CONTAMINANT TRANSPORT MODELING I

TWO-DIMENSIONAL PLUMES IN UNIFORM GROUND-WATER FLOW

E-005

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ABSTRACT

Analytical solutions for two-dimensional plumes in uniform ground-water flow are presented for two types of contaminant transport problems. The first is a vertically-averaged solution for a line source of contamination which fully penetrates the saturated thickness of an aquifer of infinite areal extent. The second solution is a horizontally-averaged solution for a line source located at the water table of an aquifer of infinite depth.

An interactive Fortran computer code has been developed to evaluate the steady-state or transient concentration distributions for both types of two-dimensional plumes. The user is provided with options to modify the definition of a given problem and, therefore, can gain some insight into the effects of physical and chemical parameters on the extent of a contaminant plume.

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INTRODUCTION

Relatively simple analytical methods can often be used to evaluate ground-water contamination problems, depending upon the complexity of the system and the availability of field data. Analytical models can also serve as valuable tools in developing parameters for more sophisticated numerical models. Although the numerical evaluation of analytical solution to a ground-water problem may be mathematically complex, analytical models are well suited for interactive use on digital computers. Many analytical solutions to ground-water contamination problems can be coded on programmable hand-held calculators. In general, very few input parameters are required to define a given problem and numerical results can be calculated in a few seconds.

This report presents analytical solutions to two ground-water pollution problems--two-dimensional plumes in uniform ground-water flow. An interactive computer code has been developed which enables the user to modify the definition of a given problem, and thus gain some insight into the effects of various parameters on the extent of a contaminant plume.

(3)

SECTION I

MATHEMATICAL DEVELOPMENT

The differential equation describing the conservation of mass of a component in a saturated, homogeneous aquifer with uniform, steady flow in the x-direction can be written as:

$$\frac{\partial C_T}{\partial t} + V\frac{\partial(\theta C)}{\partial x} = D_x\frac{\partial^2(\theta C)}{\partial x^2} + D_y\frac{\partial^2(\theta C)}{\partial y^2} + D_z\frac{\partial^2(\theta C)}{\partial z^2} + r_t \tag{1}$$

C = component mass per unit volume of fluid phase $\qquad$ M/L^3

C_T = total component mass per unit volume of aquifer $\qquad$ M/L^3

D_x = dispersion coefficient in x-direction $\qquad$ L^2/t

D_y = dispersion coefficient in y-direction $\qquad$ L^2/t

D_z = dispersion coefficient in z-direction $\qquad$ L^2/t

r_t = rate of generation of mass per unit volume of aquifer $\qquad$ M/L^3t

V = Darcy, or seepage, velocity in the x-direction $\qquad$ L/t

x,y,z = rectangular coordinates at the point of interest $\qquad$ L

θ = porosity of porous media

$\quad$ = volume of voids per unit volume of aquifer $\qquad$ L^3/L^3

The total mass of a component per unit volume of aquifer is distributed as dissolved solute in the fluid phase and adsorbed solute on the solid matrix. Let

C_s = component mass per unit mass of solid $\qquad$ M/M

and

(4)

ρ_B = bulk density of the aquifer

= mass of solids per unit volume of the aquifer $\quad$ M/L^3

The total component mass per unit volume of aquifer can be expressed as

$$\frac{\text{Mass}}{\text{Unit Vol.}} = \left[\frac{\text{Volume of voids}}{\text{Unit Volume of aquifer}}\right]\left[\frac{\text{Component Mass}}{\text{Volume of voids}}\right]$$

$$+ \left[\frac{\text{Mass of solids}}{\text{Unit volume of aquifer}}\right]\left[\frac{\text{Component Mass}}{\text{Mass of solids}}\right]$$

or

$$C_T = \theta C + \rho_B C_s \qquad (2)$$

and the rate of accumulation of mass in the aquifer becomes

$$\frac{\partial C_T}{\partial t} = \theta \frac{\partial C}{\partial t} + \rho_B \frac{\partial C_s}{\partial t} \qquad (3)$$

In general, $C_s = f(C)$ and

$$\frac{\partial C_s}{\partial t} = \frac{dC_s}{dC} \frac{\partial C}{\partial t} \qquad (4)$$

For a linear equilibrium adsorption isotherm

$$\frac{dC_s}{dC} = K_d \quad \frac{M/M}{M/L^3} \qquad (5)$$

where K_d is a distribution constant.

The change in concentration per unit volume of porous media, $\partial C_T/\partial t$, can be written in terms of fluid phase concentration, C, by substituting Equations 4 and 5 into Equation 3. Therefore,

(5)

$$\frac{\partial C_T}{\partial t} = \theta \frac{\partial C}{\partial t} + \rho_B K_d \frac{\partial C}{\partial t}$$

or

$$\frac{\partial C_T}{\partial t} = (\theta + \rho_B K_d) \frac{\partial C}{\partial t} \tag{6}$$

The rate of generation per unit volume of porous media is also distributed between the solid and liquid phases, or

$$\left(\frac{\text{Rate of mass generated}}{\text{Unit volume of aquifer}}\right) = \left(\frac{\text{Rate of mass generated}}{\text{Unit volume of fluid}}\right)\left(\frac{\text{Volume of fluid}}{\text{Volume of aquifer}}\right)$$

$$+ \left(\frac{\text{Rate of mass generated}}{\text{Unit mass of solid}}\right)\left(\frac{\text{Mass of solid}}{\text{Volume of aquifer}}\right)$$

Now, the rate of change in total mass per unit volume of aquifer due to reaction can be written as

$$r_t = \frac{\partial C_T}{\partial t} = \theta \frac{\partial C}{\partial t} + \rho_B \frac{\partial C_s}{\partial t} \tag{7}$$

The concentration on the solid, C_s, is related to the concentration in the liquid, C, through the linear adsorption isotherm assumed previously, and

$$r_t = \frac{\partial C_T}{\partial t} = (\theta + \rho_B K_d) \frac{\partial C}{\partial t} \tag{8}$$

Assuming first order decay kinetics, the rate of change in fluid concentration due to reaction can be expressed as

$$\frac{\partial C}{\partial t} = -\lambda C \tag{9}$$

where λ is a rate constant (1/t), and

$$r_t = (\theta + \rho_B K_d) \lambda C \tag{10}$$

Equation 1, can now be written in terms of the fluid concentration. Substituting Equations 6 and 10 and recalling that for a homogeneous porous medium the porosity, θ, is constant, Equation 1 becomes

$$(1 + \frac{\rho_B}{\theta} K_d) \frac{\partial C}{\partial t} + V \frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_x \frac{\partial^2 C}{\partial z^2} - (1 + \frac{\rho_B}{\theta} K_d) \lambda C \tag{11}$$

Defining a "retardation coefficient" as

$$R_d = 1 + \frac{\rho_B}{\theta} K_d \tag{12}$$

the differential equation describing the conservation of mass in the aquifer becomes

$$R_d \frac{\partial C}{\partial t} + V \frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} = R_d \lambda C \tag{13}$$

Solutions of Equation 13 for two types of ground-water contamination problems are presented in the following paragraphs. The first is a vertically-averaged solution which describes a contaminant plume in the z-y plane (Figure 1). The second is a horizontally-averaged solution, describing a contaminant plume in the x-z plane (Figure 2).

Vertically-Averaged Solutions

The vertically averaged solutions apply to a homogeneous aquifer of infinite aerial extent and finite depth. The contaminant is assumed to be well mixed over the saturated thickness. The source of contamination is a vertical line source located at the origin of a coordinate system in the
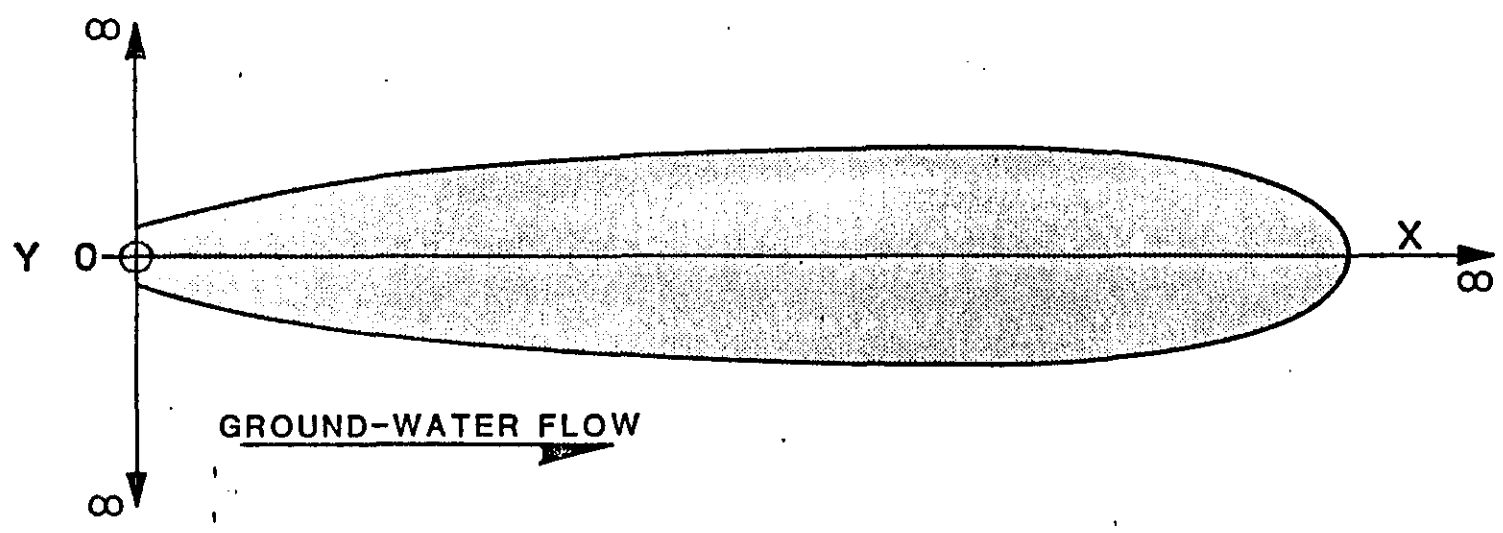
(7)

Figure 1. Coordinate System for vertically averaged solution.
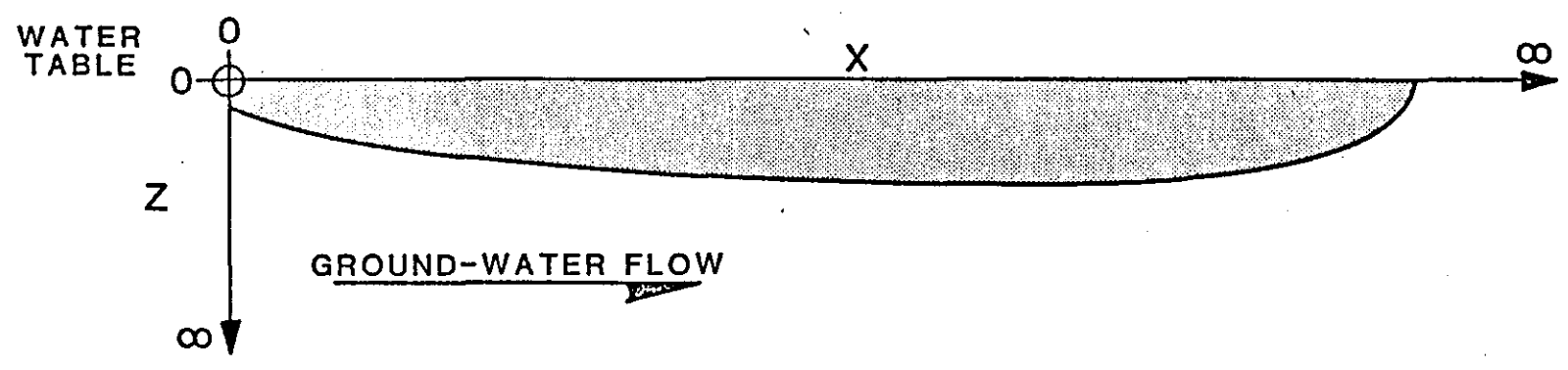

Figure 2. Coordinate system for horizontally averaged solution.

x-y plane. This conceptual model would apply to an injection well which fully penetrates the saturated zone.

Wilson and Miller (1978) have also applied this solution down-stream from a contaminant source at the surface of the water table. For a relatively thin saturated zone, vertical dispersion will result in mixing vertically. The concentration distribution can be considered as being two-dimensional in a horizontal plane at distances downstream of the source sufficient for the concentration distribution to become uniform with depth. Mathematically, the problem is treated as a semi-infinite aquifer with a line source at the origin.

