PLUME 3D
Three-Dimensional Plumes In Uniform Ground Water Flow

By

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PROJECT SUMMARY

PLUME3D: THREE-DIMENSIONAL PLUMES IN UNIFORM GROUND WATER FLOW

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Introduction

This document describes a mathematical model and the associated computer program which can be used to estimate concentration and distributions in a leachate plume which emanates from one or more point sources. The model includes both linear adsorption and first-order reactions.

The use of the computer program is fairly simple, but represents only one tool which can aid in the analysis and understanding of ground-water contamination problems. The user must select the appropriate tools for the problem at hand, based on a sound understanding of the principles of ground water hydrology, the physical problem, and the assumptions and limitations ofthe mathematical model.

Model Formulation

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

$$R_d \frac{\partial C}{\partial t} + V^* \frac{\partial C}{\partial_x} = D_x^* \frac{\partial^2 C}{\partial y^2} + D_z^* \frac{\partial^2 C}{\partial z^2} - R_d \lambda C \quad (1)$$

where

C	=	component mass per unit of fluid phase	M/L^3
D_x^*	=	dispersion coefficient in x-direction	L^2/t
D_y^*	=	dispersion coefficient in y-direction	L^2/t
D_z^*	=	dispersion coefficient in z-direction	L^2/t
R_d	=	retardation coefficient	
V^*	=	average interstitial velocity in x-direction	L/t
x,y,z	=	retangular coordinates	L
λ	=	first-order decay constant	$1/t$

The retardation coefficient accounts for partitioning of the component between the fluid and solid phases using a linear adsorption isotherm, and is defined as

$$R_d = 1 + \frac{\rho_B}{\theta} K_d \qquad (2)$$

where

ρ_B	=	bulk density of the aquifer	M/L^3
θ	=	effective porosity	
K_d	=	distribution constant for a linear adsorption isotherm	$\frac{M/M}{M/L^3}$

A closed-form analytical solution to Equation 1 for an infinite aquifer with a continuous point source of strength M_0 at the origin can be written as (Hunt, 1978; Turner, 1972)

$$C_c = \frac{M_o \exp\left(\frac{1}{2} \frac{V^* x}{D_x^*}\right)}{8 \pi \Theta R \sqrt{D_y D_z}} \left\{ \exp\left(\frac{1}{2} \frac{RU}{D_x}\right) \operatorname{erfc}\left(\frac{1}{2} \frac{R_d R + Ut}{\sqrt{R_d D_x^* t}}\right) + \exp\left(- \frac{1}{2} \frac{RU}{D_x^*}\right) \operatorname{erfc}\left(\frac{1}{2} \frac{R_d R - Ut}{\sqrt{R_d D_x^* t}}\right) \right\} \tag{2}$$

where

$$R = x^2 + \frac{D_x^*}{D_y^*} y^2 + \frac{D_x^*}{D_z^*} z^2 \quad {}^{1/2} \tag{3}$$

and

$$U = V^* \left(1 + \frac{4 D_x^* R_d \lambda}{V^{*2}}\right)^{1/2} \tag{4}$$

The steady-state solution for a continuous point source is (Hunt, 1978)

$$C_{c,\infty} = \frac{C_o Q}{4 \pi \Theta R \sqrt{D_y^* D_z^*}} \exp\left(\frac{1}{2} \frac{V^* x}{D_x^*} - \frac{UR}{D_x^*}\right) \tag{5}$$

Equations 2 and 5 can be used to calculate the concentrations in a leachate plume under the following assumptions and limitations:

1. The ground-water flow regime is completely saturated.
2. All aquifer properties are constant and uniform throughout the aquifer.
3. The ground-water flow is horizontal, continuous, and uniform throughout the aquifer.
4. The aquifer is infinite in extent.
5. The leachate source is a point located at the origin of the coordinate system.

6. The mass flow rate of the source is constant.

7. At zero time the concentration of leachate in the aquifer is zero.

The assumptions of an infinite aquifer depth and a uniform source mass rate can be overcome by using the principles of superposition in space and time, respectively (Walton, 1962). Both of these provisions have been incorporated in the computer program developed in this project. Superposition is also used to include multiple sources.

Computer Program

The closed-form analytical solutions for the two-dimensional plumes as presented above have been incorporated in an interactive computer program. The source code has been written in a subset of FORTRAN 77 and can be compiled with FORTRAN IV, FORTRAN 66, as well as FORTRAN 77 compilers. As a result, the code is almost entirely independent of hardware and operating systems. Those changes which may be required to implement the code on a given system, such as assigning logical devices are clearly identified.

The program has been developed for interactive use and requires input data under two modes of operation -- "Basic Input Data" and "Edit." The basic input data listed in Table 1 are required to initiate a new problem. The user is prompted for the required data through a series of input commands.

