2555E+00	0.2560E+00	0.2561E+00	0.2560E+00	0.2555E+00
0.2550E+00	0.2545E+00	0.2544E+00					
0.2683E+00	0.2685E+00	0.2689E+00	0.2695E+00	0.2700E+00	0.2702E+00	0.2700E+00	0.2695E+00
0.2689E+00	0.2685E+00	0.2683E+00					
0.2735E+00	0.2737E+00	0.2741E+00	0.2747E+00	0.2752E+00	0.2754E+00	0.2752E+00	0.2747E+00
0.2741E+00	0.2737E+00	0.2735E+00					
0.2696E+00	0.2698E+00	0.2703E+00	0.2709E+00	0.2713E+00	0.2715E+00	0.2713E+00	0.2709E+00
0.2703E+00	0.2698E+00	0.2696E+00					
0.2572E+00	0.2574E+00	0.2578E+00	0.2584E+00	0.2588E+00	0.2590E+00	0.2588E+00	0.2584E+00
0.2578E+00	0.2574E+00	0.2572E+00					
0.2373E+00	0.2375E+00	0.2379E+00	0.2384E+00	0.2388E+00	0.2390E+00	0.2388E+00	0.2384E+00
0.2379E+00	0.2375E+00	0.2373E+00					
0.2115E+00	0.2116E+00	0.2120E+00	0.2124E+00	0.2128E+00	0.2130E+00	0.2128E+00	0.2124E+00
0.2120E+00	0.2116E+00	0.2115E+00					
0.1813E+00	0.1814E+00	0.1818E+00	0.1822E+00	0.1825E+00	0.1826E+00	0.1825E+00	0.1822E+00
0.1818E+00	0.1814E+00	0.1813E+00					
0.1484E+00	0.1485E+00	0.1488E+00	0.1491E+00	0.1494E+00	0.1495E+00	0.1494E+00	0.1491E+00
0.1488E+00	0.1485E+00	0.1484E+00					
0.1144E+00	0.1145E+00	0.1147E+00	0.1149E+00	0.1151E+00	0.1152E+00	0.1151E+00	0.1149E+00
0.1147E+00	0.1145E+00	0.1144E+00					

COMPUTED AVERAGE DAILY EVAPOTRANSPIRATION FOR TIME STEP 800 = 0.9730E-02 FT/DAY (5/18/1963)

CONCENTRATION DISTRIBUTION AT 1600. DAYS MG/L

0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00					
0.7241E-02	0.7241E-02	0.7243E-02	0.7245E-02	0.7246E-02	0.7246E-02	0.7246E-02	0.7245E-02
0.7243E-02	0.7241E-02	0.7241E-02					
0.1649E-01	0.1649E-01	0.1649E-01	0.1650E-01	0.1650E-01	0.1650E-01	0.1650E-01	0.1650E-01
0.1649E-01	0.1649E-01	0.1649E-01					
0.2849E-01	0.2850E-01	0.2850E-01	0.2851E-01	0.2852E-01	0.2852E-01	0.2852E-01	0.2851E-01
0.2850E-01	0.2850E-01	0.2849E-01					
0.4363E-01	0.4364E-01	0.4365E-01	0.4366E-01	0.4367E-01	0.4367E-01	0.4367E-01	0.4366E-01
0.4365E-01	0.4364E-01	0.4363E-01					
0.6179E-01	0.6180E-01	0.6181E-01	0.6183E-01	0.6184E-01	0.6185E-01	0.6184E-01	0.6183E-01
0.6181E-01	0.6180E-01	0.6179E-01					
0.8257E-01	0.8257E-01	0.8259E-01	0.8261E-01	0.8263E-01	0.8264E-01	0.8263E-01	0.8261E-01
0.8259E-01	0.8257E-01	0.8257E-01					
0.1053E+00	0.1053E+00	0.1053E+00	0.1054E+00	0.1054E+00	0.1054E+00	0.1054E+00	0.1054E+00
0.1053E+00	0.1053E+00	0.1053E+00					
0.1291E+00	0.1291E+00	0.1292E+00	0.1292E+00	0.1292E+00	0.1292E+00	0.1292E+00	0.1292E+00
0.1292E+00	0.1291E+00	0.1291E+00					
0.1530E+00	0.1531E+00	0.1531E+00	0.1531E+00	0.1532E+00	0.1532E+00	0.1532E+00	0.1531E+00
0.1531E+00	0.1531E+00	0.1530E+00					
0.1759E+00	0.1759E+00	0.1760E+00	0.1760E+00	0.1761E+00	0.1761E+00	0.1761E+00	0.1760E+00
0.1760E+00	0.1759E+00	0.1759E+00					
0.1965E+00	0.1965E+00	0.1966E+00	0.1967E+00	0.1967E+00	0.1967E+00	0.1967E+00	0.1967E+00

0.1966E+00	0.1965E+00	0.1965E+00					
0.2136E+00	0.2136E+00	0.2137E+00	0.2138E+00	0.2138E+00	0.2138E+00	0.2138E+00	0.2138E+00
0.2137E+00	0.2136E+00	0.2136E+00					
0.2262E+00	0.2262E+00	0.2262E+00	0.2263E+00	0.2264E+00	0.2264E+00	0.2264E+00	0.2263E+00
0.2262E+00	0.2262E+00	0.2262E+00					
0.2333E+00	0.2333E+00	0.2334E+00	0.2334E+00	0.2335E+00	0.2335E+00	0.2335E+00	0.2334E+00
0.2334E+00	0.2333E+00	0.2333E+00					
0.2345E+00	0.2345E+00	0.2346E+00	0.2347E+00	0.2347E+00	0.2348E+00	0.2347E+00	0.2347E+00
0.2346E+00	0.2345E+00	0.2345E+00					
0.2298E+00	0.2298E+00	0.2299E+00	0.2299E+00	0.2300E+00	0.2300E+00	0.2300E+00	0.2299E+00
0.2299E+00	0.2298E+00	0.2298E+00					
0.2193E+00	0.2193E+00	0.2194E+00	0.2195E+00	0.2195E+00	0.2195E+00	0.2195E+00	0.2195E+00
0.2194E+00	0.2193E+00	0.2193E+00					
0.2039E+00	0.2039E+00	0.2039E+00	0.2040E+00	0.2040E+00	0.2041E+00	0.2040E+00	0.2040E+00
0.2039E+00	0.2039E+00	0.2039E+00					
0.1845E+00	0.1846E+00	0.1846E+00	0.1847E+00	0.1847E+00	0.1847E+00	0.1847E+00	0.1847E+00
0.1846E+00	0.1846E+00	0.1845E+00					
0.1631E+00	0.1631E+00	0.1631E+00	0.1632E+00	0.1632E+00	0.1632E+00	0.1632E+00	0.1632E+00
0.1631E+00	0.1631E+00	0.1631E+00					

COMPUTED AVERAGE DAILY EVAPOTRANSPIRATION FOR TIME STEP 1000 = 0.1073E-01 FT/DAY (6/21/1964)