The vertically averaged formulation of Equation 13 is

$$R_d \frac{\partial C}{\partial t} + V \frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - R_d \lambda C \tag{14}$$

The boundary conditions can be stated mathematically as follows:

$$\text{For } t \leq 0 \qquad C = 0 \qquad x \geq 0 \qquad |y| \geq 0 \tag{15a}$$

$$\text{For } t > 0 \qquad C = C_o \qquad x = 0 \qquad y = 0 \tag{15b}$$

$$C = 0 \qquad x = 0 \qquad |y| > 0 \tag{15c}$$

$$\frac{\partial C}{\partial x} = 0 \qquad x \rightarrow \infty \qquad |y| \geq 0 \tag{15d}$$

$$\frac{\partial C}{\partial y} = 0 \qquad x \geq 0 \qquad |y| \rightarrow \infty \tag{15e}$$

where C_o is the concentration of the contaminant source.

A solution of Equation 14 with the boundary conditions defined by Equation 15 can be written as (Wilson and Miller, 1978)

$$C = \frac{C_o Q' \; EXP \left(\frac{Vx}{2D_x}\right)}{4\pi\theta(D_x D_y)^{\frac{1}{2}}} \; W(U,B) \tag{16}$$

where

$$U = \frac{\left(\frac{Vx}{D_x}\right)^2 + \frac{D_x}{D_y}\left(\frac{Vy}{D_x}\right)^2}{\frac{4V^2t}{R_dD_x}}$$

(17)

$$B = \frac{1}{2}\left[\left(\frac{Vx}{D_x}\right)^2 + \frac{D_x}{D_y}\left(\frac{Vy}{D_x}\right)^2\right]^{\frac{1}{2}}\left[1 + \frac{4D_xR_d\lambda}{V^2}\right]^{\frac{1}{2}}$$

(18)

and Q' ($L^3/t/L$) is the volumetric contaminant source rate per unit depth of the saturated zone.

The function $W(U,B)$ is defined as

$$W(U,B) = \int_u^\infty \frac{1}{\xi} EXP\left(-\xi - \frac{B^2}{4\xi}\right) d\xi$$

(19)

where ξ is a dummy integration variable. This function is often referred to as the Hantush (1956, 1964) "well function."

The steady-state solution of Equation 14 and 15 can be obtained by noting as $t \to \infty$, $U \to 0$ and the well function (Hantush, 1956) can be expressed as

$$W(0,B) = 2K_o(B)$$

(20)

At steady state the vertically averaged solution can be written as

$$C = \frac{C_oQ' \, EXP\left(\frac{Vx}{2D_x}\right)}{2\pi\theta(D_xD_y)^{\frac{1}{2}}} K_o(B)$$

(21)

where $K_o(B)$ is the modified Bessel function of the second kind of order zero.

(10)

The units of the variables in Equations 16 and 21 can be eliminated by defining the following dimensionless groups:

Modified Peclet Numbers - $\dfrac{\text{Convective Mass Transport}}{\text{Dispersive Mass Transport}}$

$$Pe_x = \frac{Vx}{D_x} \qquad \frac{L}{t} \cdot L \cdot \frac{t}{L^2} = 1 \qquad (22)$$

$$Pe_y = \frac{Vy}{D_x} \qquad\qquad (23)$$

Damköhler Group II - $\dfrac{\text{Mass decay rate}}{\text{Mass dispersion rate}}$

$$D_k = \frac{D_x R_d}{v^2} \qquad \frac{L^2}{t} \cdot \frac{t^2}{L^2} \cdot \frac{1}{t} = 1 \qquad (24)$$

Number of Pore Volumes Injected - $\dfrac{\text{Mass transport rate}}{\text{Mass accumulation rate}}$

$$I = \frac{v^2 t}{R_d D_x} \qquad \frac{L^2}{t^2} \cdot \frac{t}{1} \cdot \frac{t}{L^2} \qquad (25)$$

Dimensionless Source Term - $\dfrac{\text{Mass injection rate}}{\text{Mass diffusion rate}}$

$$\Gamma = \frac{Q'}{\theta(D_x D_y)^{\frac{1}{2}}} \qquad \frac{L^3}{t} \frac{1}{L} \cdot \frac{t}{L^2} = 1 \qquad (26)$$

Dimensionless Concentration

$$\gamma = \frac{C}{C_o} \qquad \frac{M}{L^3} \cdot \frac{L^3}{M} \qquad (27)$$

Note that the number of pore volumes injected can be written as

$$I = \frac{v^2 t}{D_x R_d} = \left(\frac{VL}{D_x}\right)^2 \left(\frac{D_x t}{R_d L^2}\right) \qquad (28)$$

where L is a characteristic length defined as

$$L^2 = x^2 + \frac{D_x}{D_y} y^2 \qquad (29)$$

(11)

The first group on the right-hand-side of Equation 28 is the Modified Peclet number

$$Pe_{xy} = \frac{VL}{D_x} = \left[\left(\frac{Vx}{D_x}\right)^2 + \frac{D_x}{D_y} \left(\frac{Vy}{D_x}\right)^2 \right]^{\frac{1}{2}}$$

or

$$Pe_{xy} = \left(Pe_x^{\,2} + \beta\, Pe_y^{\,2}\right)^{\frac{1}{2}} \tag{30}$$

where

$$\beta = \frac{D_x}{D_y}$$

The second group on the right-hand-side of Equation 28 is a dimensionless time variable,

$$\tau = \frac{D_x t}{R_d L} \tag{31}$$

The transient and steady-state solutions to Equation 14 which are given by Equations 16 and 21 can be written in terms of dimensionless variables defined above. The transient solution is

$$\gamma = \frac{\Gamma}{4\pi} \; EXP(\tfrac{1}{2}Pe_x) \; W(U,B) \tag{32}$$

and at steady state

$$\gamma = \frac{\Gamma}{2\pi} \; EXP(\tfrac{1}{2}Pe_x) \; K_o(B) \tag{33}$$

with

$$U = \frac{Pe_{xy}^{\,2}}{4I} \tag{34}$$

and

$$B = \tfrac{1}{2}Pe_{xy}(1 + 4D_k)^{\frac{1}{2}} \tag{35}$$

(12)

The values of dimensionless concentrations evaluated using Equation 32 or Equation 33 are valid for any consistent set of units. It is also important to note non-dimensionalizing the problem reduces the twelve dimensional variables involved in Equation 16 to five dimensionless groups in Equation 32.

<u>Horizontally-Averaged Solutions</u>. The horizontally averaged solutions apply to aquifers of finite width and infinite length and depth. The contaminant is assumed to be well mixed over the width of the aquifer. The source of contamination is a line source located at the origin of a coordinate system in the x-y plane, which represents the water table. An example of a problem which would fit this conceptual model is seepage from a canal perpendicular to the direction of ground water flow.

The solution could also be applied to aquifers with a finite depth of a saturated zone. However, the solution only applies from the source downstream to the point where dispersion spreads the contaminant to the bottom of the saturated zone.

The horizontally-averaged formulation of Equation 13 is

$$R_d \frac{\partial C}{\partial t} + V \frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} + D_z \frac{\partial^2 C}{\partial z^2} - R_d \lambda C \tag{36}$$

with boundary conditions

For $t \leq 0$	$C = 0$	$x \geq 0$	$z \geq 0$	(37a)
For $t > 0$	$C = C_o$	$x = 0$	$z = 0$	(37b)
	$C = 0$	$x = 0$	$z > 0$	(37c)
	$\frac{\partial C}{\partial x} = 0$	$x \to \infty$	$z \geq 0$	(37d)
	$\frac{\partial C}{\partial z} = 0$	$x \geq 0$	$z \geq 0$	(37e)

(13)

$$\frac{\partial C}{\partial z} = 0 \qquad x > 0 \qquad z \to \infty \qquad (37f)$$

Equation 36 is identical in form to Equation 14 which describes the vertically-averaged solution. The only difference in boundary conditions between the two problems is that the x-z plane of symmetry in the vertically-averaged problem is replaced by a zero-flux x-y plane in the horizontally-averaged problem. Otherwise the form of the differential equations and boundary conditions is identical. Thus the transient solution of Equation 36 is

$$C = \frac{C_o Q'}{2\pi\theta \ (D_x D_z)^{\frac{1}{2}}} \ W(U,B) \qquad (38)$$

and at steady-state

$$C = \frac{C_o Q'}{\pi\theta \ (D_x D_z)^{\frac{1}{2}}} \ K_o(B) \qquad (39)$$

where

$$U = \frac{\left(\dfrac{Vx}{D_x}\right)^2 + \dfrac{D_x}{D_z}\left(\dfrac{Vz}{D_x}\right)^2}{\dfrac{4 \ V^2 \ t}{R_d \ D_x}} \qquad (40)$$

$$B = \frac{1}{2}\left[\left(\frac{Vx}{D_x}\right)^2 + \frac{D_x}{D_z}\left(\frac{Vz}{D_x}\right)^2\right]^{\frac{1}{2}}\left[1 + \frac{4D_x R_d \lambda}{2}\right]^{\frac{1}{2}} \qquad (41)$$

and Q' is the volumetric contaminant source rate per unit width of aquifer.

Equations 39 through 41 can be written in terms of dimensionless groups similar to those defined for the vertically-averaged solution. Let

(14)

$$Pe_z = \frac{Vz}{D_x} \qquad (42)$$

and

$$\alpha = \frac{D_x}{D_z} \qquad (43)$$

then

$$Pe_{xz} = \left(Pe_x^2 + \alpha \, Pe_z^2 \right)^{\frac{1}{2}} \qquad (44)$$

and the solutions of the transient and steady-state horizontally-averaged solutions become

$$\gamma = \frac{\Gamma}{2\pi} \, EXP(\tfrac{1}{2}Pe_x) \, W(U,B) \qquad (45)$$

and

$$\gamma = \frac{\Gamma}{\pi} \, EXP(\tfrac{1}{2}Pe_x) \, K_o(B) \qquad (46)$$

with

$$U = \frac{Pe_{xz}^2}{4I} \qquad (47)$$

and

$$B = \tfrac{1}{2}Pe_{xz}(1 + 4D_k)^{\frac{1}{2}} \qquad (48)$$

The similarity of the solutions of the vertically-averaged and horizontally-averaged problems facillitates their numerical evaluation using a common computational algorithm. For the same numerical values of the

(15)

independent variables, concentration values for the horizontally-averaged solutions are obtained by doubling the vertically-averaged solution values.

An interactive computational code has been developed to calculate transient and steady-state concentrations for both types of problems. The computer program is discussed in Section III of this report.

Superposition - The differential equation describing component mass concentration in a porous medium, Equation 1, is a linear partial differential equation. The principal of superposition can be used directly to solve complex ground-water contamination problems in terms of the simplier solutions described above. Unfortunately, the scattered applications of this principle are not explained in any single reference. Some texts indicate that superposition means that any sum of solutions is also a solution. Superposition is commonly used to generate a linear no-flow boundary condition through the use of "image wells" or to simulate multiple sources and sinks, (Walton; 1962, 1970). The principle of superposition is also complicated by referring to the "Dunhamel theorem," the "Faltung integral," and/or "convolution integrals." These terms often have no apparent physical interpretation. For the purposes of this report, "superposition in space" will refer to the approximation of sources of finite area as the sum of a finite number of line sources or the generation of no-flow boundaries using image wells. "Superposition in time" will refer to the approximation of a variable source rate of contamination as the sum of a finite number of constant source rates distributed in time.

Both the horizontally-averaged and vertically-averaged solutions can be used to simulate aquifers of finite width or depth, respectively, or plane sources of finite width. Applications of this type require a thorough understanding of the physical interpretation of the principal of superposition.

(16)

However, superposition in the time is relatively straight forward, and the provision to approximate a non-uniform source rate for a contaminant has been included in the computer program discussed in Section III.