Once the basic input data have been entered, the problem as currently defined is listed and the program enters the "edit" mode. The two character edit commands listed in Table 2 can be used to redefine the problem, run the calculations, and terminate the program.

The program has been written to require a minimum of machine resources and will run on both 8 and 16 bit microcomputers under CP/M, MS-DOS, and PC-DOS as well as larger minicomputers and mainframe machines.

Summary

The models and computer codes developed in this project are intended to serve as additional tools in the analysis of ground-water contamination problems. The user must select the best tool for the problem at hand based on a sound understanding of the principles of ground-water hydrology, the physical problem, and the limitations of the mathematical model(s). Unfortunately, these computer programs cannot substitute for an understanding of the processes and mechanisms of solute transport in ground-water systems or sound judgement based on training and experience.

References

Hunt, B., 1978, "Dispersive Sources in Uniform Ground-Water Flow," Journal of The Hydraulics Division, ASCE, Vol. 104, No. HY1, pp. 75-85.

Turner, G. A., 1972, Heat and Concentration Waves, Academic Press, New York, New York, 233 pp.

Walton, W. C., 1962, "Selected Analytical Methods for Well and Aquifer Evaluation," Bulletin 49, Illinois State Water Survey, Urbana, Illinois, 81 pp.

TABLE 1

Input Data Required for the Analytical
Three-Dimensional Plume Model

Title - Units for length, time, and concentration
Saturated thickness (for aquifer of finite depth)
Effective porosity
Ground water interstitial velocity
Retardation coefficient
Longitudinal dispersion coefficient
Transverse dispersion coefficient
Vertical dispersion coefficient
First-order decay constant
Type of solution (transient or steady-state)
Number of sources
Location and rate schedules for each source
Coordinates of observation points
Observation times (for transient solution)

TABLE 2

EDIT COMMANDS

Command	Variable changed/Execution
ST	Saturated Thickness
PO	Porosity
VX	New Seepage Velocity
RD	Retardation Coefficient
DE	Decay Constant
DX	X-Dispersion Coefficient
DY	Y-Dispersion Coefficient
DZ	Z-Dispersion Coefficient
RT	Source Rate Schedule
OB	Observation Points
XC	X-Coordinates
ZC	Z-Coordinates
YC	Y-Coordinates
TC	Observation Times
AS	Aquifer Sectioning
CS	Change Solution/Sources
MU	Menu of Edit Commands
LI	List input data
RN	Run
NP	New Problem
DN	Done

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DISCLAIMER

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INTRODUCTION

This document describes a mathematical model and the associated computer program which can be used to estimate concentration distributions in a leachate plume which emanates from a point source. The model includes both linear adsorption and first-order reactions.

The use of the computer program is fairly simple, but represents only one tool which can aid in the analysis and understanding of ground-water contamination problems. The user must select the appropriate tools for the problem at hand, based on a sound understanding of the principles of ground-water hydrology, the physical problem, and the assumptions and limitations of the mathematical model.

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

$$R_d \frac{\partial C}{\partial t} + V^* \frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - R_d \lambda C \qquad (1)$$

where

C =	component mass per unit volume of fluid phase	M/L^3
D_x =	dispersion coefficient in x-direction	L^2/t
D_y =	dispersion coefficient in y-direction	L^2/t
D_z =	dispersion coefficient in z-direction	L^2/t
R_d =	retardation coefficient	
V^* =	average interstitial velocity in x-direction	L/t
x,y,z =	rectangular coordinates	L
λ =	first-order decay constant	$1/t$

The retardation coefficient accounts for partitioning of the component between the fluid and solid phases using a linear adsorption isotherm, and is defined as

$$R_d = 1 + \frac{\rho_B}{\theta} K_d \qquad (2)$$

where

ρ_B = bulk density of the aquifer M/L^3

Θ = effective porosity

K_d = distribution constant for a linear adsorption isotherm $\frac{M/M}{M/L^3}$

Analytical Solution

A closed-form analytical solution to Equation 1 can be obtained by making a change of variables. Let

$$\tau = t/R_d \tag{3}$$

and

$$X = x - V^* \tau \tag{4}$$

Then Equation 1 is transformed to

$$\frac{\partial C}{\partial \tau} = D_x \frac{\partial^2 C}{\partial X^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - R_d \lambda C \tag{5}$$

with boundary conditions

$$C(X,y,z,o) = 0 \tag{6a}$$

$$C(X,y,\pm\infty,\tau) = 0 \tag{6b}$$

$$C(X,\pm\infty,z,\tau) = 0 \tag{6c}$$

$$C(\pm\infty, y, z, \tau) = 0 \tag{6d}$$

Equation 5 is a special form of the analogous equations in heat conduction, for which solutions are given by Carslaw and Jaeger (1959). The solution for an instantaneous point source of strength M_o at the origin is

$$C_i = \frac{M_o}{8\theta\sqrt{\pi^3 t^3 D_x D_y D_z}} \exp\left(- \frac{x^2}{4D_x \tau} - \frac{y^2}{4D_y \tau} - \frac{z^2}{4D_z \tau} - R_d \lambda \tau\right) \tag{7}$$