CONCENTRATION DISTRIBUTION AT 2000. DAYS MG/L

0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00					
0.3837E-02	0.3838E-02	0.3838E-02	0.3838E-02	0.3838E-02	0.3838E-02	0.3838E-02	0.3838E-02
0.3838E-02	0.3838E-02	0.3837E-02					
0.1129E-01	0.1129E-01	0.1129E-01	0.1129E-01	0.1129E-01	0.1129E-01	0.1129E-01	0.1129E-01
0.1129E-01	0.1129E-01	0.1129E-01					
0.2100E-01	0.2100E-01	0.2100E-01	0.2100E-01	0.2100E-01	0.2100E-01	0.2100E-01	0.2100E-01
0.2100E-01	0.2100E-01	0.2100E-01					
0.3297E-01	0.3297E-01	0.3297E-01	0.3297E-01	0.3297E-01	0.3297E-01	0.3297E-01	0.3297E-01
0.3297E-01	0.3297E-01	0.3297E-01					
0.4732E-01	0.4732E-01	0.4732E-01	0.4732E-01	0.4732E-01	0.4732E-01	0.4732E-01	0.4732E-01
0.4732E-01	0.4732E-01	0.4732E-01					
0.6371E-01	0.6371E-01	0.6371E-01	0.6371E-01	0.6371E-01	0.6371E-01	0.6371E-01	0.6371E-01
0.6371E-01	0.6371E-01	0.6371E-01					
0.8159E-01	0.8159E-01	0.8160E-01	0.8160E-01	0.8160E-01	0.8160E-01	0.8160E-01	0.8160E-01
0.8160E-01	0.8159E-01	0.8159E-01					
0.1004E+00	0.1004E+00	0.1004E+00	0.1004E+00	0.1004E+00	0.1004E+00	0.1004E+00	0.1004E+00
0.1004E+00	0.1004E+00	0.1004E+00					
0.1195E+00	0.1195E+00	0.1195E+00	0.1195E+00	0.1195E+00	0.1195E+00	0.1195E+00	0.1195E+00
0.1195E+00	0.1195E+00	0.1195E+00					
0.1383E+00	0.1383E+00	0.1383E+00	0.1383E+00	0.1383E+00	0.1383E+00	0.1383E+00	0.1383E+00
0.1383E+00	0.1383E+00	0.1383E+00					
0.1561E+00	0.1561E+00	0.1561E+00	0.1561E+00	0.1561E+00	0.1561E+00	0.1561E+00	0.1561E+00
0.1561E+00	0.1561E+00	0.1561E+00					
0.1721E+00	0.1721E+00	0.1721E+00	0.1721E+00	0.1721E+00	0.1721E+00	0.1721E+00	0.1721E+00
0.1721E+00	0.1721E+00	0.1721E+00					
0.1857E+00	0.1857E+00	0.1857E+00	0.1857E+00	0.1857E+00	0.1857E+00	0.1857E+00	0.1857E+00
0.1857E+00	0.1857E+00	0.1857E+00					
0.1960E+00	0.1960E+00	0.1960E+00	0.1960E+00	0.1960E+00	0.1960E+00	0.1960E+00	0.1960E+00
0.1960E+00	0.1960E+00	0.1960E+00					
0.2027E+00	0.2027E+00	0.2027E+00	0.2027E+00	0.2027E+00	0.2027E+00	0.2027E+00	0.2027E+00
0.2027E+00	0.2027E+00	0.2027E+00					
0.2055E+00	0.2055E+00	0.2055E+00	0.2055E+00	0.2055E+00	0.2055E+00	0.2055E+00	0.2055E+00
0.2055E+00	0.2055E+00	0.2055E+00					
0.2043E+00	0.2043E+00	0.2043E+00	0.2043E+00	0.2043E+00	0.2043E+00	0.2043E+00	0.2043E+00
0.2043E+00	0.2043E+00	0.2043E+00					
0.1995E+00	0.1995E+00	0.1995E+00	0.1995E+00	0.1995E+00	0.1995E+00	0.1995E+00	0.1995E+00
0.1995E+00	0.1995E+00	0.1995E+00					
0.1918E+00	0.1918E+00	0.1918E+00	0.1918E+00	0.1918E+00	0.1918E+00	0.1918E+00	0.1918E+00
0.1918E+00	0.1918E+00	0.1918E+00					
0.1825E+00	0.1825E+00	0.1825E+00	0.1825E+00	0.1825E+00	0.1825E+00	0.1825E+00	0.1825E+00
0.1825E+00	0.1825E+00	0.1825E+00					

COMPUTED AVERAGE DAILY EVAPOTRANSPIRATION FOR TIME STEP 1200 = 0.1141E-01 FT/DAY (7/26/1965)

CONCENTRATION DISTRIBUTION AT 2400. DAYS MG/L

0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
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COMPUTED AVERAGE DAILY EVAPOTRANSPIRATION FOR TIME STEP 1400 = 0.9420E-02 FT/DAY (8/30/1966)

[illegible]

COMPUTED AVERAGE DAILY EVAPOTRANSPIRATION FOR TIME STEP 1600 = 0.5594E-02 FT/DAY (10/ 4/1967)

[illegible]

0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00					
0.2467E-02	0.2467E-02	0.2467E-02	0.2467E-02	0.2467E-02	0.2467E-02	0.2467E-02	0.2467E-02
0.2467E-02	0.2467E-02	0.2467E-02					
0.6063E-02	0.6063E-02	0.6063E-02	0.6063E-02	0.6063E-02	0.6063E-02	0.6063E-02	0.6063E-02
0.6063E-02	0.6063E-02	0.6063E-02					

COMPUTED AVERAGE DAILY EVAPOTRANSPIRATION FOR TIME STEP 2000 = 0.3348E-03 FT/DAY (12/12/1969)

[illegible]

0.1102E+00	0.1102E+00	0.1102E+00					
0.1203E+00	0.1203E+00	0.1203E+00	0.1203E+00	0.1203E+00	0.1203E+00	0.1203E+00	0.1203E+00
0.1203E+00	0.1203E+00	0.1203E+00					
0.1304E+00	0.1304E+00	0.1304E+00	0.1304E+00	0.1304E+00	0.1304E+00	0.1304E+00	0.1304E+00
0.1304E+00	0.1304E+00	0.1304E+00					
0.1403E+00	0.1403E+00	0.1403E+00	0.1403E+00	0.1403E+00	0.1403E+00	0.1403E+00	0.1403E+00
0.1403E+00	0.1403E+00	0.1403E+00					
0.1503E+00	0.1503E+00	0.1503E+00	0.1503E+00	0.1503E+00	0.1503E+00	0.1503E+00	0.1503E+00
0.1503E+00	0.1503E+00	0.1503E+00					

SATURATED ZONE TRANSPORT PARAMETERS

AQUIFER VELOCITY----- = 0.2000 FT/DAY
LONGITUDINAL DISPERSION COEFFICIENT----- = 0.5000 FT2/DAY
TRANSVERSE DISPERSION COEFFICIENT----- = 0.0500 FT2/DAY
HALF LENGTH SOURCE----- = 5.0000 FT
AQUIFER THICKNESS----- = 10.0000 FT

FIRST ORDER DECAY COEFFICIENT----- = 0.0000 1/DAY
RETARDATION FACTOR----- = 1.0000

TOTAL NUMBER OF X POSITIONS----- = 7
TOTAL NUMBER OF Y POSITIONS----- = 3
TOTAL NUMBER OF SIMULATIONS----- = 10

FOR TIME = 500. DAYS

X FT	Y FT	CONCENTRATION (ppm)
0.00	0.00	0.000000
0.00	5.00	0.000000
0.00	10.00	0.000000
2.50	0.00	0.000000
2.50	5.00	0.000000
2.50	10.00	0.000000
5.00	0.00	0.000000
5.00	5.00	0.000000
5.00	10.00	0.000000
10.00	0.00	0.000000
10.00	5.00	0.000000
10.00	10.00	0.000000
50.00	0.00	0.000007
50.00	5.00	0.000006
50.00	10.00	0.000005
100.00	0.00	0.000079
100.00	5.00	0.000069
100.00	10.00	0.000057
500.00	0.00	0.000000
500.00	5.00	0.000000
500.00	10.00	0.000000

FOR TIME = 1000. DAYS

X FT	Y FT	CONCENTRATION (ppm)
0.00	0.00	0.000000
0.00	5.00	0.000000
0.00	10.00	0.000000
2.50	0.00	0.000000
2.50	5.00	0.000000
2.50	10.00	0.000000
5.00	0.00	0.000000
5.00	5.00	0.000000
5.00	10.00	0.000000
10.00	0.00	0.000000
10.00	5.00	0.000000
10.00	10.00	0.000000
50.00	0.00	0.000041
50.00	5.00	0.000038
50.00	10.00	0.000035
100.00	0.00	0.001665