Consider the variable source of contamination shown in Figure 3a. The solutions of the governing differential equation presented in this report are of the form

$$C(x,y,t) = C_o Q' \ f(x,y,t) = \dot{Q}' \ f(x,y,t) \tag{49}$$

where $\dot{Q}'$ is the source mass rate per unit length. The principle of super-position in time can be written for any position as

$$c(x,y,t) = \sum_{i=1}^{n} \dot{Q}'_n \ f(x,y,t_n) \tag{50}$$

Now, the variable rate schedule shown in Figure 3a can be decomposed into a series of positive and negative mass rates as shown in Figure 3b. The concentration at a point x,y at the end of the simulation can be evaluated as

$$
\begin{aligned}
C(x,y,t) = \ & \dot{Q}'_1 \ f(x,y,t_1) \quad -\dot{Q}'_1 \ f(x,y,t_2) \\
+ \ & \dot{Q}'_2 \ f(x,y,t_2) \quad -\dot{Q}'_2 \ f(x,y,t_3) \\
+ \ & \dot{Q}'_3 \ f(x,y,t_3) \quad -\dot{Q}'_3 \ f(x,y,t_4) \\
+ \ & \dot{Q}'_4 \ f(x,y,t_4)
\end{aligned}
\tag{51}
$$

In general terms

$$C(x,y,t) = \sum_{i=1}^{n} (\dot{Q}'_n - \dot{Q}'_{n-1}) \ f(x,y,t_n) \tag{52}$$

with $\dot{Q}'_0 = 0$

(17)
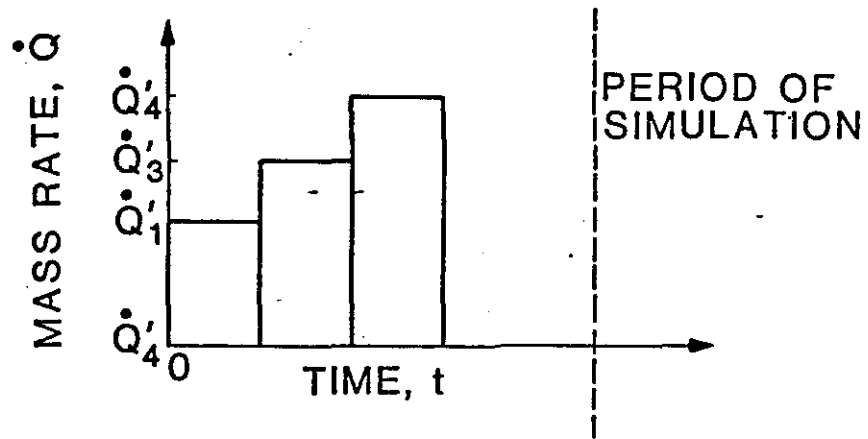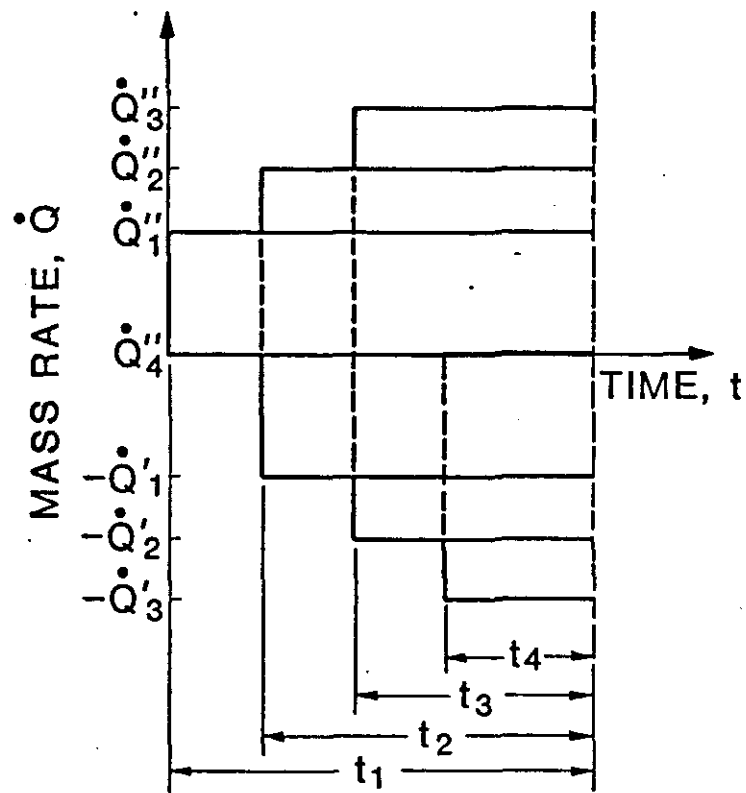
Figure 3.   Decomposition of a variable source rate using
            superposition in time.

(18)

Note the time corresponding to a given source rate is the period beginning with the start of the given rate to the end of the simulation period — the time is not the duration of a given rate.

A continuous non-uniform rate schedule may be approximated as closely as desired by increasing the number of discrete rates in the source rate schedule. In theory an infinite number of discrete rates would be required. An understanding of the physical problem and the assumptions incorporated in the mathematical model are the best guidelines for decomposing a continuous non-uniform source of contamination.

SECTION II

APPLICATIONS

The case history of ground-water contamination with hexavalent chrom-
ium described by Perlmutter and Lieber (1970), will be used as an example of
the application of a two-dimensional plume model. The contaminant plume has
been modeled numerically by Pinder (1973) and analytically by Wilson and
Miller (1978). Details of the hydrologic system are described in the above
references. A brief summary of the problem is presented in the following
paragraphs.

The aquifer is assumed to have a saturated thickness of 33.52 m with a
porosity of 0.35. Perlmutter and Lieber (1970) estimated the average seepage
velocity to be approximately 0.366 m/dy. Using Pinder's (1973) values of
dispersivity, α_x = 21.3 m and α_y = 4.27 m, the x and y dispersion coefficients
are

$$D_x = (21.3m)(0.366m/dy) = 7.70 \ m^2/dy$$

and

$$D_y = (4.27m)(0.366m/dy) = 1.56 \ m^2/dy$$

The source of contamination consisted of three metal-plating-waste disposal
ponds as shown in Figure 4. The mass rate of chromium entering the aquifer
has been estimated at 23.6 kg/dy during the nine year period from 1941 through
1949 (Perlmutter and Lieber, 1970). Chromium is believed to be a conservative
contaminant, thus absorption and degradation can be neglected. The vertically-
averaged model parameters are summarized as follows:

(20)
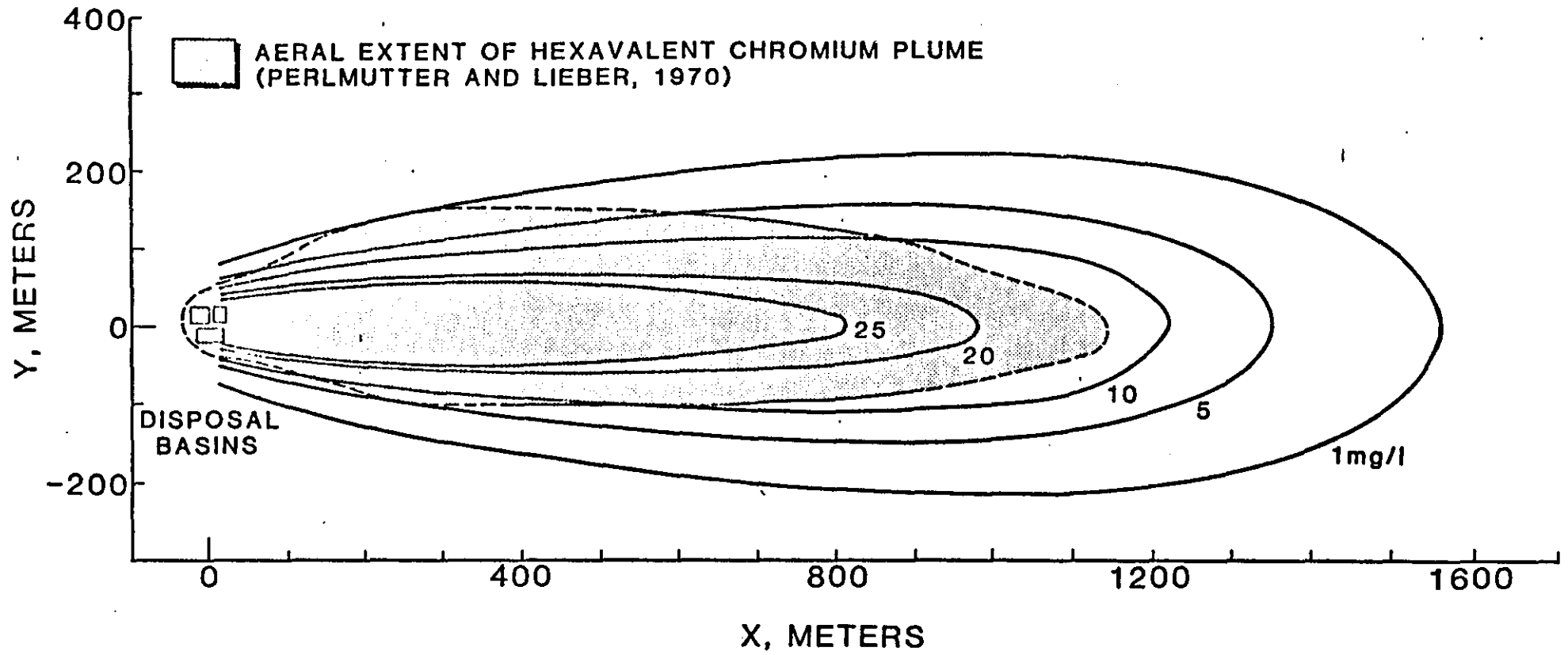
Figure 4. Results of hexavalent chromium plume simulation at 2800 days.

Aquifer porosity	0.35
Seepage velocity	0.366 m/dy
Retardation coefficient	1.0
x-Dispersion coefficient	7.79 m^2/dy
y-Dispersion coefficient	1.56 m^2/dy
Decay constant	0.0 1/dy

The contaminant source rate is assumed to be constant, and only one rate period is required. The mass rate can be converted to units of concentration times volume rate per unit depth as

$$\frac{23.6 \text{ kg}}{\text{dy}} \cdot \frac{10^6 \text{ mg}}{\text{kg}} \cdot \frac{\text{m}^3}{10^3 \text{l}} \cdot \frac{1}{33.52 \text{ m}} = 704 \text{ (mg/l) } (\text{m}^3/\text{dy})/\text{m}$$

for approximately nine years or 3,280 days.

The numerical results for the horizontally-averaged solution are summarized in Figure 4. The shape and general extent of the predicted plume are in fair agreement with the observed extent of contamination considering the availability of field data and the assumptions which have been made in characterizing the problem as two-dimensional uniform flow with a continuous line source.

Superposition in time will be illustrated using data for the aquifer contaminated with chromium described above. Rather than a continuous source of contamination from the disposal ponds, an "accidental spill" of high strength waste will be simulated. The contaminant source will be assumed to be an "instantaneous line source" of strength 704 (mg/l)(m^3/m). The source rate schedule for the horizontally-averaged model is constructed as follows:

(22)
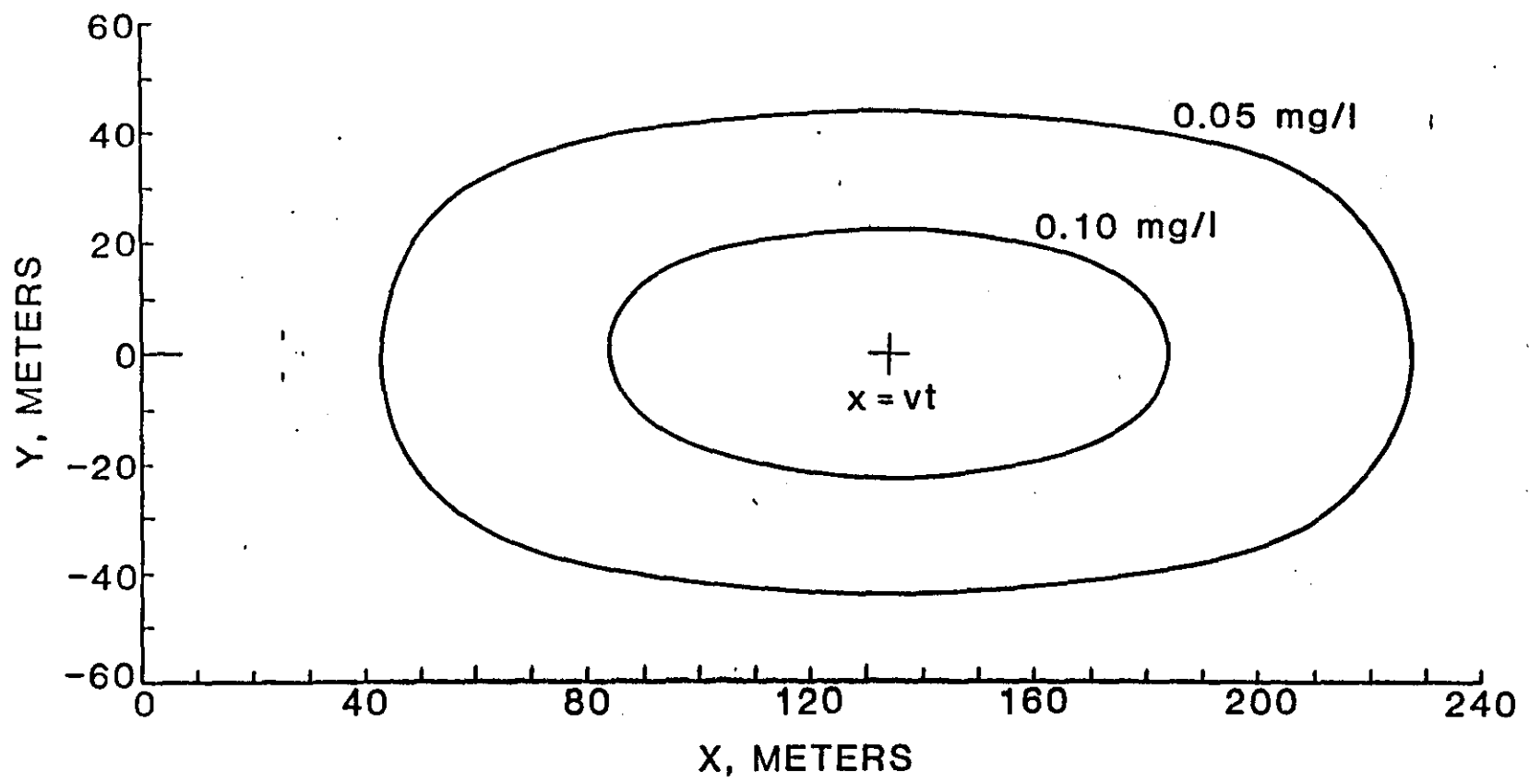
Figure 5. Results of hexavalent chromium spill simulation at 365 days.