In terms of the untransformed variables,

$$C_i = \frac{M_o}{8\theta\sqrt{\pi^3 t^3 D_x D_y D_z}} \exp\left(- \frac{(x - V^* t/R_d)^2}{4D_x t/R_d} - \frac{y^2}{4D_y t/R_d} - \frac{z^2}{4D_z t/R_d} - \lambda t\right) \tag{8}$$

The solution for a continuous point source is obtained by integrating Equation 8 with respect to time and letting $C_oQ = dM_o/dt$, or

$$C_c = \frac{1}{8\theta\sqrt{\pi^3 D_x D_y D_z}} \int_o^t C_oQ\, t^{-3/2} \exp\left(- \frac{(x - V^* t/R_d)^2}{4D_x t/R_d} - \frac{y^2}{4D_y t/R_d} - \frac{z^2}{4D_z t/R_c} - \lambda t\right) dt \tag{9}$$

Equation 9 can be rearranged slightly to

$$C_c = \frac{\exp \frac{1}{2} \frac{V^* x}{D_x}}{8\theta \sqrt{\pi^3 D_x D_y D_z}} \int_0^t C_o Q \quad t^{-3/2} \exp\left(- \frac{R_d R^2}{4D_x t} - \frac{U^2 t}{4D_x R_d}\right) dt \qquad (10)$$

where

$$R^2 = x^2 + \frac{D_x}{D_y} y^2 + \frac{D_x}{D_z} z^2 \qquad (11)$$

and

$$U = V^* \left(1 + \frac{4D_x R_d \lambda}{V^{*2}}\right)^{1/2} \qquad (12)$$

Turner (1972) gives the solution to Equation 10 as

$$C_c = \frac{C_o Q \exp\left(\frac{1}{2} \frac{V^* x}{D_x}\right)}{8\pi\theta R \sqrt{D_y D_z}} \left\{ 2 \cosh\left(\frac{1}{2} \frac{RU}{D_x}\right) + \exp\left(\frac{1}{2} \frac{RU}{D_x}\right) \operatorname{erf}\left[\frac{1}{2}\left(\frac{U^2 t}{D_x R_d}\right)^{1/2} - \frac{1}{2}\left(\frac{R_d R^2}{D_x t}\right)^{1/2}\right] - \exp\left(- \frac{1}{2} \frac{RU}{D_x}\right) \operatorname{erf}\left[\frac{1}{2}\left(\frac{U^2 t}{D_x R_d}\right)^{1/2} + \frac{1}{2}\left(\frac{R_d R^2}{D_x t}\right)^{1/2}\right] \right\}$$

(13)

which can be simplified somewhat to yield

$$C_c = \frac{C_o\ Q\ \exp\left(\frac{1}{2}\ \frac{V^* x}{D_x}\right)}{8\pi\theta R\ \sqrt{D_y\ D_z}} \left\{ \exp\left(\frac{1}{2}\frac{RU}{D_x}\right)\ \text{erfc}\ \left(\frac{1}{2}\ \frac{R_d\ R + Ut}{\sqrt{R_d\ D_x\ t}}\right) \right.$$

$$\left. + \exp\left(-\frac{1}{2}\frac{RU}{D_x}\right)\ \text{erfc}\ \left(\frac{1}{2}\ \frac{R_d\ R - Ut}{\sqrt{R_d\ D_x\ t}}\right) \right\} \qquad (14a)$$

for $x > 0$.

For $x < 0$, only the first term, $\exp\ (V^* x/D_x)$, has the sign of x altered, because the value of the integral in Equation 10 is the same for both positive and negative values of x. Therefore

$$C_c = \frac{C_o\ Q\ \exp\left(-\frac{1}{2}\ \frac{V^* x}{D_x}\right)}{8\pi\theta R\ \sqrt{D_y\ D_z}} \left\{ \exp\left(-\frac{1}{2}\frac{RU}{D_x}\right)\ \text{erfc}\ \left(\frac{1}{2}\ \frac{R_d\ R + Ut}{\sqrt{R_d\ D_x\ t}}\right) \right.$$

$$\left. + \exp\left(-\frac{1}{2}\frac{RU}{D_x}\right)\ \text{erfc}\ \left(\frac{1}{2}\ \frac{R_d\ R - Ut}{\sqrt{R_d\ D_x t}}\right) \right\} \qquad (14b)$$

for $x < 0$.