100.00	5.00	0.001552
100.00	10.00	0.001397
500.00	0.00	0.000000
500.00	5.00	0.000000
500.00	10.00	0.000000

FOR TIME = 1500. DAYS

X FT	Y FT	CONCENTRATION (ppm)
0.00	0.00	0.000000
0.00	5.00	0.000000
0.00	10.00	0.000000
2.50	0.00	0.000000
2.50	5.00	0.000000
2.50	10.00	0.000000
5.00	0.00	0.000000
5.00	5.00	0.000000
5.00	10.00	0.000000
10.00	0.00	0.000000
10.00	5.00	0.000000
10.00	10.00	0.000000
50.00	0.00	0.000020
50.00	5.00	0.000020
50.00	10.00	0.000019
100.00	0.00	0.002003
100.00	5.00	0.001964
100.00	10.00	0.001855
500.00	0.00	0.000000
500.00	5.00	0.000000
500.00	10.00	0.000000

FOR TIME = 2000. DAYS

X FT	Y FT	CONCENTRATION (ppm)
0.00	0.00	0.000000
0.00	5.00	0.000000
0.00	10.00	0.000000
2.50	0.00	0.000000
2.50	5.00	0.000000
2.50	10.00	0.000000
5.00	0.00	0.000000
5.00	5.00	0.000000
5.00	10.00	0.000000
10.00	0.00	0.000000
10.00	5.00	0.000000
10.00	10.00	0.000000
50.00	0.00	0.000002
50.00	5.00	0.000002
50.00	10.00	0.000002
100.00	0.00	0.000387
100.00	5.00	0.000394
100.00	10.00	0.000383
500.00	0.00	0.000002
500.00	5.00	0.000003
500.00	10.00	0.000003

FOR TIME = 2500. DAYS

X FT	Y FT	CONCENTRATION (ppm)
0.00	0.00	0.000000
0.00	5.00	0.000000
0.00	10.00	0.000000
2.50	0.00	0.000000
2.50	5.00	0.000000
2.50	10.00	0.000000
5.00	0.00	0.000000
5.00	5.00	0.000000
5.00	10.00	0.000000
10.00	0.00	0.000001
10.00	5.00	0.000001
10.00	10.00	0.000001
50.00	0.00	0.000285
50.00	5.00	0.000248
50.00	10.00	0.000206
100.00	0.00	0.003437
100.00	5.00	0.003003

100.00	10.00	0.002516
500.00	0.00	0.000219
500.00	5.00	0.000242
500.00	10.00	0.000249

FOR TIME = 3000. DAYS

X FT	Y FT	CONCENTRATION (ppm)
0.00	0.00	0.000000
0.00	5.00	0.000000
0.00	10.00	0.000000
2.50	0.00	0.000000
2.50	5.00	0.000000
2.50	10.00	0.000000
5.00	0.00	0.000000
5.00	5.00	0.000000
5.00	10.00	0.000000
10.00	0.00	0.000000
10.00	5.00	0.000000
10.00	10.00	0.000000
50.00	0.00	0.000041
50.00	5.00	0.000038
50.00	10.00	0.000034
100.00	0.00	0.001670
100.00	5.00	0.001559
100.00	10.00	0.001405
500.00	0.00	0.001876
500.00	5.00	0.002060
500.00	10.00	0.002125

FOR TIME = 3500. DAYS

X FT	Y FT	CONCENTRATION (ppm)
0.00	0.00	0.000000
0.00	5.00	0.000000
0.00	10.00	0.000000
2.50	0.00	0.000000
2.50	5.00	0.000000
2.50	10.00	0.000000
5.00	0.00	0.000000
5.00	5.00	0.000000
5.00	10.00	0.000000
10.00	0.00	0.000000
10.00	5.00	0.000000
10.00	10.00	0.000000
50.00	0.00	0.000012
50.00	5.00	0.000012
50.00	10.00	0.000011
100.00	0.00	0.001181
100.00	5.00	0.001159
100.00	10.00	0.001094
500.00	0.00	0.002945
500.00	5.00	0.003227
500.00	10.00	0.003325

FOR TIME = 4000. DAYS

X FT	Y FT	CONCENTRATION (ppm)
0.00	0.00	0.000000
0.00	5.00	0.000000
0.00	10.00	0.000000
2.50	0.00	0.000000
2.50	5.00	0.000000
2.50	10.00	0.000000
5.00	0.00	0.000000
5.00	5.00	0.000000
5.00	10.00	0.000000
10.00	0.00	0.000000
10.00	5.00	0.000000
10.00	10.00	0.000000
50.00	0.00	0.000001
50.00	5.00	0.000001
50.00	10.00	0.000001
100.00	0.00	0.000119
100.00	5.00	0.000121
100.00	10.00	0.000118

500.00	0.00	0.002492
500.00	5.00	0.002730
500.00	10.00	0.002813

FOR TIME = 4500. DAYS

X FT	Y FT	CONCENTRATION (ppm)
0.00	0.00	0.000000
0.00	5.00	0.000000
0.00	10.00	0.000000
2.50	0.00	0.000000
2.50	5.00	0.000000
2.50	10.00	0.000000
5.00	0.00	0.000000
5.00	5.00	0.000000
5.00	10.00	0.000000
10.00	0.00	0.000000
10.00	5.00	0.000000
10.00	10.00	0.000000
50.00	0.00	0.000000
50.00	5.00	0.000000
50.00	10.00	0.000000
100.00	0.00	0.000046
100.00	5.00	0.000048
100.00	10.00	0.000047
500.00	0.00	0.001666
500.00	5.00	0.001824
500.00	10.00	0.001879

FOR TIME = 5000. DAYS

X FT	Y FT	CONCENTRATION (ppm)
0.00	0.00	0.000000
0.00	5.00	0.000000
0.00	10.00	0.000000
2.50	0.00	0.000000
2.50	5.00	0.000000
2.50	10.00	0.000000
5.00	0.00	0.000000
5.00	5.00	0.000000
5.00	10.00	0.000000
10.00	0.00	0.000000
10.00	5.00	0.000000
10.00	10.00	0.000000
50.00	0.00	0.000000
50.00	5.00	0.000000
50.00	10.00	0.000000
100.00	0.00	0.000000
100.00	5.00	0.000000
100.00	10.00	0.000000
500.00	0.00	0.001555
500.00	5.00	0.001705
500.00	10.00	0.001758

MAX. CONCENTRATION : 0.3437E-02 MG/L AT 2500 DAYS

EFFLUENT CONCENTRATION AT WATER TABLE

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AT EVERY 200 TIME STEPS

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AT LATERAL DISTANCE = 0.0000 FT

TIME DAYS	DISCHARGE FT/DAY	CHEMICAL CONC. MG/
400.	0.6774E-02	0.1309E-0
800.	0.9149E-02	0.3602E-0
1200.	0.8919E-02	0.1144E+0
1600.	0.4050E-02	0.1631E+0
2000.	0.3866E-02	0.1825E+0
2400.	0.2186E-02	0.1876E+0
2800.	0.1796E-02	0.1857E+0
3200.	0.3429E-02	0.1760E+0
3600.	0.1241E-02	0.1635E+0
4000.	0.2085E-02	0.1503E+0

AT LATERAL DISTANCE = 1.0000 FT

TIME DAYS	DISCHARGE FT/DAY	CHEMICAL CONC. MG/
400.	0.6774E-02	0.1337E-0
800.	0.9149E-02	0.3615E-0
1200.	0.8919E-02	0.1145E+0
1600.	0.4050E-02	0.1631E+0
2000.	0.3866E-02	0.1825E+0
2400.	0.2186E-02	0.1876E+0
2800.	0.1796E-02	0.1857E+0
3200.	0.3429E-02	0.1760E+0
3600.	0.1241E-02	0.1635E+0
4000.	0.2085E-02	0.1503E+0