Rate 1:   704 (mg/l) (m^3/dy)/m for 365 days

Rate 2:   0 (mg/l) (m^3/dy)/m for 364 days

Other model parameters are identical to those used in the first example. The results of the simulation are summarized in Figure 5, which shows the center of mass of the plume moving down-gradient at the seepage velocity and spreading longitudinally and transversely by diffusion.

The results of the simulation using superposition in time were compared with the concentrations calculated using

$$C = \frac{C_o Q'}{4\pi\theta t (D_x D_y)^{\frac{1}{2}}} \; \text{EXP} \left\{ - \frac{(x-Vt)^2}{4D_x t} - \frac{y^2}{4D_y t} - \lambda t \right\} \tag{53}$$

which is the solution of Equation 14 for an instantaneous line source of strength $C_o Q'$ (m/L^3) (L^3/L). The values of concentration and errors in approximating the instantaneous source through superposition in time are presented in Table 1. Note that the finite duration of the source results is slightly higher concentrations up-gradient from the center of mass than concentrations down-gradient. For an instantaneous source the concentration distribution should be symmetrical about a y-z plane through the center of mass located at x = Vt. A better approximation can be obtained by injecting the same total mass of contaminant over a shorter period of time; but for purposes of illustrating superposition in time, the errors in the example problem are not significant.

The two example problems presented above are intended to illustrate the application of the two-dimensional plume models developed in this report. These models are tools which can aid in the analysis of ground-water contamination problems. The user must select the best tool for the

(24)

TABLE 1

COMPARISON OF CONCENTRATIONS CALCULATED USING SUPERPOSITION IN TIME AND AN ANALYTICAL SOLUTION FOR AN INSTANTANEOUS LINE SOURCE

MODEL PARAMETERS

Aquifer Porosity	0.35
Seepage Velocity	0.366 m/dy
Retardation Coefficient	1.0
x-Dispersion Coefficient	7.79 m^2/dy
y-Dispersion Coefficient	1.56 m^2/dy
First-Order Decay Constant	0.0 1/dy
Source Strength	704.0 (mg/1) (m^3/m)

Concentration at 365 days, mg/1

Superposition
(Equation 53)
% Error

y (meters)	x(meters)				
	73.59	103.59	133.59 (= Vt)	163.59	193.59
20.0	0.0919 (.0917) .22	0.1165 (.1162) .26	0.1259 (.1258) .08	0.1163 (.1162) .01	0.0916 (.0917) −.11
10.0	0.0878 (.0877) .11	0.1115 (.1112) .27	0.1206 (.1204) .17	0.1113 (.1112) .09	0.0876 (.0877) −.11
0.0	0.0771 (.0769) .26	0.0977 (.0975) .21	0.1057 (.1055) .19	0.0975 (.0975) .0	0.0768 (.0769) −.13

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problem at hand, based on a sound understanding of the principles of ground-
water hydrology, the physical problem, and the limitations of the mathema-
tical model(s).

SECTION III

PROGRAM PLUME

Program PLUME evaluates the analytical solution of the differential
equation describing concentration distributions in a two-dimensional plume
in uniform ground-water flow. The program has been designed for interact-
ive use and requires input data under two modes of operation - "Basic Input
Data" and "Edit."

Basic Input Data

Basic input data are required to initiate a new problem using the PLUME
program. The user is prompted for the required data through a series of in-
put commands described below. Numeric data may be entered through the key-
board with or without decimal points and multiple data entries should be
separated by a comma(s). The first basic input command is:

ENTER TITLE

?

Any valid keyboard characters can be used. The first 60 characters will be
retained for further problem identification.

The second input command is used to select the vertically-averaged solu-
tion or the horizontally-averaged solution. The command is:

ENTER COORDINATE SYSTEM

XY FOR VERTICALLY-AVERAGED SOLUTION

XZ FOR HORIZONTALLY-AVERAGED SOLUTION

?

Either of the indicated responses is valid.

The next three input commands define the units for all variables used in the calculations. Any consistent set of units may be used.

ENTER UNITS FOR LENGTH (2 CHARACTERS)

?

Any valid keyboard characters can be used. The first two characters will be retained for identifying the units of the length dimensions which may be required for other input data or output listings.

ENTER UNITS FOR TIME (2 CHARACTERS)

?

Any valid keyboard characters can be used. The first two characters will be retained for identifying the units of the time dimensions which may be required for other input data or output listings.

ENTER UNITS FOR CONCENTRATION (6 CHARACTERS)

?

The first six characters of any valid keyboard entries will be retained for identifying the concentration units used for data input and output.

The remaining input commands are used to initialize all variables for a given problem. They include both aquifer and contaminant parameters. Input data errors which may interrupt the computational sequence are detected by the program and a command is issued to reenter the data for the appropriate variable.

ENTER AQUIFER POROSITY

?

Enter the volume void fraction.

ENTER SEEPAGE VELOCITY

?

The seepage, or Darcy, velocity must be entered with dimensions of L/t in
the units requested. Numerical values must be greater than zero.

ENTER RETARDATION COEFFICIENT

?

The retardation coefficient includes the effects of absorption of the tracer
on the solid matrix (see Section II for discussion). The numerical value
must be greater than 1.0, or equal to 1.0 if absorption is neglected.

ENTER X AND Y DISPERSION COEFFICIENTS (L^2/t)

?,?

Dispersion coefficients have dimensions of L^2/t and must be entered in the
units requested. Numerical values must be greater than zero.

ENTER DECAY CONSTANT, (1/t)

?

The first order decay constant has dimensions of (1/t) and must be entered
in the units requested. The decay constant must be greater than, or equal
to, zero.

The next two input commands are used to set up the source rate schedule.
A nonuniform source is accommodated through superposition of a series of uni-
form source rates (see Section II for discussion).

ENTER NUMBER OF SOURCE RATES

?

The number of uniform source rates used to approximate a nonuniform rate
schedule is entered. If a negative or zero value is entered, the steady

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state concentration will be evaluated.

ENTER MASS RATE N (M/L^3) $(L^3/t/L)$ AND TIME, (t)

?,?

The source mass rate is entered in units of concentration times the volume-
tric rate per unit depth of saturated thickness of the aquifer. Note the
actual source concentration and rate are not required, but the units must
be consistent. The time units must also be consistent and the time variable
is the interval from the start of a new source rate to the "time of recon-
ning."

The last two basic input commands are used to define the matrix of ob-
servation points, or coordinates at which concentration will be evaluated.

ENTER XFIRST, XLAST, DELTAX (L)

?,?,?

The input units for the coordinates must also be in the units requested.
XFIRST must be a positive value. A zero entry for DELTAX will result in a
Single X-coordinate observation. Results of calculations for multiple x-co-
ordinates will be listed from XFIRST to XLAST.

ENTER YFIRST, YLAST, DELTAY (L)

?,?,?

Any of the numerical values used to define the y-coordinates of obser-
vation points may be positive or negative. If the x-z coordinate system
has been selected, a command to enter the z-coordinates, rather than the
y-coordinates, will be issued.

ENTER ZFIRST, ZLAST, DELTAX (L)

?,?,?

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Values of ZFIRST must be greater than, or equal to, zero.

Edit Commands

Once the basic input data have been entered" the problem as currently

defined is listed and the program enters the "edit" mode. The edit commands

are listed in Table 2. The request for information is:

ENTER NEXT COMMAND?

One of the responses from Table 2 should be given. If the response is in-

correct or improperly formulated the statement

ERROR IN LAST COMMAND -- REENTER

?

is issued. Error messages for invalid numerical data will be issued as

described under the Basic Input Commands.

The request for information will be repeated until one of the responses

LI, RN, NP, or DN is entered.

LI will list the problem as currently defined.

RN will initiate the calculation of concentrations and

print the results.

NP will request a complete new problem definition using

the "Basic Input Data" dialog.

DN will terminate the program.

Listings of the dialog and the results for the two example problems

discussed in Section II are included in Appendix E.

Although many tests for valid input data and properly formulated edit

commands have been coded in the program, the user is encouraged to correct

TABLE 2

EDIT COMMANDS FOR PLUME

Command	Variable Changed/Execution
VX	New Seepage Velocity
RD	Retardation Coefficient
DE	Decay Constant
DX	X-Dispersion Coefficient
DY	Y-Dispersion Coefficient
DZ	Z-Dispersion Coefficient
PO	Porosity
OB	X-and Y-Coordinates
XC	X-Coordinates
YC	Y-Coordinates
ZC	Z-Coordinates
RT	Source Rate Schedule
NP	New Problem
RN	Run
DN	Done
LI	List Input Data

"keyboard errors" before the data are transmitted. These precautions will serve to minimize the frustration of program termination as a result of fatal errors during execution of the numerical computations.

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APPENDIX A

Description of Program PLUME

Program PLUME has been written in an unextended Fortran computer code in an effort to make the program transportable between computer systems. The computer code consists of a main program and several function subroutines which are required to evaluate the Hantush well function. The program has been documented "internally" through the liberal use of comment statements.

The main program has been divided into three sections. A listing of the computer code is presented in Appendix C. Section I provides for the "Basic Input Data" as described in Section III of this report. The numerical evaluation of concentration at specified grid coordinates is accomplished in Section II of the main program which contains the code for the analytical solution of the governing differential equations. Section III provides for problem redefinition and control of execution under the "Edit" mode discussed in the body of this report.

Eight function subroutines are used to evaluate the Hantush well function using the numerical methods described in Appendix B. Listings of the computer codes are presented in Appendix D. FUNCTION W(U,B) evaluates the Hantush well function for $B \leq 20$. For $B > 20$ the term $EXP(Pe_x/2) W(U,B)$ in Equation 45 is evaluated using FUNCTION WELPRD (U,B,PEX). This procedure is used to avoid taking the direct product of very large numbers, $EXP(Pe_x/2)$, and very small numbers, $W(U,B)$, for large values of B.

FUNCTION GAUSS is a 24-point Gauss-Legendre quadrature numerical integration scheme which is used to evaluate the Hantush well function

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using either Equation B-6 or Equation B-7. FUNCTION FUNCTN evaluates

the integrand of Equations B-6 and B-7.

The four remaining function subroutines are used to evaluate

mathematical functions using rational approximations or polynomial

approximations. They are:

FUNCTION BIO   (Z)   Modified Bessel function of the first
                             kind of order zero.

FUNCTION BKO   (Z)   Modified Bessel function of the second
                             kind of order zero.

FUNCTION E1LOG   (Z)   Natural logrithm of the exponential
                             integral.

FUNCTION ERFC   (Z)   Complimentary error function.

These four function subroutines are support FUNCTION W(U,B) and/or

FUNCTION WELPRD (U,B,PEX). If system subroutines are available for

these functions they may be substituted for the function subroutines

provided with Program PLUME.