The steady-state solution for a continuous point source is found from Equation 8 as (Hunt, 1978)

$$C_{c,\infty} = \int_0^\infty C_i \, dt \tag{15}$$

and the limit of Equation 12 as $t \rightarrow \infty$ is

$$C_{c,\infty} = \frac{C_o Q}{4\pi\theta R \sqrt{D_y D_z}} \exp\left(\frac{1}{2} \frac{V^* x}{D_x} - \frac{UR}{D_x}\right) \tag{16}$$

Equations 14 and 16 describe the transient and steady-state concentration distributions arising from a continuous point source in an infinite aquifer with uniform ground-water flow.

Assumptions and Limitations

Equations 14 and 16 can be used to calculate the concentrations in a leachate plume under the following assumptions and limitations:

1. The ground-water flow regime is completely saturated.
2. All aquifer properties are constant and uniform throughout the aquifer.
3. The ground-water flow is horizontal, continuous, and uniform throughout the aquifer.
4. The aquifer is infinite in extent.
5. The leachate source is a point located at the origin of the coordinate system.
6. The mass flow rate of the source is constant.
7. At zero time the concentration of leachate in the aquifer is zero.

The assumptions of an infinite aquifer depth and a uniform source mass rate can be overcome by using the principles of superposition in space and time, respectively (Walton, 1962). Both of these provisions have been incorporated in the computer program described in the next section.

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 "Duhamel 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 or volume as the sum of a finite number of point 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.

The three-dimensional solutions presented above can be used to simulate aquifers of finite width or depth or sources of finite volume. Applications of this type require a thorough understanding of the physical interpretation of the principal of superposition.

However, some applications are relatively straight forward, and the computer program provides for the approximation of a non-uniform source rate using superposition in time. Multiple sources and aquifers of finite thickness are also included using superposition in space.

Consider the variable source of contamination shown in Figure 1. The solutions of the governing differential equation presented in this report are of the form

$$C(x,z,t) = C_0 Q' \; f(x,z,t) = \dot{Q}' \; f(x,z,t) \tag{17}$$

where Q' is the source mass rate per unit length. The principle of superposition in time can be written for any position as

$$C(x,z,t) = \sum_{i=1}^{n} \dot{Q}_i' \; f(x,z,t_i) \tag{18}$$

Now, the variable rate schedule shown in Figure 1a can be decomposed into a series of positive and negative mass rates as shown in Figure 1b. The concentration at a point x,y,z at the end of the simulation, t_s, can be evaluated as

$$\begin{aligned} C(x,y,z,t) = {} & \dot{Q}_1' \; f(x,y,z,t_1) - \dot{Q}_1' \; f(x,y,z,t_2) \\ & + \dot{Q}_2' \; f(x,y,z,t_2) - \dot{Q}_2' \; f(x,y,z,t_3) \\ & + \dot{Q}_3' \; f(x,y,z,t_3) - \dot{Q}_3' \; f(x,y,z,t_4) \\ & + \dot{Q}_4' \; f(x,y,z,t_4) \end{aligned} \tag{19}$$