AT LATERAL DISTANCE = 2.0000 FT

TIME DAYS	DISCHARGE FT/DAY	CHEMICAL CONC. MG/
400.	0.6774E-02	0.1410E-0
800.	0.9149E-02	0.3649E-0
1200.	0.8919E-02	0.1147E+0
1600.	0.4050E-02	0.1631E+0
2000.	0.3866E-02	0.1825E+0
2400.	0.2186E-02	0.1876E+0
2800.	0.1796E-02	0.1857E+0
3200.	0.3429E-02	0.1760E+0
3600.	0.1241E-02	0.1635E+0
4000.	0.2085E-02	0.1503E+0

AT LATERAL DISTANCE = 3.0000 FT

TIME DAYS	DISCHARGE FT/DAY	CHEMICAL CONC. MG/
400.	0.6774E-02	0.1500E-0
800.	0.9149E-02	0.3691E-0
1200.	0.8919E-02	0.1149E+0
1600.	0.4050E-02	0.1632E+0

2000.	0.3866E-02	0.1825E+01
2400.	0.2186E-02	0.1876E+01
2800.	0.1796E-02	0.1857E+01
3200.	0.3429E-02	0.1760E+01
3600.	0.1241E-02	0.1635E+01
4000.	0.2085E-02	0.1503E+01

AT LATERAL DISTANCE = 4.0000 FT

TIME DAYS	DISCHARGE FT/DAY	CHEMICAL CONC. MG/L
400.	0.6774E-02	0.1573E-01
800.	0.9149E-02	0.3724E-01
1200.	0.8919E-02	0.1151E+01
1600.	0.4050E-02	0.1632E+01
2000.	0.3866E-02	0.1825E+01
2400.	0.2186E-02	0.1876E+01
2800.	0.1796E-02	0.1857E+01
3200.	0.3429E-02	0.1760E+01
3600.	0.1241E-02	0.1635E+01
4000.	0.2085E-02	0.1503E+01

AT LATERAL DISTANCE = 5.0000 FT

TIME DAYS	DISCHARGE FT/DAY	CHEMICAL CONC. MG/L
400.	0.6774E-02	0.1601E-01
800.	0.9149E-02	0.3737E-01
1200.	0.8919E-02	0.1152E+01
1600.	0.4050E-02	0.1632E+01
2000.	0.3866E-02	0.1825E+01
2400.	0.2186E-02	0.1876E+01
2800.	0.1796E-02	0.1857E+01
3200.	0.3429E-02	0.1760E+01
3600.	0.1241E-02	0.1635E+01
4000.	0.2085E-02	0.1503E+01

AT LATERAL DISTANCE = 6.0000 FT

TIME DAYS	DISCHARGE FT/DAY	CHEMICAL CONC. MG/L
400.	0.6774E-02	0.1573E-01
800.	0.9149E-02	0.3724E-01
1200.	0.8919E-02	0.1151E+01
1600.	0.4050E-02	0.1632E+01
2000.	0.3866E-02	0.1825E+01
2400.	0.2186E-02	0.1876E+01
2800.	0.1796E-02	0.1857E+01
3200.	0.3429E-02	0.1760E+01
3600.	0.1241E-02	0.1635E+01
4000.	0.2085E-02	0.1503E+01

AT LATERAL DISTANCE = 7.0000 FT

TIME DAYS	DISCHARGE FT/DAY	CHEMICAL CONC. MG/L
400.	0.6774E-02	0.1500E-01
800.	0.9149E-02	0.3691E-01
1200.	0.8919E-02	0.1149E+01
1600.	0.4050E-02	0.1632E+01
2000.	0.3866E-02	0.1825E+01
2400.	0.2186E-02	0.1876E+01
2800.	0.1796E-02	0.1857E+01
3200.	0.3429E-02	0.1760E+01

3600.	0.1241E-02	0.1635E+00
4000.	0.2085E-02	0.1503E+00

AT LATERAL DISTANCE = 8.0000 FT

TIME DAYS	DISCHARGE FT/DAY	CHEMICAL CONC. MG/L
400.	0.6774E-02	0.1410E-02
800.	0.9149E-02	0.3649E-01
1200.	0.8919E-02	0.1147E+00
1600.	0.4050E-02	0.1631E+00
2000.	0.3866E-02	0.1825E+00
2400.	0.2186E-02	0.1876E+00
2800.	0.1796E-02	0.1857E+00
3200.	0.3429E-02	0.1760E+00
3600.	0.1241E-02	0.1635E+00
4000.	0.2085E-02	0.1503E+00

AT LATERAL DISTANCE = 9.0000 FT

TIME DAYS	DISCHARGE FT/DAY	CHEMICAL CONC. MG/L
400.	0.6774E-02	0.1337E-01
800.	0.9149E-02	0.3615E-01
1200.	0.8919E-02	0.1145E+00
1600.	0.4050E-02	0.1631E+00
2000.	0.3866E-02	0.1825E+00
2400.	0.2186E-02	0.1876E+00
2800.	0.1796E-02	0.1857E+00
3200.	0.3429E-02	0.1760E+00
3600.	0.1241E-02	0.1635E+00
4000.	0.2085E-02	0.1503E+00

AT LATERAL DISTANCE = 10.0000 FT

TIME DAYS	DISCHARGE FT/DAY	CHEMICAL CONC. MG/L
400.	0.6774E-02	0.1309E-01
800.	0.9149E-02	0.3602E-01
1200.	0.8919E-02	0.1144E+00
1600.	0.4050E-02	0.1631E+00
2000.	0.3866E-02	0.1825E+00
2400.	0.2186E-02	0.1876E+00
2800.	0.1796E-02	0.1857E+00
3200.	0.3429E-02	0.1760E+00
3600.	0.1241E-02	0.1635E+00
4000.	0.2085E-02	0.1503E+00