APPENDIX B

NUMERICAL EVALUATION OF THE HANTUSH WELL FUNCTION

The Hantush well function can be defined as

$$W(U,B) = \int_u^\infty \frac{1}{\xi} \, \text{EXP} \left(-\xi - \frac{B^2}{4\xi} \right) d\xi \qquad (B-1)$$

or the reciprocal relation

$$W(U,B) = 2K_o(B) - \int_{B^2/4U}^\infty \frac{1}{\xi} \, \text{EXP} \left(-\xi - \frac{B^2}{4\xi} \right) d\xi \qquad (B-2)$$

where ξ is a dummy integration variable (Hantush, 1964). Using the identity

$$\int_a^\infty f(\xi) \, d\xi = \int_0^\infty f(\xi) \, d\xi - \int_0^a f(\xi) \, d\xi \qquad (B-3)$$

Equation B-1 can be rewritten as

$$W(U,B) = \int_0^\infty \frac{1}{\xi} \, \text{EXP} \left(-\xi - \frac{B^2}{4\xi} \right) d\xi - \int_0^u \frac{1}{\xi} \left(-\xi - \frac{B^2}{4\xi} \right) d\xi \qquad (B-4)$$

Now

$$\int_0^\infty \frac{1}{\xi} \, \text{EXP} \left(-\xi - \frac{B^2}{4\xi} \right) d\xi = 2K_o(B) \qquad (B-5)$$

where K_o is the modified Bessel function of the second kind of order zero. Substituting Equation B-5 into Equation B-4, the well function becomes

$$W(U,B) = 2K_o(B) - \int_0^u \frac{1}{\xi} \, \text{EXP} \left(-\xi - \frac{B^2}{4\xi} \right) d\xi \qquad (B-6)$$

The reciprocal relation, Equation B-2, can also be written in terms of finite limits. Using the relationship given by Equations B-4 and B-5, the reciprocal relation can be expressed as

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$$W(U,B) = \int_0^{B^2/4U} \frac{1}{\xi} \, \text{EXP} \left(-\xi - \frac{B^2}{4\xi} \right) d\xi \qquad (B-7)$$

For $0 < B \leq 20$, values of $W(U,B)$ for $0 < U < B/2$ are obtained from Equation B-6 by first evaluating the value of the integrand using a 24-point Gauss-Legendre numerical integration scheme. For $B/2 \leq U < \infty$, the reciprocal relation, Equation B-7, is evaluated using the same numerical integration scheme.

For $0 < B \leq 0.1$, values of $W(U,B)$ are obtained from the series expansions presented by Hantush and Jacob (1955). For $U \leq 1$

$$W(U,B) = 2K_0(B) - I_0(B)E_1\left(\frac{B^2}{4U}\right) \qquad (B-8)$$

$$+ \text{EXP}\left(-\frac{B^2}{4U}\right) \left[0.57721566 + \ln(U) + E_1(U) + \frac{U}{4}\frac{B^2}{4}\left(1 - \frac{U}{9}\right) \right]$$

and for $U > 1$

$$W(U,B) = I_0(B)E_1(U) - \text{EXP}(-U) \left[\frac{B^2}{4}\left[\frac{1}{U} - \frac{1}{36U^2}\right] + \frac{B^4}{16}\left[\frac{1}{4U} - \frac{1}{4U^2}\right] \right]$$

$$(B-9)$$

where I_0 is the modified Bessel function of the first kind of order zero, E is the exponential integral, and 0.57721566 is Euler's constant.

For $B > 20$, the third order approximation for $W(U,B)$ presented by Wilson and Miller (1979) is used to evaluate the well function. The approximation is

$$W(U,B) = \left(\frac{\pi}{2B}\right)^{\frac{1}{2}} \text{EXP}(-B) \left[\left(1 - \frac{1}{8B}\right) \text{ERFC}(-\beta) + \frac{\beta}{4B\pi^{\frac{1}{2}}} \text{EXP}\left(-\beta^2\right) \right]$$

$$(B-10)$$

where

$$\beta = \frac{B-2U}{(4U)^{\frac{1}{2}}}$$

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and ERFC is the complimentary error function.

Now, for large positive values of β,

$$W(U,B) = 2 \left[\frac{\pi}{2B}\right]^{\frac{1}{2}} EXP\ (-B)\ \left[1 - \frac{1}{8B}\right] \tag{B-11}$$

and an asymptotic expansion for $K_o(B)$ can be written as

$$K_o(B) = \left[\frac{\pi}{2B}\right]^{\frac{1}{2}} EXP\ (-B)\ \left[1 - \frac{1}{8B}\right] + \frac{9}{2\ (8B)^2} + \ldots \tag{B-12}$$

Thus for $B > 20$ and $\beta > 7.5$ the well function is approximated as

$$W(U,B) - 2K_o(B) \tag{B-13}$$

Note that this approximation is equivalent to the relation

$$W(0,B) = 2K_o(B) \tag{B-14}$$

Evaluation of the Hantush well function using the methods described in the previous paragraphs have been checked for both accuracy and continuity of the function between the various approximations. The Gauss-Legendre quadrature scheme was checked using up to 48 quadrature points. A maximum of 24 quadrature points yielded results accurate to four significant figures in the mantissa over the entire range of arguments which require numerical integration. The other approximations for $W(U,B)$ are also accurate to four significant figures in the mantissa.

APPENDIX C

Listing of Program PLUME

```
C         TWO-DIMENSIONAL PLUME IN UNIFORM GROUND-WATER FLOW
C             JAN WAGNER
C             SCHOOL OF CHEMICAL ENGINEERING
C             OKLAHOMA STATE UNIVERSITY
C             STILLWATER, OK  74078
C             PHONE (405) 624-5280
C             JULY, 1981
C
          DIMENSION CXYT(51,51),Q(20),T(20),TITLE(30),X(51),Y(51),IC(16)
          INTEGER TITLE
          DATA IC/'DE','VX','RD','DX','DY','DZ','PO','OB','XC','YC','ZC',
         1'RT','NP','RN','DN','LI'/
          DATA KPRO1/'XY'/, KPRO2/'XZ'/, KHARY/'Y'/, KHARZ/'Z'/
          DATA NPAGE/1/
C
C         READ DEVICE: NI=1       WRITE DEVICE: NO=1
          NI=1
          NO=1
C
C         MAXIMUM NUMBER OF OBSERVATION POINTS IN EACH COORDINATE
C         DIRECTION HAS BEEN SET AT 50
C             DIMENSION C(N,N), X(N), Y(N) -- WHERE N=MAXPTS+1
          MAXPTS = 50
C
C         MAXIMUM NUMBER OF SOURCE RATES FOR SUPERPOSITION IN TIME
C         HAS BEEN SET AT 20
C             DIMENSION Q(20),T(20)
          MAXRT = 20
C
C
C **** SECTION I -- BASIC INPUT DATA
C
C         READ TITLE
        1 WRITE(NO,3)
        3 FORMAT(3X,'ENTER TITLE',/' ?')
          READ(NI,5) (TITLE(I), I=1,30)
        5 FORMAT(30A2)
C
C         SELECT VERTICALLY OR HORIZONTALLLY AVERAGED SOLUTION
          KFLOW = 3
          WRITE(NO,7)
        7 FORMAT(3X,'ENTER COORDINATE SYSTEM',/,
         16X,'XY FOR VERTICALLY-AVERAGED SOLUTION',/,
         26X,'XZ FOR HORIZONTALLY-AVERAGED SOLUTION',/,' ?')
        8 READ(NI,9) KNTL
        9 FORMAT(A2)
          IF(KNTL.EQ.KPRO1) KFLOW=1
          IF(KNTL.EQ.KPRO2) KFLOW=2
          GO TO (12,12,10), KFLOW
       10 WRITE(NO,11)
       11 FORMAT(3X,'ERROR IN PROBLEM SELECTION -- REENTER',/,' ?')
          GO TO 8
       12 CONTINUE
          KHAR = KHARY
```

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```
      IF(KFLOW.EQ.2) KHAR=KHARZ
C
C     DEFINE UNITS
      WRITE(NO,15)
   15 FORMAT(3X,'ENTER UNITS FOR LENGTH (2 CHARACTERS)',/,' ?')
      READ(NI,25) IL
   25 FORMAT(A2)
      WRITE(NO,35)
   35 FORMAT(3X,'ENTER UNITS FOR TIME (2 CHARACTERS)',/,' ?')
      READ(NI,25) IT
      WRITE(NO,45)
   45 FORMAT(3X,'ENTER UNITS FOR CONCENTRATION (6 CHARACTERS)',/,' ?')
      READ(NI,26) IM1,IM2,IM3
   26 FORMAT(3A2)
C
C     ENTER DATA FOR FIRST PROBLEM
C
C     POROSITY
      WRITE(NO,55)
   55 FORMAT(3X,'ENTER AQUIFER POROSITY',/,' ?')
      READ(NI,56) P
   56 FORMAT(F10.0)
   57 IF(P.GT.0.0.AND.P.LT.1.0) GO TO 60
      WRITE(NO,58)
   58 FORMAT(3X,'POROSITY MUST BE GREATER THAN ZERO',
     1' AND LESS THAN ONE -- REENTER',/,' ?')
      READ(NI,56) P
      GO TO 57
C
C     SEEPAGE VELOCITY
   60 WRITE(NO,65) IL,IT
   65 FORMAT(3X,'ENTER SEEPAGE VELOCITY, 'A2,'/',A2,/,' ?')
      READ(NI,56) V
   66 IF(V.GT.0.0) GO TO 70
      WRITE(NO,67)
   67 FORMAT(3X,'SEEPAGE VELOCITY MUST BE GREATER THAN ZERO',
     1' -- REENTER',/,' ?')
      READ(NI,56) V
      GO TO 66
C
C     RETARDATION COEFFICIENT
   70 WRITE(NO,75)
   75 FORMAT(3X,'ENTER RETARDATION COEFFICIENT',/,' ?')
      READ(NI,56) RD
   76 IF(RD.GE.1.0) GO TO 80
      WRITE(NO,77)
   77 FORMAT(3X,'RETARDATION COEFFICIENT MUST BE GREATER THAN OR',
     1' EQUAL TO ONE',/,' -- REENTER',/,' ?')
      READ(NI,56) RD
      GO TO 76
C
C     DISPERSION COEFFICIENTS
   80 WRITE(NO,85) KHAR,IL,IT
   85 FORMAT(3X,'ENTER X AND ',A1,' DISPERSION COEFFICIENTS, SQ ',A2,
```

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```
    1'/',A2,/,' ?,?')
 86 FORMAT(2F10.0)
    READ(NI,86) DX,DY
 87 IF(DX.GT.0.0) GO TO 89
    WRITE(NO,88) _
 88 FORMAT(3X,'X DISPERSION COEFFICIENT MUST BE GREATER THAN ZERO',
    1' -- REENTER',/,' ?')
    READ(NI,56) DX
    GO TO 87
 89 IF(DY.GT. 0.0) GO TO 92
 90 WRITE(NO,91) KHAR
 91 FORMAT(3X,A1,' DISPERSION COEFFICIENT MUST BE GREATER THAN ZERO',
    1' -- REENTER',/,' ?')
    READ(NI,56) DY
    GO TO 89
C
C     FIRST-ORDER DECAY CONSTANT
 92 WRITE(NO,95) IT
 95 FORMAT(3X,'ENTER DECAY CONSTANT, 1/',A2,/,' ?')
    READ(NI,56) DECAY
C
C     SOURCE RATE SCHEDULE
    Q(1) = 0.0
    T(1) = 0.0
    WRITE(NO,105) MAXRT
105 FORMAT(3X,'ENTER THE NUMBER OF SOURCE RATES (MAXIMUM OF',I4,')',/,
   16X,'0 FOR STEADY-STATE SOLUTION',/,' ?')
100 READ(NI,106) N
106 FORMAT(I4)
    IF(N.LE.MAXRT) GO TO 110
    WRITE(NO,107) N,MAXRT
107 FORMAT(3X,I3,' SOURCE RATES EXCEED MAXIMUM OF',I4,' -- REENTER',/,
   1' ?')
    GO TO 100
110 CONTINUE
    IF(N.LE.0) GO TO 121
    MT = N + 1
    DO 120  I=1,N
      M = I + 1
      WRITE(NO,115) I,IM1,IM2,IM3,IL,IT,IL,IT
115     FORMAT(3X,'ENTER MASS RATE ',I2,' (',3A2,')(CU ',A2,'/',
   1           A2,'/',A2,')   AND TIME, (',A2,')',/,' ?,?')
      READ(NI,116) Q(M),T(M)
116     FORMAT(2F10.0)
117     IF(T(M).GT.0.0) GO TO 119
      WRITE(NO,118)
118     FORMAT(3X,'TIME MUST BE GREATER THAN ZERO -- REENTER',/,' ?')
      READ(NI,56) T(M)
      GO TO 117
119     CONTINUE
120 CONTINUE
    GO TO 124
121 WRITE(NO,122) IM1,IM2,IM3,IL,IT,IL
122 FORMAT(3X,'ENTER STEADY-STATE MASS RATE, (',3A2,')(CU ',A2,
```

```
      1'/',A2,'/',A2,')',/,' ?')
       READ(NI,56) Q(1)
       MT = 1
   124 CONTINUE
C                        —
C      COORDINATES OF THE OBSERVATION POINTS
       WRITE(NO,125) IL
   125 FORMAT(3X,'ENTER XFIRST, XLAST, DELTAX  (',A2,')' ,/,' ?,?,?')
       READ(NI,126) XF,XL,DELX
   126 FORMAT(3F10.0)
       DELX = ABS(DELX)
   127 IF(XF.GT.0.0.AND.DELX.LE.1.0E-06) GO TO 132
       IF(XF.GT.0.0) GO TO 130
       WRITE(NO,128)
   128 FORMAT(3X,'XFIRST MUST BE GREATER THAN ZERO -- REENTER',/' ?')
       READ(NI,56) XF
       GO TO 127
   130 IF(XL.GT.0.0) GO TO 133
       WRITE(NO,131)
   131 FORMAT(3X,'XLAST MUST BE GREATER THAN ZERO -- REENTER',/,' ?')
       READ(NI,56) XL
       GO TO 130
   132 XL = XF
   133 CONTINUE
       IF(KFLOW.EQ.2) GO TO 136
       WRITE(NO,135) IL
   135 FORMAT(3X,'ENTER YFIRST, YLAST, DELTAY  (',A2,')',/,' ?,?,?')
       READ(NI,126) YF,YL,DELY
       DELY = ABS(DELY)
       GO TO 143
   136 WRITE(NO,137) IL
   137 FORMAT(3X,'ENTER ZFIRST, ZLAST, DELTAZ  (',A2,')',/,' ?,?,?')
       READ(NI,126) YF,YL,DELY
       DELY = ABS(DELY)
   138 IF(YF.GE.0.0.AND.DELY.LE.1.0E-06) GO TO 142
       IF(YF.GE.0.0) GO TO 140
       WRITE(NO,139)
   139 FORMAT(3X,'ZFIRST MUST NOT BE LESS THAN ZERO -- REENTER',/,' ?')
       READ(NI,56) YF
       GO TO 138
   140 IF(YL.GT.0.0) GO TO 143
       WRITE(NO,141)
   141 FORMAT(3X,'ZLAST MUST BE GREATER THAN ZERO -- REENTER',/,' ?')
       READ(NI,56) YL
       GO TO 140
   142 YL = YF
   143 CONTINUE
C
C      LIST PROBLEM DEFINITION
       WRITE(NO,147) NPAGE
   147 FORMAT(1H1,2X,'PLUME I',
      1/3X,'PAGE ',I3///)
       NPAGE = NPAGE + 1
       WRITE(NO,145) (TITLE(I), I=1,30),IL,IT,V,IL,IT,DX,KHAR,IL,IT,DY,P
```