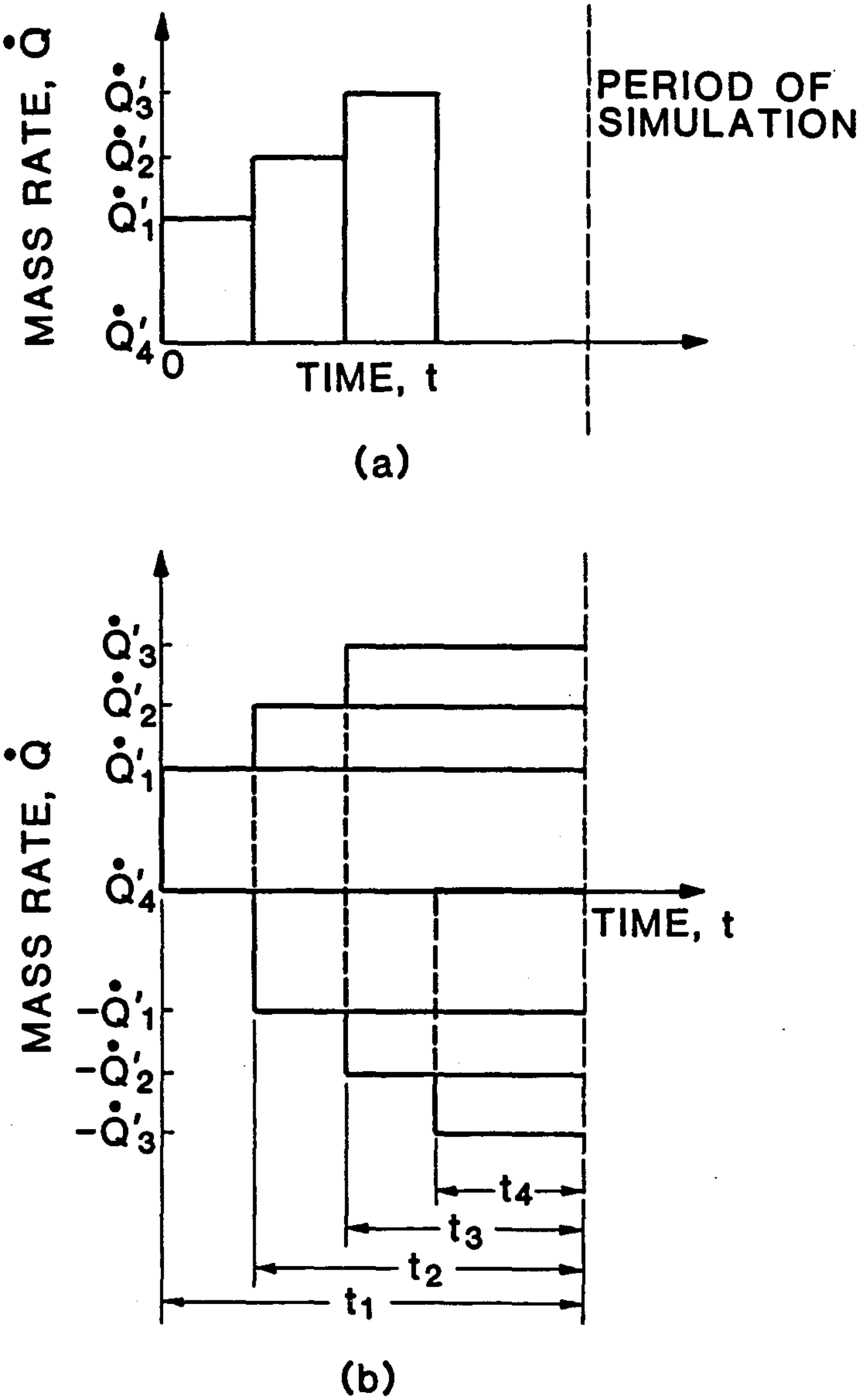


Figure 1. Decomposition of a variable source rate using superposition in time.

In general terms

$$C(x,y,z,t_s) = \sum_{i=1}^{n} (\dot{Q}'_i - \dot{Q}'_{i-1}) \; f(x,y,z,t_i) \tag{20}$$

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

Note the time corresponding to a given source rate, t_i, is the period beginning with the start of the given rate to the end of the simulation period; time is not the duration of a given rate. For ease of application, Equation 20 can be rewritten as

$$C(x,y,z,t_s) = \sum_{k=1}^{n} (\dot{Q}'_k - \dot{Q}'_{k-1}) \; f(x,y,z,t_s-t_{k-1}) \tag{21}$$

where t_{k-1} is the time corresponding to the end of mass rate Q_{k-1} or the beginning of rate Q_k with $Q_o = 0$ and $t_o = 0$.

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.

The influence of geohydrologic boundaries on the movement of a tracer is similar to the influence of these boundaries on the drawdown response of an aquifer to pumping. The applications of image well theory described by Walton (1962, 1970) can be extended to the horizontally-averaged solution to the solute transport problem considered in this report. The following discussion parallels Walton's examples of the use of image wells to account for barrier boundaries.

Consider the contaminant plume which would exist if the aquifer were of infinite depth as shown in Figure 2a. If the contaminant plume was to intersect an impermeable base of the aquifer as shown in Figure 2b, the vertical concentration gradient must change since there can be no transport of mass across the boundary as a result of dispersion. In mathematical terms

$$D_z \frac{\partial C}{\partial z} = 0$$

at $z = B$. Now, if an imaginary, or image, source were placed across the boundary at a distance equal to the depth of the aquifer, as shown in Figure 2c, this source would create a concentration gradient from the boundary to the image water table equal to the concentration gradient from the boundary to the real water table. A "concentration divide" would be established at boundary, and the no-transport boundary condition ($\partial C/\partial z = 0$) would be satisfied.

The imaginary system of a contaminant source and its image in an aquifer of infinite depth satisfies the boundary conditions dictated by the finite depth system. The resultant concentration distribution is the sum of concentrations in both the real and image systems as shown in Figure 2d.