DISCHARGE AND CUMM. VOL. AT WATER TABLE

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AT EVERY 200 TIME STEPS

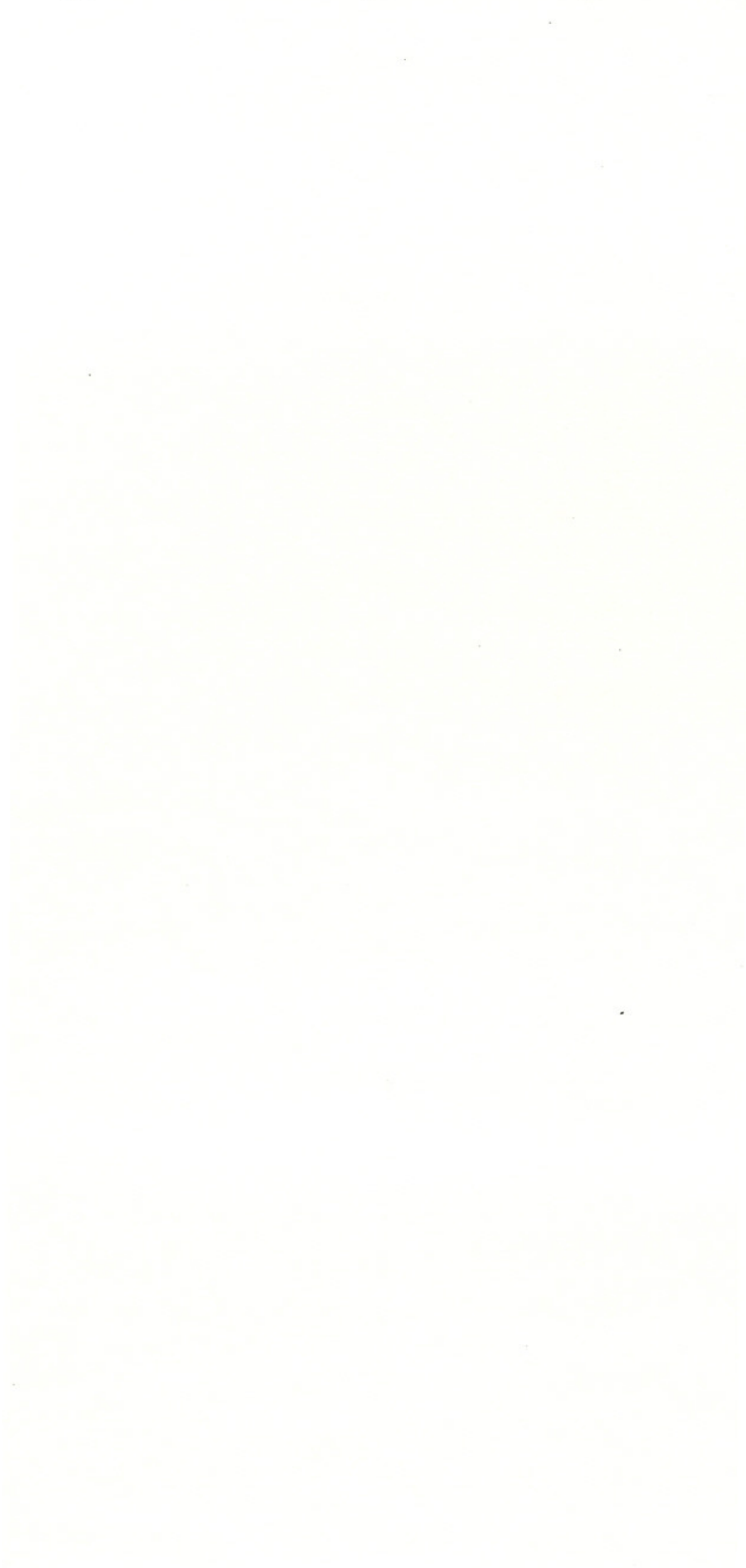
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TIME DAYS	DISCHARGE CUBIC FT/DAY	VOLUME CUBIC FT	CUMM. VOLUME CUBIC FT
400.	0.6774E-02	0.1341E-01	0.6416E+00
800.	0.9149E-02	0.1838E-01	0.2588E+01
1200.	0.8919E-02	0.1790E-01	0.4714E+01
1600.	0.4050E-02	0.8239E-02	0.6286E+01
2000.	0.3866E-02	0.7867E-02	0.7530E+01
2400.	0.2186E-02	0.4409E-02	0.8616E+01
2800.	0.1796E-02	0.3615E-02	0.9409E+01
3200.	0.3429E-02	0.6932E-02	0.1105E+02
3600.	0.1241E-02	0.2499E-02	0.1237E+02
4000.	0.2085E-02	0.4170E-02	0.1365E+02

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4. Korfiatis, G. P. and N. M. Talimcioglu, 1991, "*Model for Evaluation of the Impact of Contaminated Soil on Groundwater*", Final Report for Phase I, submitted to NJDEPE.
5. Korfiatis, G. P. and N. M. Talimcioglu, 1994, "*Model for Evaluation of the Impact of Contaminated Soil on Groundwater*", Final Report for Phase II, submitted to NJDEPE.
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Appendix: Final Report from Rutgers Group



Report - Rutgers Group

I. Introduction

This report states the progress to date of the Rutgers Research group for this project. In November of 1994 it was decided to modify the goals of the project.

A. Modifications

1. It was decided that the column studies for the phthalate esters should not be performed.
2. Batch studies and column studies of the dichlorobenzenes, the xylenes, and the BTX compounds were to be substituted for the column studies for the phthalate esters.

B. Summary of Progress to Date

During the second year batch studies for the phthalate esters were performed, a manuscript was prepared for publication, modification of the research goals occurred, preparation for the performance of the column studies occurred, data for an alternative soil-after characteristic curve were collected using a pressure plate apparatus, new soil was collected, soil property analyses were collected, and a development of soil organic matter determination modification was initiated.

II. Phthalate Ester Batch Studies

Batch studies were performed with dimethyl phthalate ester and diethyl phthalate ester on both the cohanscy and towacco soils. These batch studies covered a wide range of liquid phase concentrations up to the saturation concentration of dimethyl phthalate ester and diethyl phthalate ester. The resulting isotherms showed BET like multi-layer adsorption.

At the suggestion of the grant officer a manuscript summarizing the batch study data was prepared. The data were analyzed using a number of different isotherm models and were fitted to these models using a Levingberg-Marquardt non-linear curve fitting algorithm. It was noted that there was a high correlation between organic carbon content and the total amount of analyte adsorbed. The test of the manuscript is presented below as a summary of the phthalate ester batch studies. The pertinent tables and figures are appended.

Adsorption of Phthalate Esters on Soil at Near Saturation Conditions

by J. G. Hunter and C. G. Uchirin

Introduction

Esters of the phthalic acids are common environmental contaminants which are known causes of health problems. They have been implicated in mammalian hepatotoxicity (Rao et al 1993), mammalian testicular atrophy (Fukuoka et al 1993), mammalian teratogenicity (Ema et al 1992), and plant toxicity (Herring and Bering 1988). Phthalate esters are environmentally ubiquitous contaminants with a variety of industrial uses including carriers for pesticides and insect repellents, in cosmetics fragrances, lubricants, defoaming agents and as plastisizers (Russell and McDuffie 1986). However, little has been published concerning their adsorption behavior.

Esters of the phthalic acids are common environmental contaminants which are known causes of health problems. They have been implicated in mammalian hepatotoxicity (Rao et al 1993), mammalian testicular atrophy (Fukuoka et al 1993), mammalian teratogenicity (Ema et al 1992), and plant toxicity (Herring and Bering 1988). Phthalate esters are environmentally ubiquitous contaminants with a variety of industrial uses including carriers for pesticides and insect repellents, in cosmetics fragrances, lubricants, defoaming agents and as plastisizers (Russell and McDuffie 1986). However, little has been published concerning their adsorption behavior.

Contaminant movement through a subsurface matrix is intimately tied to the adsorption behavior of the particular contaminant. Russell and McDuffie (1986) examined adsorption behavior for several phthalic acid esters. They concluded that the adsorption of phthalic acid esters to soil followed a linear isotherm type of behavior. These investigators limited their investigation to a range of concentrations well below saturation. Hughes (1990) also investigated the adsorption behavior of several phthalic acid esters on soil and found their adsorption behavior to conform with the Langmuir isotherm equation. Hughes used concentration up to 50 % of the saturation concentration of the phthalic acid esters examined.

In general there has been little attention paid to the adsorption behavior of environmental contaminants on soils at their solubility limit in water. This is of concern in cases where non-aqueous phase liquids (NPLs) exist and which can potentially create a saturated aqueous solution in the subsurface system. Under these conditions it is possible to experience type II BET behavior (Brunauer et al 1940), which is indicative of multimolecular layer adsorption. It was decided to investigate two phthalic acid esters (dimethyl phthalate and diethyl phthalate) over the full range of their solubilities and examine the isotherms for the common isotherm equations and for two non-linear equations, the BET isotherm equation (Brunauer et al 1938) and the Marinas and Li (1994) composite isotherm equation, both of which model multimolecular layer adsorption.

Materials and Methods

Batch studies were performed to determine the adsorption behavior of Dimethyl phthalate ester (Aldrich Chemical) and Diethyl phthalate ester (Aldrich Chemical) on two soils at constant temperature (20°C). Solutions were prepared as needed by weighing out a specific mass of the desired phthalate ester on an analytical balance in a hexane rinsed aluminum weighing pan and then rinsing the mass into 1 liter volumetric flask using 0.005 M CaCl₂. The solution was gently stirred until the phthalate ester dissolved entirely, after which point the volumetric flask was filled to the mark using 0.005 M CaCl₂.

The soils chosen were cohansay and towacco, low clay content soils with respectively a small amount or trace organic matter. Table 1 presents specific characteristics of these soils. Soil organic matter content was determined by the Walkley and Black modification of the rapid dichromate oxidation technique (Nelson and Somers 1982). Soils were air dried and then sieved through a 2 mm sieve, visible roots and pebbles were removed.