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```
    145 FORMAT(3X,30A2,//,
       18X,'SEEPAGE VELOCITY, (',A2,'/',A2,') ',25X,F10.4,/,
       28X,'X DISPERSION COEFFICIENT (',A2,'**2/',A2,')   ',13X,F10.4,/,
       38X,A1,' DISPERSION COEFFICIENT (',A2,'**2/',A2,')   ',13X,F10.4,/,
       58X,'POROSITY ',42X,F10.4)
       WRITE(NO,146) RD,IT,DECAY
    146 FORMAT(//,8X,'RETARDATION COEFFICIENT',28X,F10.4,/,
       18X,'FIRST ORDER DECAY CONSTANT (1/',A2,')',18X,F10.4)
       IF(MT.GT.1) GO TO 160
       WRITE(NO,155) IM1,IM2,IM3,IL,IT,IL,Q(1)
    155 FORMAT(//,8X,'STEADY-STATE SOURCE RATE (',3A2,')(CU ',A2,'/',
       1A2,'/',A2,')    ',F12.4)
       GO TO 171
    160 WRITE(NO,165) IM1,IM2,IM3,IL,IT,IL,IT
    165 FORMAT(//,8X,'SOURCE RATE SCHEDULE',/,
       123X,'Q(',3A2,')(CU ',A2,'/',A2,'/',A2,')       T(',A2,')',,//)
       DO 170  I=1,N
          M = I + 1
          WRITE(NO,166) I,Q(M),T(M)
    166     FORMAT(17X,I2,10X,F10.2,6X,F10.2)
    170 CONTINUE
    171 WRITE(NO,175) IL,XF,XL,DELX,KHAR,YF,KHAR,YL,KHAR,DELY
    175 FORMAT(//,8X,'OBSERVATION POINTS (',A2,')',,/,
       117X,'XFIRST =',F10.2,3X,'XLAST =',F10.2,3X,'DELX =',F10.4,/,
       217X,A1,'FIRST =',F10.2,3X,A1,'LAST =',F10.2,3X,'DEL',A1,' =',
       1F10.4)
    180 CONTINUE
C
C
C
C ***** SECTION II -- NUMERICAL EVALUATION OF CONCENTRATION AT
C                     SPECIFIED GRID COORDINATES
C
C
C
C     X-COORDINATES
      GO TO 400
    190 IX = 1
      X(IX) = XF
      IF(DELX.LE.1.0E-06) GO TO 220
      DIF = XL - XF
      IF(ABS(DIF).LE.1.0E-06) GO TO 220
      DEL = DELX
      IF(DIF.LE.0.0) DEL=-DELX
      NPTS = ABS(DIF/DEL)
      REM = DIF - DEL*FLOAT(NPTS)
      NPTS = NPTS + 1
      IF(NPTS.LE.MAXPTS) GO TO 195
      WRITE(NO,193) NPTS,MAXPTS
    193 FORMAT(3X,I3,' X-OBSERVATION POINTS EXCEEDS MAXIMUM OF',I4,
       1/,3X,'USE COMMAND XC TO CHANGE COORDINATES')
       GO TO 400
    195 CONTINUE
       DO 200  IX=2,NPTS
          X(IX) = X(IX-1) + DEL
```

```
      200 CONTINUE
          IX = NPTS
          IF(ABS(REM).LT.1.0E-06) GO TO 220
          IX = IX + 1
          X(IX) = XL
      220 CONTINUE
C
C         Y-COORDINATES
          JY = 1
          Y(JY) = YF
          IF(DELY.LE.1.0E-06) GO TO 240
          DIF = YL - YF
          IF(ABS(DIF).LE.1.0E-06) GO TO 240
          DEL = DELY
          IF(DIF.LE.0.0) DEL=-DELY
          NPTS = ABS(DIF/DEL)
          REM = DIF - DEL*FLOAT(NPTS)
          NPTS = NPTS + 1
          IF(NPTS.LE.MAXPTS) GO TO 225
          WRITE(NO,223) NPTS,MAXPTS
      223 FORMAT(3X,I3,' Y- OR Z-OBSERVATION POINTS EXCEEDS MAXIMUM OF',I4,
         1/,3X,'USE COMMAND YC OR ZC TO CHANGE COORDINATES')
          GO TO 400
      225 CONTINUE
          DO 230  JY=2,NPTS
              Y(JY) = Y(JY-1) + DEL
      230 CONTINUE
          JY = NPTS
          IF(ABS(REM).LT.1.0E-06) GO TO 240
          JY = JY + 1
          Y(JY) = YL
      240 CONTINUE
C
          DAMK = DX*DECAY*RD/(V**2)
          BETA = DX/DY
          CON1 = 1.0/(12.566371*P*((DX*DY)**0.5))
          CON2 = 1.0 + 4.0*DAMK
C
          DO 300  I=1,IX
              PEX = V*X(I)/DX
              DO 300  J=1,JY
                  PEY = V*Y(J)/DX
                  PEXY = (PEX**2 + BETA*(PEY**2))**0.5
                  IF(MT.GT.1) GO TO 245
                  B = 0.5*PEXY*(CON2**0.5)
                  C = 2.0*CON1*Q(1)*EXP(PEX/2.0 + ALOG(BK0(B)))
                  GO TO 260
      245         C = 0.0
                  DO 250  K=2,MT
                      PINJ = V*V*T(K)/(DX*RD)
                      TAU = PINJ/(PEXY**2)
                      S = Q(K) - Q(K-1)
                      U = 0.25/TAU
                      B = 0.5*PEXY*(CON2**0.5)
```

(46)

```
                   IF (B.GT.20.0) GO TO 247
                   WF = W(U,B)
                   SUMLOG = PEX/2.0 + ALOG(WF)
                   TERM = EXP(SUMLOG)
                   GO TO 249
C                  FOR LARGE VALUES OF B USE THE THIRD ORDER APPROXIMATION
C                  OF WILSON AND MILLER (1979) JOUR. HYDRAULICS DIV., ASCE,
C                  VOL 105, NO HY12, P 1565.
C
C                  NOTE:  THE TERM EXP(PEX/2) IS INCLUDED IN THE NUMERICAL
C                  APPROXIMATION FOR W(U,B) TO AVOID COMPUTATIONAL DIFFICULTIES
C                  IN TAKING THE PRODUCT  EXP(PEX/2)*W(U,B)
  247              WF = WELPRD(U,B,PEX)
                   TERM = WF
  249              IF(WF.LE.1.0E-32) TERM=0.0
                   C = C + CON1*S*TERM
  250          CONTINUE
  260      CONTINUE
           CXYT(I,J) = C
           IF(KFLOW.EQ.2) CXYT(I,J)=2.0*CXYT(I,J)
  300 CONTINUE
C
C      PRINT CONCENTRATION DISTRIBUTION
       IF(MT.EQ.1) GO TO 306
       WRITE(NO,147) NPAGE
       NPAGE = NPAGE + 1
       WRITE(NO,305) T(2),IT,IM1,IM2,IM3,IL
  305 FORMAT(13X,'CONCENTRATION DISTRIBUTION AT ',F10.2,
     1 11X,A2,' (',3A2,') ',//,' *',/,'    * X(',A2,')')
       GO TO 309
  306 WRITE(NO,147) NPAGE
       NPAGE = NPAGE + 1
       WRITE(NO,307) IM1,IM2,IM3,IL
  307 FORMAT(13X,'CONCENTRATION DISTRIBUTION AT STEADY STATE',
     1 ' (',3A2,') ',//,' *',/,'    * X(',A2,')')
  309 CONTINUE
       LIM1 = 1
       LIM2 = 7
  310 IF(LIM2.GE.IX) LIM2=IX
       WRITE(NO,315) (X(L),L=LIM1,LIM2)
  315 FORMAT('     *',4X,7F10.2)
       WRITE(NO,325) KHAR,IL
  325 FORMAT(1X,A1,'(',A2,') *',/,9X,'*')
       DO 350  J=1,JY
           WRITE(NO,335) Y(J),(CXYT(L,J),L=LIM1,LIM2)
  335 FORMAT(2X,F8.2,7F10.4)
  350 CONTINUE
       IF(LIM2.EQ.IX) GO TO 400
       LIM1 = LIM1 + 7
       LIM2 = LIM2 + 7
       IF(MT.EQ.1) GO TO 360
       WRITE(NO,147) NPAGE
       NPAGE = NPAGE + 1
       WRITE(NO,355) T(2),IT,IM1,IM2,IM3,IL
```

(47)

```
  355 FORMAT(7X,'CONCENTRATION DISTRIBUTION AT ',F10.2,
     11X,A2,' (',3A2,')    (CONTINUED)',//,' *',/,'    * X(',A2,')')
      GO TO 370
  360 WRITE(NO,147) NPAGE
      NPAGE = NPAGE + 1
      WRITE(NO,365) IM1,IM2,IM3,IL
  365 FORMAT(7X,'CONCENTRATION DISTRIBUTION AT STEADY STATE',
     1' (',3A2,')    (CONTINUED)',//,' *',/,'    * X(',A2,')')
  370 CONTINUE
      GO TO 310
  400 CONTINUE
C
C
C ***** SECTION III -- PROBLEM REDEFINITION AND CONTROL OF EXECUTION
C
C
      KNTL = 0
      WRITE(NO,405)
  405 FORMAT(//,3X,'ENTER NEXT COMMAND',/,3X, ' ?')
  410 READ(NI,415) NEXT
  415 FORMAT(A2,F10.0)
C
      DO 420  I=1,16
          IF(NEXT.EQ.IC(I)) GO TO 430
  420 CONTINUE
      WRITE(NO,425)
  425 FORMAT(3X,'ERROR IN LAST COMMAND -- REENTER',/,3X,' ?')
      GO TO 410
  430 GO TO (500,510,520,530,540,540,550,560,570,580,580,590,1,
     1190,700,143),I
C
C     NEW DECAY CONSTANT
  500 WRITE(NO,95) IT
      READ(NI,56) DECAY
      GO TO 400
C
C     NEW SEEPAGE VELOCITY
  510 WRITE(NO,65) IL,IT
      READ(NI,56) V
  515 IF(V.GT.0.0) GO TO 400
      WRITE(NO,67)
      READ(NI,56) V
      GO TO 515
C
C     NEW RETARDATION COEFFICIENT
  520 WRITE(NO,75)
      READ(NI,56) RD
  525 IF(RD.GE.1.0) GO TO 400
      WRITE(NO,77)
      READ(NI,56) RD
      GO TO 525
C
C     NEW X DISPERSION COEFFICIENT
  530 WRITE(NO,531) IL,IT
```