In theory an infinite number of image systems may be required. For example, if the plume in the infinite system intersects the water table in the image system a second no-transport boundary is encountered as shown in Figure 3. This boundary can be handled by introducing another image system across the imaginary boundary and equidistant from the first image system. This process of adding image systems could be repeated indefinitely. In practice

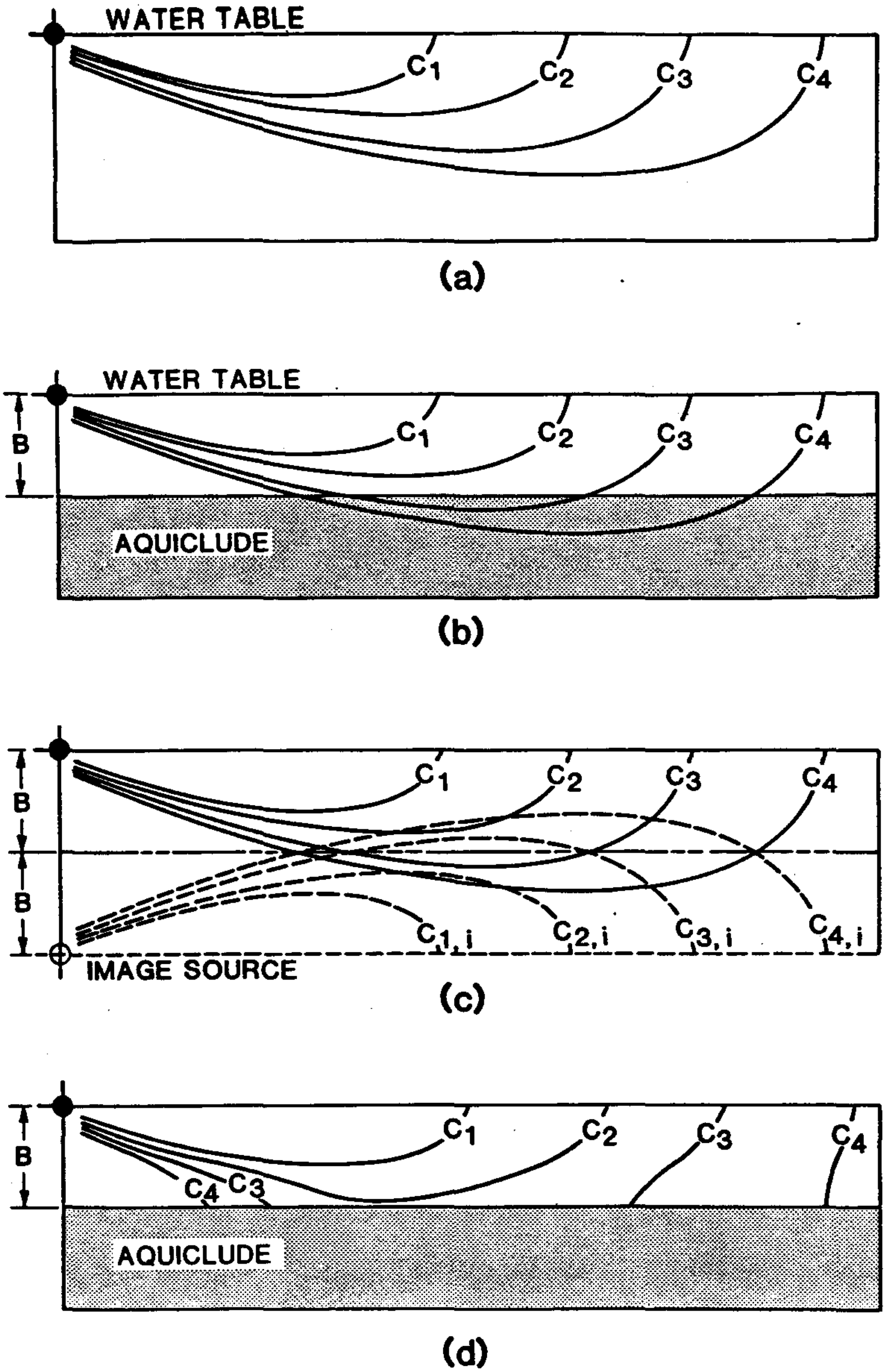
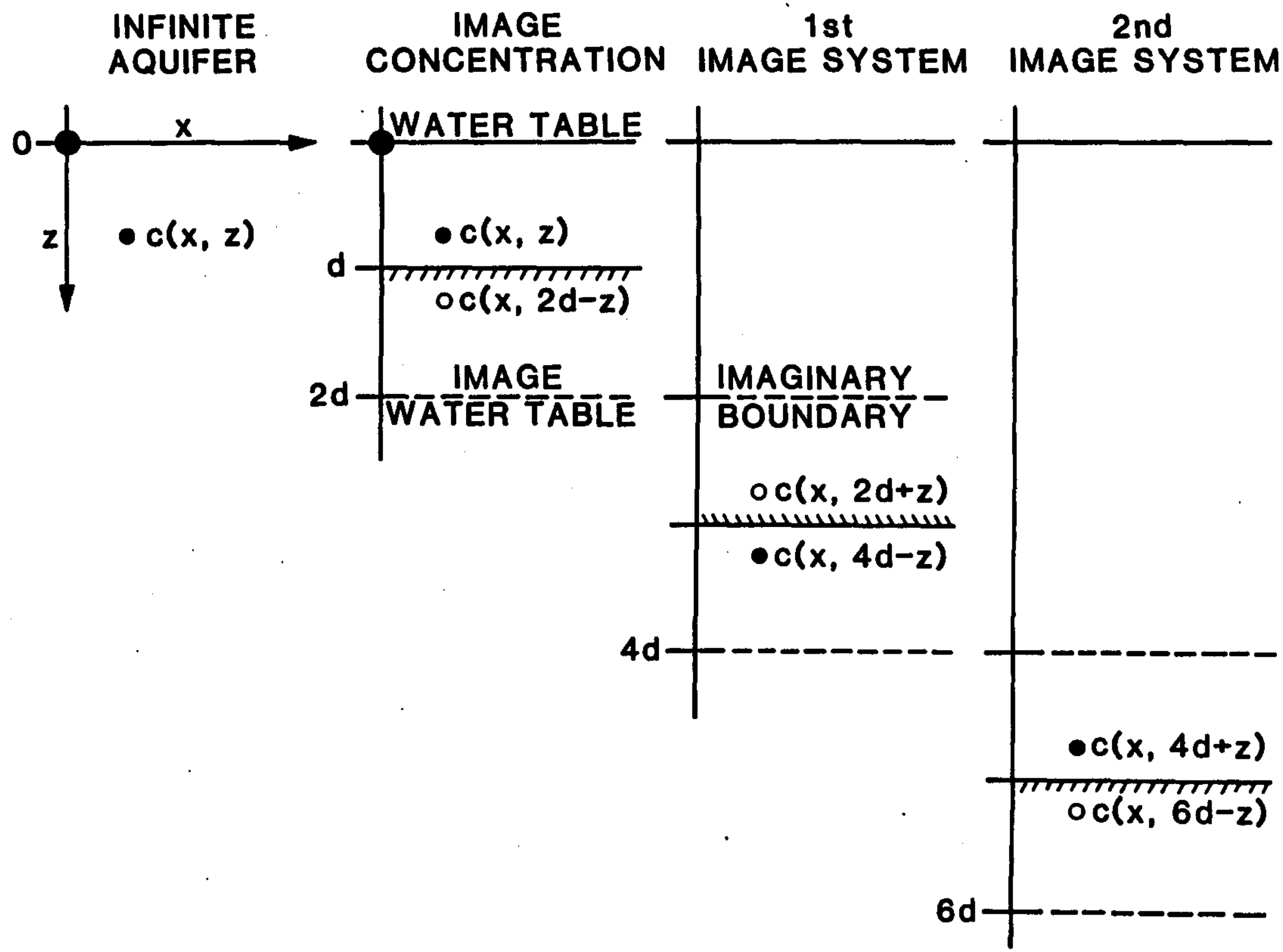