A series of batches were prepared using varying amounts of soil and different amounts of dimethyl phthalate ester solutions of different concentrations. The soils were weighed into either a 50 mL Teflon centrifuge tube or a 125 mL septum vial. The centrifuge tubes/vials with soils then had an aliquot of the phthalate ester solution added into the vial using a volumetric pipette. After addition of the solution the centrifuge tube were capped with Teflon screw top caps with fluoroelastomer o-rings while the vials were covered with solvent rinsed aluminum foil and were sealed with a butyl rubber septum cap. It was discovered that there was significant adsorption of diethyl phthalate ester by the Teflon centrifuge tubes, therefore it was decided to do all the batch studies for diethyl phthalate ester in glass containers. A series of batches were prepared using varying amounts of soil and different amounts of solutions of increasing concentrations. The soils were weighed into either a 55 mL or a 125 mL septum vial. The vials with soils then had an aliquot of the phthalate ester solution added into the vial using a volumetric pipette. After addition of the solution the vials were covered with solvent rinsed aluminum foil and were sealed with a butyl rubber septum cap. The samples were attached to shaker table and gently shaken for 48 hours.

The samples in the centrifuge tube were then centrifuged at 3000 rpm and a 10 mL aliquot was removed and placed, along with 10 mL of hexane (pesticide grade), into 22 mL crimp top vial which was sealed with aluminum and butyl rubber septum cap. The samples in the crimp top vials were allowed to settle and then a 20 mL aliquot was removed and placed into a 22 mL crimp top vial which was sealed with aluminum and butyl rubber septum cap and then centrifuged at 3000 rpm after which a 10 mL aliquot was removed and placed, along with 10 mL of hexane (pesticide grade), into 22 mL crimp top vial which was sealed with aluminum and butyl rubber septum cap. The 22 mL crimp top vial containing the sample and the hexane were then shaken for 15 minutes on a wrist action shaker.

After the samples were allowed to settle, aliquots of the extracts were placed into 2 mL screw top vials for analysis. The extracts were then analyzed on a Hewlett-Packard model gas chromatograph according to the procedures set forth in Method 8061 Phthalate Esters by Capillary Gas Chromatography with Electron Capture Detection (GC/ECD) from USEPA Document SW-846 (USEPA 1990) with a modification in which a flame ionization detector was substituted for an electron capture detector.

The equilibrium concentration of the soil fraction was calculated from the difference of the equilibrium concentration of the liquid phase after exposure to the soil from the initial concentration of the liquid phase when added.

The results were fitted to the linear, Freundlich, and Langmuir Isotherm equations using both linear regression on linearized versions of the equations and were also fitted using a Levinberg-Marquardt non-linear curve fitting routine from the software package MathCAD (Mathsoft 1991). The BET and Marinas and Li composite Isotherm equations were fitted using the same Levinberg-Marquardt non-linear curve fitting routine.

Results and Discussion

Isotherms were analyzed for the linear, Langmuir, Freundlich, BET, and a composite isotherm recently proposed by Marinas and Li (1994). Linear regression was performed for the linear isotherm and the linearized forms of the Langmuir, Freundlich, and BET. The equations for these isotherms are provided in Table 2 while the fitted parameters and the r^2 values are presented in Table 3. Furthermore, non-linear regression was performed using a Levinberg-Marquardt algorithm on the Langmuir, Freundlich, BET, and Marinas and Li isotherms; the fitted parameters and "fit" values are presented in Table 3. The isotherms for the dimethyl phthalic acid ester and diethyl phthalic acid are presented in Figures 1 and 2 respectively. For the non-linear regression it is not feasible to calculate r^2 values and thus a quantity which we shall refer to as "fit" was used in place of r^2 . The "fit" is calculated according to an equation provided in the MathCAD Statistical Package. The "fit" values for both the linearized forms and the non-linear fitted parameters are provided so that there is a common basis of comparison for the various isotherm equations.

The dimethyl phthalate isotherm data on cohansey soil showed a good fit (0.838) to the linear isotherm model; a poor fit (0.472 for the non-linear regressed parameters) to the Langmuir isotherm model; a good fit (0.838 for the non-linear regressed parameters check) to the Freundlich isotherm model; a good fit to the (0.932 for the non-linear regressed parameters) BET isotherm model; and the best fit (0.986) to the Marinas and Li composite model. The high fit values for the BET and Marinas and Li composite models is undoubtedly due to the BET type II adsorption exhibited in this isotherm (see Figure 1). The BET type II adsorption is indicative of the formation of multiple layers of adsorbate upon the adsorbent.

The dimethyl phthalate on Towacco soil isotherm data showed a poor fit (meaningless value) to linear isotherm model; a poor fit (0.481 for the non-linear regressed parameters check) to the Langmuir isotherm model; a poor fit (0.535 for the non-linear regressed parameters check) to the Freundlich isotherm model; a poor fit (0.453 for the non-linear regressed parameters) to the BET isotherm model; and a best fit to the composite (0.573) isotherm model. While the BET type II adsorption exhibited by this

isotherm (see Figure 1) likely explains the best fit to the Marinas and Li composite model, the overall poor fit of the Towacco data to any model demands explanation. The simplest explanation is the difference in organic matter between the two soil: the best "fits" overall belong to the high organic matter cohansey while the poorest belong to the low organic matter towacco. If organic matter is the chief explanation for the difference between the two soils then we should expect this to be reflected in differences between the adsorptive capacities or rates of adsorption of the two soils.

Each isotherm has its own adsorptive capacity or rate of adsorption term. Each term for each isotherm will be compared for the two soils. The rate of adsorption term for the linear isotherm is K. The linear isotherm K is $0.51((\text{mg/kg})/(\text{mg/L}))$ for the cohansey soil, and is much less at $0.07((\text{mg/kg})/(\text{mg/L}))$ for the towacco soil. The capacity term for the Langmuir isotherm is Q. The Langmuir isotherm Q is 1108 mg/kg for cohansey soil, and slightly lower at 900 mg/kg for the towacco soil. The pseudo-rate of adsorption term for the Freundlich isotherm is also generally symbolized by K. The Freundlich isotherm K is $5.7((\text{mg/kg})/(\text{mg/L})^n)$ for the cohansey soil, and vastly less at $0.0003((\text{mg/kg})/(\text{mg/L})^n)$ for the Towacco soil. The capacity term for the BET isotherm, like the Freundlich, is generally symbolized by Q. The BET isotherm Q is 282 mg/kg for the cohansey soil, and much less at 7.8 mg/kg for the Towacco soil. The capacity term for the composite isotherm is Cs1. The composite isotherm Cs1 is 630 mg/kg for the cohansey soil, and at 128 mg/kg is considerably less for the Towacco soil. The dimethyl phthalate ester capacity and rate of adsorption terms for all isotherms are uniformly higher for the cohansey soil than for the towacco soil. It has been shown (Karickhoff 1984) that soil organic matter is correlated to the rate of adsorption. These results indicate that capacity as well as rate of adsorption can be correlated to soil organic matter.

The diethyl phthalate isotherm data on cohansey soil showed a good fit (0.706) to linear isotherm model; a good fit the (0.782 for the non-linear regressed parameters) to the Langmuir isotherm model; a good fit (0.693 for the non-linear regressed parameters check) to Freundlich isotherm model; a good fit (0.709 for the non-linear regressed parameters) to the BET isotherm model; and the best fit (0.995) to the Marinas and Li composite model. The exceptionally high fit value for the Marinas and Li composite model is demonstrates its strength. This isotherm does not clearly demonstrate BET Type II behavior and has a nearly linear nature. The K2 term in the Marinas and Li composite isotherm is an equilibrium constant which expresses the favorability of multi-layer adsorption. Thus extremely low K2 value of 4.81×10^{-11} indicates that multi-layer adsorption is highly disfavored.