```
      531 FORMAT(3X,'ENTER X DISPERSION COEFFICIENT, SQ ',A2,
     1'/',A2,/,' ?')
          READ(NI,56) DX
      535 IF(DX.GT.0.0) GO TO 400
          WRITE(NO,88)
          READ(NI,56) DX
          GO TO 535
C
C     NEW Y OR Z DISPERSION COEFFICIENT
      540 WRITE(NO,541) KHAR,IL,IT
      541 FORMAT(3X,'ENTER ',A1,' DISPERSION COEFFICIENT, SQ ',A2,
     1'/',A2,/,' ?')
          READ(NI,56) DY
      545 IF(DY.GT.0.0) GO TO 400
          WRITE(NO,91) KHAR
          READ(NI,56) DY
          GO TO 545
C
C     NEW POROSITY
      550 WRITE(NO,55)
          READ(NI,56) P
      555 IF(P.GT.0.0.AND.P.LT.1.0) GO TO 400
          WRITE(NO,58)
          READ(NI,56) P
          GO TO 555
C
C     NEW SET OF X AND Y OBSERVATIONS
      560 KNTL = 1
C
C     NEW SET OF X OBSERVATIONS
      570 WRITE(NO,125) IL
          READ(NI,126) XF,XL,DELX
          DELX = ABS(DELX)
      572 IF(XF.GT.0.0.AND.DELX.LE.1.0E-06) GO TO 574
          IF(XF.GT.0.0) GO TO 573
          WRITE(NO,128)
          READ(NI,56) XF
          GO TO 572
      573 IF(XL.GT.0.0) GO TO 575
          WRITE(NO,131)
          READ(NI,56) XL
          GO TO 573
      574 XL = XF
      575 CONTINUE
          IF(KNTL.GT.0) GO TO 580
          GO TO 400
C
C     NEW SET OF Y OR Z OBSERVATIONS
      580 IF(KFLOW.EQ.2) GO TO 581
          WRITE(NO,135) IL
          READ(NI,126) YF,YL,DELY
          DELY = ABS(DELY)
          GO TO 400
      581 WRITE(NO,137) IL
```

```
      READ(NI,126) YF,YL,DELY
      DELY = ABS(DELY)
  582 IF(YF.GE.0.0.AND.DELY.LE.1.0E-06) GO TO 584
      IF(YF.GE.0.0) GO TO 583
      WRITE(NO,139)
      READ(NI,56) YF
      GO TO 582
  583 IF(YL.GT.0.0) GO TO 585
      WRITE(NO,141)
      READ(NI,56) YL
      GO TO 583
  584 YL = YF
  585 GO TO 400
C
C     NEW SOURCE RATE SCHEDULE
  590 WRITE(NO,595) N
  595 FORMAT(3X,I3,' SOURCE RATES IN CURRENT SCHEDULE -- ',
     1'ENTER RATE TO BE CHANGED',/,3X,
     2'(ENTER 0 TO REDEFINE ENTIRE RATE SCHEDULE)',
     3/,3X,' ?')
      READ(NI,596) NEW
  596 FORMAT(I2)
      IF(NEW.LE.0) GO TO 600
      MEW = NEW + 1
      WRITE(NO,597) NEW,IM1,IM2,IM3,IL,IT,IL,T(MEW),IT
  597 FORMAT(3X,'ENTER NEW MASS RATE',I3,' (',3A2,')(CU ',A2,'/',
     1A2,'/',A2,') FOR LAST',F10.2,' ',A2,/,3X,' ?')
      READ(NI,598) Q(MEW)
  598 FORMAT(F10.0)
      GO TO 400
C
C     REDEFINE ENTIRE RATE SCHEDULE
  600 WRITE(NO,105) MAXRT
  605 READ(NI,106) N
      IF(N.LE.MAXRT) GO TO 610
      WRITE(NO,107) N,MAXRT
      GO TO 605
  610 CONTINUE
      IF(N.LE.0) GO TO 630
      MT = N + 1
      DO 620  I=1,N
         M = I + 1
         WRITE(NO,115) I,IM1,IM2,IM3,IL,IT,IL,IT
         READ(NI,116) Q(M),T(M)
  617    IF(T(M).GT.0.0) GO TO 619
         WRITE(NO,118)
         READ(NI,56) T(M)
         GO TO 617
  619    CONTINUE
  620 CONTINUE
      GO TO 400
  630 WRITE(NO,122) IM1,IM2,IM3,IL,IT,IL
      READ(NI,56) Q(1)
      MT = 1
```

```
       GO TO 400
700 STOP
    END
```

APPENDIX D

LISTING OF UTILITY FUNCTION SUBROUTINES

```
      FUNCTION W(U,B)
C     EVALUATION OF THE HANTUSH WELL FUNCTION
C     THIS VERSION HANDLES ARGUMENTS OVER THE ENTIRE RANGE
      REAL*8 A1,A2,FUNCTN,GAUSS,DZ
      EXTERNAL FUNCTN
      COMMON BF
      BF=B
      IF(B.GT.0.1) GO TO 200
      IF(U.GT.1.0) GO TO 100
C
C     FOR B < 0.1  USE APRROXIMATIONS PRESENTED BY
C     HANTUSH, M.S. AND C.E. JACOB (1955)
C     TRANSACTIONS AMERICAN GEOPHYSICAL UNION,
C     VOL 36, NO. 1 PP. 95 - 100.
C
C
      IF(U.LE.1.0E-10) GO TO 50
C
C
C     EQUATION 12, FOR U < 1.0
C
C
      CON = B*B/(4.0*U)
      TERM1 = 2.0*BK0(B)
      BI0LOG = ALOG(BI0(B))
      TERM2 = EXP(BI0LOG + E1LOG(CON))
      E1U = EXP(E1LOG(U))
      SUM = 0.57721566 + ALOG(U) + E1U + (U*B*B/16.0)*(1.0 - U/9.0)
      SUMLOG = ALOG(SUM)
      TERM3 = EXP(SUMLOG - CON)
      W = TERM1 - TERM2 + TERM3
      RETURN
   50 W = 2.0*BK0(B)
      RETURN
C
C     RECIPROCAL RELATION, EQUATION 17, FOR U > 1.0
C
C
  100 BI0LOG = ALOG(BI0(B))
      TERM1 = EXP(BI0LOG + E1LOG(U))
      SUM = (B*B/4.0)*(1.0/U - 1.0/(36.0*U*U))
     1        + ((B*B/4.0)**2)*(1.0/(4.0*U) - 1.0/(4.0*U*U))
      SUMLOG = ALOG(SUM)
      TERM2 = EXP(SUMLOG - U)
      W = TERM1 - TERM2
      RETURN
C
C
  200 CONTINUE
C     FOR 0.1 < B < 20.0  USE NUMERICAL INTEGRATION
C     FOR U < B/2, W(U,B) = 2K0(B)-INT(0--U) FUNCTION
C     FOR U > B/2  W(U,B) = INT(0--B**2/4U) FUNCTION
C
C
```

(53)

```
A1 = 0.0
A2 = U
B2 = B/2.0D00
IF(U.GE.B2) A2=B2*B2/U
DZ = GAUSS(A1,A2,FUNCTN)
Z = DZ
BK0B = 2.0*BK0(B)
W = BK0B - Z
IF(U.GE.B2) W=Z
RETURN
END
```

(54)

```
      FUNCTION FUNCTN(Z)
C     INTEGRAND OF HANTUSH WELL FUNCTION
      REAL*8 DB,Z,ARG,FUNCTN
      COMMON BF
      DB=BF
      ARG = DLOG(Z) + Z + DB*DB/(4.0D00*Z)
      FUNCTN = DEXP(-ARG)
      RETURN
      END
```

```
      FUNCTION GAUSS(A,B,FUNCTN)
C
C     NUMERICAL INTEGRATION  BY 24 POINT GAUSS-LEGENDRE QUADRATURE
C     ZEROS AND WEIGHTING FACTORS ARE FROM TABLE 25.4, P916, OF
C     ABRAMOWITZ AND STENGUN(1966)
C
      REAL*8 A,B,C,D,FUNCTN,GAUSS,SUM,W,Z
      DIMENSION Z(12),W(12)
C
C
C
      DATA Z/0.064056892862065,0.191118867473616,0.315042679696163,
     1       0.433793507626045,0.545421471388839,0.648093651936975,
     2       0.740124191578554,0.820001985973902,0.886415527004401,
     3       0.938274552002732,0.974728555971309,0.995187219997021/
C
      DATA W/0.127938195346752,0.125837456346828,0.121670472927803,
     1       0.115505668053725,0.107444270115965,0.097618652104113,
     2       0.086190161531953,0.073346481411080,0.059298584915436,
     3       0.044277438817419,0.028531388628933,0.012341229799987/
C
C
C.....SET UP INITIAL PARAMETERS
      C = (B-A)/2.0D00
      D = (B+A)/2.0D00
C
C.....ACCUMULATE THE SUM IN THE 24-POINT FORMULA
      SUM = 0.0
      DO 5  J = 1, 12
           IF(Z(J).EQ.0.0) SUM = SUM + W(J)*FUNCTN(D)
           IF(Z(J).NE.0.0) SUM = SUM + W(J)*(FUNCTN(Z(J)*C + D)
     1                                  + FUNCTN(-Z(J)*C + D))
    5  CONTINUE
C
C.....MAKE INTERVAL CORRECTION AND RETURN
      GAUSS = C*SUM
      RETURN
      END
```

```fortran
      FUNCTION WELPRD(U,B,PEX)
C     THIS FUNCTION SUBROUTINE EVALUATES EXP(PEX/2)*W(U,B)
C     USING THE THIRD-ORDER APPROXIMATION FOR W(U,B) PRESENTED
C     BY WILSON AND MILLER (1979) JOUR. HYDRAULICS DIV., ASCE,
C     VOL 105,NO HY12, P 1565.
C                         —
      REAL*8 DI, FZ, TERMI, TERMO, SUM, Z
C
C     WRITE DEVICE: NO=1
      NO = 1
      PAR = (B-2.0*U)/((4.0*U)**0.5)
      IF(ABS(PAR).GT.7.5) GO TO 50
      TERM1 = (1.0 - 1.0/(8.0*B))*ERFC(-PAR)
      TERM2 = (PAR/(7.0898154*B))/EXP(PAR**2)
C     W = ((1.5707963/B)**0.5)*EXP(-B)*(TERM1+TERM2)
C     WELPRD = EXP(PEX/2)*W(U,B)
C             = ((1.5707963/B)**0.5)*EXP(PEX/2 - B)*(TERM1+TERM2)
      SUMLOG = ALOG(TERM1 + TERM2)
      WELOG = 0.5*(0.45158271 - ALOG(B)) + (PEX/2.0 - B) + SUMLOG
      IF(WELOG.LT.-72.0) GO TO 20
      WELPRD = EXP(WELOG)
      RETURN
   20 CONTINUE
      WELPRD = 1.0E-32
      RETURN
   50 CONTINUE
      IF(PAR.LT.0.0) GO TO 100
C     FOR B>20 AND PAR>7.5 W(U,B)=2K0(B)
      W = 2.0*BK0(B)
      WELOG = PEX/2.0 + ALOG(W)
      WELPRD = EXP(WELOG)
      RETURN
  100 CONTINUE
C     FOR PAR<-7.5 AN ASYMPTOTIC EXPANSION FOR ERFC(-PAR) IS UTILIZED
C     SEE SECTION 7.1 OF ABRAMOWITZ AND STEGUN (1966)
      COEFLG = PEX/2.0 - B - PAR*PAR - ALOG(-PAR) - 0.5*ALOG(2.0*B)
     1          + ALOG(1.0 - 0.1250/B)
      IF(COEFLG.LT.-72.0) GO TO 200
      Z = -PAR
      FZ = 2.0D00*Z*Z
      SUM = 1.0D00
      TERMO = 1.0D00
      DO 120  I=2,50
          DI = I
          TERMI = -TERMO*(2.0D00*DI-3.0D00)/FZ
          IF(DABS(TERMI).GT.DABS(TERMO)) GO TO 150
          SUM = SUM + TERMI
          TEST = TERMI/SUM
          IF(ABS(TEST).LT.1.0E-16) GO TO 150
          TERMO = TERMI
  120 CONTINUE
      WRITE(NO,500)
  500 FORMAT(6X,'*** WARNING -- ASYMPTOTIC APPROXIMATION FOR ERFC IN',/,
     1        6X,'                    FUNCTION WELPRD DID NOT CONVERGE WITH ',/,
```

(57)

```
      2      6X,'                          50 TERMS IN THE SUMMATION')
  150 SUMLOG = DLOG(SUM)
      WELOG = COEFLG + SUMLOG
      WELPRD = EXP(WELOG)
      RETURN        -
  200 CONTINUE
C     FOR LARGE NEGATIVE VALUES OF PAR, ERFC(-PAR) -> 0
      WELPRD = 1.0E-32
      RETURN
      END
```