Figure 2. Use of image sources to account for aquifers of finite depth.



$$c'(x, z) = c(x, z) + \sum_{n=1}^{\infty}\left[c(x, 2nd-z) + c(x, 2nd+z)\right]$$

Figure 3. Superposition in space to account for barrier boundaries.

only a few image systems are required. The computer program automatically introduces an appropriate number of image systems.

SECTION II

COMPUTER PROGRAM

The computer program evaluates the analytical solution of the differential equation describing concentration distributions in a three-dimensional plume with uniform ground-water flow. The program has been designed for interactive 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 PLUME3D program. The user is prompted for the required data through a series of input commands described below. Numeric data may be entered through the keyboard with or without decimal points and multiple data entries should be separated by 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 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 dimension 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 dimension 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 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 SATURATED THICKNESS, (0 FOR INFINITE THICKNESS), L
?

The saturated thickness must be entered in the units requested with dimensions of L. If a zero or negative value is entered, the calculations will be carried out assuming an aquifer of infinite depth. The program automatically includes up to 20 image wells for aquifers of finite depth.

ENTER AQUIFER POROSITY
?

Enter the volume void fraction.

ENTER SEEPAGE VELOCITY, L/t
?

The seepage, or interstitial, 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. The numerical value must be greater than 1.0, or equal to 1.0 if absorption is neglected.

ENTER X DISPERSION COEFFICIENT, SQ L/t
?

Dispersion coefficients have dimensions of L^2/t and must be entered in the units requested. Numerical values must be greater than zero. The next two commands will ask for the Y and Z dispersion coefficients, respectively. They also have dimensions of L^2/T and must be entered in the units requested. Numerical values must be greater than zero.

ENTER Y DISPERSION COEFFICIENT, SQ L/t
?

ENTER Z DISPERSION COEFFICIENT, SQ L/t
?

The subsequent command is:

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.