The diethyl phthalate isotherm data on towacco soil showed a good fit (0.836) to linear isotherm model; a good fit the (0.793 for the non-linear regressed parameters check) to the Langmuir isotherm model; a good fit (0.831 for the non-linear regressed parameters check) to Freundlich isotherm model; a good fit (0.539 for the non-linear regressed parameters) to the BET isotherm model; and the best fit (0.903) to the Marinas and Li composite model. The Marinas and Li composite isotherm equation for diethyl phthalate ester on Towacco soil, like that for diethyl phthalate ester on cohansey soil, has an extremely low K2 value (2.15×10^{-9}) again indicating that multi-layer adsorption is highly disfavored. Isotherms for diethyl phthalate, in contrast to dimethyl phthalate, do not have universally superior fit for cohansey soil. Indeed, three of the five isotherms have slightly superior fits for the towacco soil. This would seem to contradict the observation that organic matter is of central importance in the adsorption of phthalate esters by soils. However, the Marinas and Li composite isotherm still provides the best fit values for both the cohansey and towacco soils, and of the two soils cohansey provides the highest fit value. This would agree with the thesis that organic matter is of central importance to adsorption phenomenon. To, again, test the importance of organic matter in the adsorption of diethyl phthalic acid ester we again can examine the capacity terms for the various isotherms.

We shall now turn examine the adsorptive capacity or rate of adsorption terms for each isotherm equation for the adsorption of diethyl phthalate onto the cohansey and towacco soils. The linear isotherm K is $1.35((\text{mg/kg})/(\text{mg/L}))$ for the cohansey soil, and is much less at $0.14((\text{mg/kg})/(\text{mg/L}))$ for the towacco soil. The Langmuir isotherm Q is 1014 mg/kg for cohansey soil, and much lower at 525 mg/kg for the towacco soil. The Freundlich isotherm K is $3.13((\text{mg/kg})/(\text{mg/L})^n)$ for the cohansey soil, and vastly less at

0.00065 ((mg/kg)/(mg/L)ⁿ) for the Towacco soil. The BET isotherm Q is 171 mg/kg for the cohansey soil, and much less at 19.2 mg/kg for the Towacco soil. The composite isotherm Csl is 1210 mg/kg for the cohansey soil, and at 111 mg/kg is considerably less for the Towacco soil. The diethyl phthalate ester capacity and rate of adsorption terms for all isotherms are uniformly higher for the cohansey soil than for the towacco soil. Thus the capacity and rate of adsorption terms reinforce the interpretation that the amount of organic matter is of central importance in determining adsorption. If soil organic matter behaves as a organic phase into which organic compounds partition then we should expect this to be reflected in the degree of adsorption of chemicals with different degrees of polarity. The greater degree of non-polarity of diethyl phthalate ester is reflected in its greatly lower solubility in water (solubility of 928 mg/L, Leyder and Boulanger 1983) than that of dimethyl phthalate ester (solubility of 4000 mg/L, Howard et al 1985). Therefore, it should be expected that the more non-polar compound (diethyl phthalate ester) should be more heavily adsorbed than the more polar compound (dimethyl phthalate ester).

There are two possible modes of comparing the behavior of dimethyl phthalate ester and diethyl phthalate ester on the towacco (low organic) soil: capacity and fit of the various isotherm equations. Diethyl phthalate ester provided higher fit for all models than did dimethyl phthalate ester. Upon examination, it may be seen that the capacity terms for three of the five models are highest for diethyl phthalate ester, however, the model which provides the best fit for both esters, the Marinas and Li composite model, is slightly higher for dimethyl phthalate ester.

Do the two esters behave in a similar way on the high organic soil? There are, again, two possible modes of comparison: capacity and fit of the isotherms. Diethyl phthalate ester provided higher fit for three of the five models, however dimethyl phthalate ester provided the best for the composite isotherm. Upon examination the capacity terms for three of the five models are highest for diethyl phthalate ester, furthermore, the model which provides the best fit for both esters, the Marinas and Li composite model, is much higher for diethyl phthalate ester, this suggests that diethyl phthalate ester has a significantly higher affinity for organic matter. This higher affinity for organic matter is probably a reflection of the decreased polarity of the diethyl phthalate ester molecule which would increase non-polar partitioning into the organic matter (Karickhoff 1984).

The composite isotherm provides the best fit in all cases. This may mean that it is simply a better model of the adsorption process. However, it should be noted that this may merely reflect an inherent mathematical flexibility of the Marinas and Li composite isotherm.

Conclusions

As hypothesized multi-molecular layer adsorption, as represented by the BET type II isotherms of dimethyl phthalic acid ester, can occur in aqueous-soil systems. Furthermore, the importance of soil organic carbon has been re-affirmed in this study. Finally the Marinas and Li composite isotherm has been demonstrated to be the best overall model for the adsorption of dimethyl phthalic acid ester and diethyl phthalic acid ester onto soil from aqueous solution.

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III. Analytical Preparations

An analytical system of the analysis of the dichlorobenzenes was developed. This system has been tested by the performance of percent recovery studies.

IV. Soil Column Preparations

Preparation for the soil column analyses has been conducted. The record of programming for the data loggers had been lost and it was thus necessary to develop a new set of programs for the data loggers. The programming of the data loggers is complete and a new computer data acquisition method (Softwarewedge By TAL Enterprises) is being tested.

V. Soil Sampling And Soil Properties Testing

(performed by the Soil Testing Laboratory - New Jersey Agricultural Experiment Station, Cook College, Rutgers The State University of New Jersey)

The cohansey soil used in the batch studies was tested. The results are presented below:

Test of Original Cohansey 10/18/94

Soil pH : 3.5

Soil Organic Matter: 1.88

A new batch of cohansey was obtained from the Rutgers Blueberry and Cranberry Research station. This batch was dried and sifted and has been analyzed, along with a sample of the previous cohansey batch for a variety soil properties. The results are presented below:

Soil Testing 2/2/95

Soil Parameters	Soil pH	Soil Organic Matter	Texture	% Sand	% Silt	% Clay
Original Cohansey	3.4	2.30	Sand	89	8	3
New Cohansey	3.9	1.33	Sand	91	4	5
Sand Fractions	%>2 mm	% 2-1 mm	% 1 - 0.5 mm	% 0.5 - 0.25 mm	% 0.25- 0.10 mm	% 0.10 - 0.05 mm
Original Cohansey	0.0	3.0	15.7	39.2	37.3	4.8
New Cohansey	0.0	1.0	19.8	44.0	31.5	3.6

Variability between sampling events is inevitable in soil sampling. However there is considerable variation in the organic content of the cohansey soil, not only between old and new, but also between two different analyses of the old batch. In view of the importance of soil organic content in adsorption it was decided to investigate this phenomenon more closely. The Soil organic matter testing involves taking relatively small sample (5 gm) of soil for testing. After consultation with Dr. Harry S. Motto of the Soil Testing Laboratory - New Jersey Agricultural Experiment Station, Cook College, Rutgers The State University of New Jersey it is hypothesized that sampling error in taking the sub-sample is the likely cause of the organic matter variability. To test this samples of both the old and the new cohansey are being ground to below 150 micrometers (by the Rutgers group). It is believed that this will results in a more accurate soil organic matter analysis.

VI. Soil Pressure Plate Analysis of Cohansey and Towacco

The cohansey and towacco soils were analyzed using a 5 bar pressure plate apparatus. The 5 bar pressure plate apparatus consists of pressure vessel with a porous ceramic plate the whole of which can be pressurized at accurate small increments. The saturated soil samples are weighed before being placed in the unit and are weighed after each pressure setting thus yielding the moisture content at each given pressure. The soil moisture retention curves to be developed from this will be compared with the soil moisture retention curves developed from the column studies. The results are presented below.