```
      FUNCTION BI0(Z)
C     EVALUATION OF THE NATURAL LOG OF A MODIFIED BESSEL
C     FUNCTION OF THE FIRST KIND OF ORDER ZERO
C     POLYNOMIAL APPROXIMATIONS ARE USED FOR I0(Z)
C     SEE SECTION 9.8 OF ABRAMOWITZ AND STEGUN (1966)
      DIMENSION A(9)
      DATA A/0.9189385,4.32105045,6.09540829,6.45308739,4.6926023,
     13.88357842,3.63608323,4.10583047,5.540702353/
      NO = 1
      IF(Z.LE.0.0) GO TO 200
      T = Z/3.75
      IF(Z.GT.3.75) GO TO 100
      T2 = T*T
      T4 = T2*T2
      T6 = T2*T4
      T8 = T2*T6
      T10 = T2*T8
      T12 = T2*T10
      BI0 = 1.0 + 3.5156229*T2 + 3.0899424*T4 + 1.2067492*T6
     1          + 0.2659732*T8 + 0.0360768*T10+ 0.0045813*T12
      RETURN
  100 CONTINUE
      SUM = 0.0
      DO 150  I=1,9
      SIGN = (-1.0)**(I+1)
      IF(I.EQ.2) SIGN=1.0
      ARG = -1.0*A(I) - 0.5*ALOG(Z) - FLOAT(I-1)*ALOG(T)
      SUM = SUM + SIGN*EXP(ARG)
  150 CONTINUE
      BI0LOG = ALOG(SUM) + Z
      BI0 = EXP(BI0LOG)
      RETURN
  200 CONTINUE
      IF(Z.LT.0.0) GO TO 300
      BI0 = 1.0
      RETURN
  300 WRITE(NO,305) Z
  305 FORMAT(6X,'ARGUEMENT OF BESSEL FUNCTION I0(Z) IS NEGATIVE',/,
     116X,'Z = ',E12.6,'  -- PROGRAM TERMINATED')
      STOP
      END
```

```fortran
      FUNCTION BK0(Z)
C     EVALUATION OF MODIFIED BESSEL FUNTION OF SECOND KIND
C     OF ORDER ZERO
C     POLYNOMIAL APPROXIMATIONS ARE USED FOR K0(Z)
C     SEE SECTION 9.8 OF ABRAMOWITZ AND STEGUN (1966)
      NO = 1
      IF(Z.LE.0.0) GO TO 200
      T = Z/2.0
      T2 = T*T
      T4 = T2*T2
      T6 = T2*T4
      T8 = T2*T6
      T10 = T2*T8
      T12 = T2*T10
      IF(Z.GT.2.0) GO TO 100
      BK0 = -1.0*ALOG(T)*BI0(Z) - 0.57721566
     1      + 0.42278420*T2 + 0.23069756*T4 + 0.03488590*T6
     2      + 0.00262698*T8 + 0.00010750*T10+ 0.0740E-04*T12
      RETURN
  100 CONTINUE
      SUM = (1.25331414 - 0.07832358/T + 0.02189568/T2
     1      - 0.01062446/(T*T2) + 0.00587872/T4
     2      - 0.00251540/(T*T4) + 0.00053208/T6)
      BK0LOG = ALOG(SUM) - Z - 0.5*ALOG(Z)
      BK0 = EXP(BK0LOG)
      RETURN
  200 CONTINUE
      WRITE(NO,205) Z
  205 FORMAT(6X,'ARGUEMENT OF BESSEL FUNCTION K0(Z) IS LESS THAN',
     1' OR EQUAL TO ZERO',/,6X,'Z = ',E12.6,'  -- PROGRAM TERMINATED')
      STOP
      END
```

```fortran
      FUNCTION ERFC(Z)
C     RATIONAL APPROXIMATION OF THE COMPLIMENTARY ERROR FUNCTION
C     SEE SECTION 7.1 OF ABRAMOWITZ AND STEGUN (1966)
      IF(ABS(Z).GT.7.5) GO TO 30
C     THE FOLLOWING IDENTITIES ARE USED TO HANDLE NEGATIVE ARGUMENTS
C        ERFC( Z) = 1 - ERF(Z)
C        ERFC(-Z) = -ERFC(Z) = 1 + ERF(Z)
C
      X = Z
C     NEGATIVE ARGUMENTS
      IF (Z.LT.0.0) X = -Z
      ERFC =       1.0/((1.0 + 0.070523*X + 0.042282*(X**2)
     1                   + 0.009270*(X**3) + 0.000152*(X**4)
     2                   + 0.000276*(X**5) + 0.000043*(X**6))**16)
C     NOTE: 2-ERF(X) = ERFC(-X) = ERFC(Z) FOR Z<0
      IF (Z.LT.0.0) ERFC = 2.0 - ERFC
      RETURN
C
C     FOR Z>7.5, ERFC(Z)<2.32E-22 AND IS SET TO 0
   30 ERFC = 0.0
      RETURN
      END
```

```
      FUNCTION E1LOG(Z)
C     EVALUATION OF THE NATURAL LOG OF THE EXPONENTIAL INTEGRAL
C     POLYNOMIAL APPROXIMATIONS ARE USED FOR E1(Z)
C     SEE SECTION 5.1 OF ABRAMOWITZ AND STEGUN (1966)
      NO = 1
      IF(Z.LE.0.0) GO TO 200
      Z2 = Z*Z
      Z3 = Z*Z2
      IF(Z.GT.1.0) GO TO 100
C     ARGUEMENTS LESS THAN UNITY
      E1 = - 0.57721566    + 0.99999193*Z     - 0.24991055*Z2
     1     + 0.05519968*Z3 - 0.00976004*Z2*Z2 + 0.00107857*Z2*Z3
     2     - ALOG(Z)
      E1LOG = ALOG(E1)
      RETURN
  100 CONTINUE
C     ARGUEMENTS GREATER THAN UNITY
      E1LOG =    ALOG(Z2*Z2 +   8.5733287401*Z3 + 18.0590169730*Z2
     1                      +   8.6347608925*Z  +  0.2677737343    )
     2         - ALOG(Z2*Z2 +   9.5733223454*Z3 + 25.6329561486*Z2
     3                      +  21.0996530827*Z  +  3.9584969228    )
     4         - ALOG(Z) - Z
      E1 = EXP(E1LOG)
      RETURN
  200 WRITE(NO,205) Z
  205 FORMAT(6X,'ARGUEMENT OF EXPONENTIAL INTEGRAL IS LESS THAN',
     1' OR EQUAL TO ZERO',/,6X,'Z = ',E12.6,3X,'  -- PROGRAM',
     2' TERMINATED')
      STOP
      END
```

APPENDIX E

EXAMPLE PROBLEMS

The two example problems presented in the following pages are discussed in Section II of this report. The first demonstrates the application of Program PLUME to a continuous source of contamination. The second example approximates an instantaneous source using the principal of superposition in time as discussed in Section I.

```
   ENTER TITLE
?HEXAVALENT CHROMIUM PLUME

   ENTER COORDINATE SYSTEM
      XY FOR VERTICALLY-AVERAGED SOLUTION
      XZ FOR HORIZONTALLY-AVERAGED SOLUTION
?XY

   ENTER UNITS FOR LENGTH (2 CHARACTERS)
? M

   ENTER UNITS FOR TIME (2 CHARACTERS)
?DY

   ENTER UNITS FOR CONCENTRATION (6 CHARACTERS)
?MG/L

   ENTER AQUIFER POROSITY
?0.35

   ENTER SEEPAGE VELOCITY,   M/DY
?0.366

   ENTER RETARDATION COEFFICIENT
?1.0

   ENTER X AND Y DISPERSION COEFFICIENTS, SQ  M/DY
?,?7.79,1.56

   ENTER DECAY CONSTANT, 1/DY
?0.0

   ENTER THE NUMBER OF SOURCE RATES (MAXIMUM OF  20)
      0 FOR STEADY-STATE SOLUTION
?1

   ENTER MASS RATE  1 (MG/L  )(CU  M/DY/ M)  AND TIME, (DY)
?,?704.,2800.

   ENTER XFIRST, XLAST, DELTAX  ( M)
?,?,?200.,1200.,200.

   ENTER YFIRST, YLAST, DELTAY  ( M)
?,?,?150.,-150.,50.
```

(64)

HEXAVALENT CHROMIUM PLUME

SEEPAGE VELOCITY, (M/DY)	.3660
X DISPERSION COEFFICIENT (M**2/DY)	7.7900
Y DISPERSION COEFFICIENT (M**2/DY)	1.5600
POROSITY	.3500
RETARDATION COEFFICIENT	1.0000
FIRST ORDER DECAY CONSTANT (1/DY)	0.0000

SOURCE RATE SCHEDULE

	Q(MG/L)(CU M/DY/ M)	T(DY)
1	704.00	2800.00

OBSERVATION POINTS (M)

XFIRST =	200.00	XLAST =	1200.00	DELX =	200.0000
YFIRST =	150.00	YLAST =	-150.00	DELY =	50.0000

ENTER NEXT COMMAND
 ?RN

CONCENTRATION DISTRIBUTION AT   365.00 DY (MG/L   )

```
*
 * X( M)       _
   *         103.59    118.59    133.59    148.59    163.59
Y( M) *
       *
   20.00      .0977     .1036     .1057     .1035     .0975
   10.00      .1115     .1183     .1206     .1181     .1113
    0.00      .1165     .1235     .1259     .1234     .1163
```

ENTER NEXT COMMAND
  ?DN
STOP

CONCENTRATION DISTRIBUTION AT   2800.00 DY (MG/L   )

```
*
  * X( M)
    *       200.00 _ 400.00   600.00    800.00   1000.00   1200.00
Y( M) *
      *
  150.00      .4286    1.8443    3.4690    4.0376    2.8196    1.0355
  100.00     4.0799    8.8157   11.0693   10.4067    6.5406    2.2825
   50.00    24.5158   25.3627   23.1175   18.6409   10.8973    3.6758
    0.00    51.8244   37.0277   29.7821   22.7017   12.9321    4.3104
  -50.00    24.5158   25.3627   23.1175   18.6409   10.8973    3.6758
 -100.00     4.0799    8.8157   11.0693   10.4067    6.5406    2.2825
 -150.00      .4286    1.8443    3.4690    4.0376    2.8196    1.0355
```

ENTER NEXT COMMAND
 ?DN
STOP

(66)

```
    ENTER TITLE
?ACCIDENTAL HEXAVALENT CHROMIUM SPILL

    ENTER COORDINATE SYSTEM
        XY FOR VERTICALLY-AVERAGED SOLUTION
        XZ FOR HORIZONTALLY-AVERAGED SOLUTION
?XY

    ENTER UNITS FOR LENGTH (2 CHARACTERS)
? M

    ENTER UNITS FOR TIME (2 CHARACTERS)
?DY

    ENTER UNITS FOR CONCENTRATION (6 CHARACTERS)
?MG/L

    ENTER AQUIFER POROSITY
?0.35

    ENTER SEEPAGE VELOCITY,  M/DY
?0.366

    ENTER RETARDATION COEFFICIENT
?1.0

    ENTER X AND Y DISPERSION COEFFICIENTS, SQ  M/DY
?,?7.79,1.56

    ENTER DECAY CONSTANT, 1/DY
?0.0

    ENTER THE NUMBER OF SOURCE RATES (MAXIMUM OF  20)
        0 FOR STEADY-STATE SOLUTION
?2

    ENTER MASS RATE  1 (MG/L  )(CU  M/DY/ M)  AND TIME, (DY)
?,?704.,365.

    ENTER MASS RATE  2 (MG/L  )(CU  M/DY/ M)  AND TIME, (DY)
?,?0.,364.

    ENTER XFIRST, XLAST, DELTAX  ( M)
?,?,?73.59,193.59,30.

    ENTER YFIRST, YLAST, DELTAY  ( M)
?,?,?20.,0.,10.




                            (67)
```

ACCIDENTAL HEXAVALENT CHROMIUM SPILL

SEEPAGE VELOCITY, (M/DY)	.3660
X DISPERSION COEFFICIENT (M**2/DY)	7.7900
Y DISPERSION COEFFICIENT (M**2/DY)	1.5600
POROSITY	.3500

RETARDATION COEFFICIENT	1.0000
FIRST ORDER DECAY CONSTANT (1/DY)	0.0000

SOURCE RATE SCHEDULE

	Q(MG/L)(CU M/DY/ M)	T(DY)
1	704.00	365.00
2	0.00	364.00

OBSERVATION POINTS (M)

XFIRST =	73.59	XLAST =	193.59	DELX =	30.0000
YFIRST =	20.00	YLAST =	0.00	DELY =	10.0000

ENTER NEXT COMMAND
?RN

CONCENTRATION DISTRIBUTION AT   365.00 DY (MG/L   )

```
*
 * X( M)
   *            73.59    103.59    133.59    163.59    193.59
Y( M) *
       *
   20.00        .0771     .0977     .1057     .0975     .0768
   10.00        .0878     .1115     .1206     .1113     .0876
    0.00        .0919     .1165     .1259     .1163     .0916
```

ENTER NEXT COMMAND
?XC

ENTER XFIRST, XLAST, DELTAX   (M)
?,?,?103.59,163.59,15.

ENTER NEXT COMMAND
?RN