Towacco Pressure in Bars	Average % Moisture
0	35.5
0.5	3.5
0.75	3.3
1.0	3.1
1.5	2.4
2.0	2.0
2.5	1.8
3.0	1.7

Cohansey

Pressure in Bars

Average % Moisture

0	38.1
0.5	5.30
0.75	5.0
1.0	4.7
1.5	3.6
2.0	3.0
2.5	2.9
3.0	2.6

TABLE 1. Properties of Cohansey and Towacco Soils

Soil Property	Cohansey	Towacco
Sand (%)	90.0	92.0
Silt (%)	8.0	6.0
Clay (%)	2.0	2.0
Organic Matter (%)	4.4	<0.12
pH	3.8	8.4
Texture	Sand	Sand

TABLE 2. Adsorption Isotherm Equations

Isotherm Name	Equation	Rate or Capacity Term
Linear	$q_e = K_L \cdot C_e$	K_L
Langmuir	$q_e = \frac{b \cdot q^0 \cdot C_e}{1 + b \cdot C_e}$	q^0
Freundlich	$q_e = K_f \cdot C_e^n$	K_f
BET	$q_e = \frac{B \cdot q^0 \cdot C_e}{(C_s - C_e) \cdot [1 + (B - 1) \cdot (C_e / C_s)]}$	q^0
Composite	$q_e = \frac{K_1 \cdot q_{s,1} \cdot \frac{C_e}{C_c}}{1 + (K_1 - 1) \cdot \frac{C_e}{C_c}} + \frac{K_2 \cdot q_{s,2} \cdot \frac{C_e}{C_c}}{1 + (K_2 - 1) \cdot \frac{C_e}{C_c}}$	$q_{s,1}$

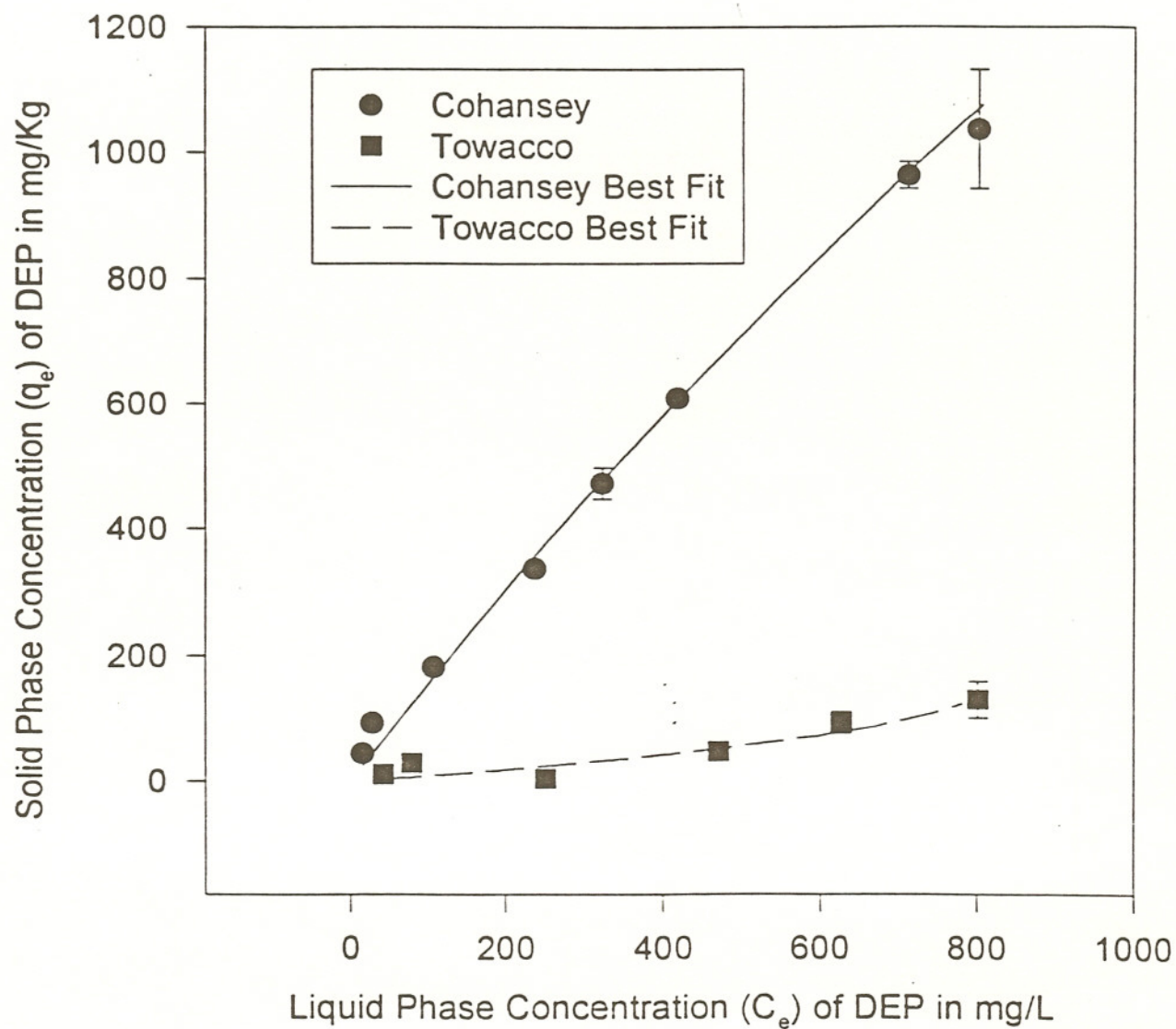
Table 3: Summary of Isotherm Equation Parameters

Isotherm Parameters	Dimethyl Phthalate Ester				Diethyl Phthalate Ester			
	Cohansey		Towacco		Cohansey		Towacco	
	Linear Regressed	Non-Linear Regressed	Linear Regressed	Non-Linear Regressed	Linear Regressed	Non-Linear Regressed	Linear Regressed	Non-Linear Regressed
Linear								
K	0.50965	-	0.06878	-	1.35	-	0.1417	-
r ²	0.9878	-	0.4826	-	0.8801	-	0.7671	-
Fit	0.838	-	-94.838	-	0.706	-	0.836	-
Langmuir								
Q	1108	1108	-154.9	900	1014	1014	16.8329	525
K	0.001510	0.002	-0.0002522	0.00008697	0.002969	0.003	0.045986	0.0006497
r ²	0.9664	-	0.9776	-	0.9794	-	0.0155	-
Fit	0.458	0.472	-3.55E+03	0.481	0.817	0.782	-0.636	0.793
Freundlich								
n	0.6867	1.027	1.053	1.658	0.7706	0.869	0.6830	1.829
K	5.7246	0.41	0.03866	0.000316	5.661	3.128	0.7069	0.0006497
r ²	0.9480	-	0.8805	-	0.9880	-	0.3813	-
Fit	0.807	0.838	-68.203	0.535	0.751	0.693	0.509	0.831
BET								
Q	291.545	282.685	6.101	7.783	0.007	171.095	0.338	19.292
B	-3.85E+01	102.416	-5.813	1.89E+18	1625	2.41E+130	9.158	6.87E+56
r ²	0.9413	-	0.455	-	0.8378	-	0.07343	-
Fit	0.652	0.932	0.394	0.453	-1.4	0.709	-1.324	0.539
Composite								
K1	-	14.542	-	3.486	-	1.217	-	0.653
Cs1	-	629.982	-	128.388	-	1.21E+03	-	111.048
K2	-	1.20E-08	-	1.76E-09	-	4.81E-11	-	2.15E-09
Cs2	-	1.79E+10	-	2.62E+09	-	7.18E+07	-	3.21E+09
Fit	-	0.986	-	0.573	-	0.995	-	0.903

Appendix I

Variable	Definition
q_e	= equilibrium solid phase concentration
C_e	= equilibrium liquid phase concentration
K_L	= linear isotherm coefficient
b	= Langmuir isotherm constant
q^0	= maximum solid phase concentration
K_f	= Freundlich isotherm constant
n	= Freundlich isotherm constant
B	= BET isotherm constant
K_1	= Composite isotherm monolayer constant
$q_{s,1}$	= Composite isotherm monolayer maximum solid phase concentration
K_2	= Composite isotherm multi-layer constant
$q_{s,2}$	= Composite isotherm multi-layer maximum solid phase concentration

Isotherms for Diethyl Phthalate Ester (DEP)



Isotherms for Dimethyl Phthalate Ester (DMP)