SELECT TRANSIENT OR STEADY-STATE SOLUTION
TR FOR TRANSIENT SOLUTION
SS FOR STEADY-STATE SOLUTION
?

Selection of the transient solution also allows the approximation of a nonuniform rate schedule by a series of uniform rates. Approximation is accomplished through superposition of a series of uniform rates. If steady-state solution is chosen, the steady state concentration will be evaluated.

ENTER THE NUMBER OF SOURCES (MAXIMUM OF N)
?

The number of sources of contaminant should be entered. The value entered must be greater than zero.

MASS RATES HAVE UNITS OF (M/L^3) (L^3/t)
TIME HAS UNITS OF t

This statement reminds the user of the units that will be used for mass rates and for time. All mass rates and time values entered must be in these units.

The next three commands will be repeated for each source.

ENTER X, Y, AND Z COORDINATES OF SOURCE I (L)
?

The input units for the coordinates must be in the units requested. The Z-coordinate must be greater than or equal to zero.

If the transient solution was chosen the following two commands will be issued.

ENTER THE NUMBER OF RATES FOR SOURCE I (MAXIMUM OF N)
?

The number of uniform rates used to approximate a nonuniform rate schedule for this source is entered. The value must be greater than zero.

SOURCE I, RATE J STARTS AT TIME t
ENTER MASS RATE AND ENDING TIME
?

The source mass rate is entered in units of concentration times the volumetric rate. Note the actual source concentration and rate are not required, but the units must be consistent. The time units must also be consistent.

If the steady-state solution has been selected, the following command will be entered instead of the two previously listed commands.

ENTER STEADY-STATE MASS RATE I
?

The next three basic input commands are used to define the matrix of observation 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. A zero entry for DELTAX will result in a single X-coordinate observation.

Results of calculations for multiple X-coordinates will be listed from XFIRST to XLAST.

ENTER YFIRST, YLAST, DELTAY (L)
?,?,?

Any of the numerical values used to define the Y-coordinates of observation points may be positive or negative.

ENTER ZFIRST, ZLAST, DELTAZ (L)
?,?,?

Both ZLAST and ZFIRST must be greater than or equal to zero and less than or equal to the saturated thickness.

ENTER PLANE FOR SECTIONING AQUIFER (XY, XZ, OR YZ)
?

The selection of a particular plane determines the presentation of the output of the program. Concentrations at the specified coordinates in the selected plane will be printed for a constant value of the third coordinate.

ENTER TFIRST, TLAST, DELTAT (t)
?,?,?

The beginning value and ending value of the time interval of contaminant transport being modeled is entered. Both TFIRST and TLAST must be positive values in the units requested. A zero entry for DELTAT will result in model output at a single value of time.

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 1 and are also listed the first time the program enters the edit mode. The request for information is:

ENTER NEXT COMMAND ?

One of the reponses from Table 1 should be given. If the response is incorrect 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 MU, LI, RN, NP, or DN is entered.

MU will list the table of edit commands.

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 using the "Basic Input Data" dialog.

DN will terminate the program.

Although many tests for valid input data and properly formulated edit commands have been embedded in the program, the user is encouraged to correct "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.

Table 1

EDIT COMMANDS

Command	Variable changed/Execution
ST	Saturated Thickness
PO	Porosity
VX	Seepage Velocity
RD	Retardation Coefficient
DE	Decay Constant
DX	X-Dispersion Coefficient
DY	Y-Dispersion Coefficient
DZ	Z-Dispersion Coefficient
RT	Source Rate Schedule
OB	Observation Points
XC	X-Coordinates
ZC	Z-Coordinates
YC	Y-Coordinates
TC	Observation Times
AS	Aquifer Sectioning
CS	Change Solution/Sources
MU	Menu of Edit Commands
LI	List Input Data
RN	Run
NP	New Problem
DN	Done

SECTION III

APPLICATIONS

The example problems presented in this document are based on the dispersal of chromium discharged to the ground water in southeastern Nassau County, New York. The hydrogeology and history of contamination have been documented by Perlmutter and Lieber (1970) and will be briefly summarized in the following paragraphs.

Site Location

The general area of the documented case history of the concentrations of contaminants in ground-water is in southeastern Nassau County, Long Island, New York (Figure 4). The detailed study area included an industrial park at South Farmingdale. During World War II, the industrial park was occupied by an aircraft company whose cadmium and chromium enriched metal plating waste was the source of much of the heavy-metal contamination in a shallow glacial aquifer.

Hydrogeology

The upper glacial aquifer which is addressed in this document extends from the water table, at depths ranging from 0 to 15 feet below the ground surface, to the top of the deeper Magothy aquifer, at depths of 80 to 140 feet below the ground surface. The upper unit consists of beds and lenses of fine to coarse sand and gravel. In some parts of the aquifer, thin lenses of fine to medium sand, as well as some silt, are interbedded with the coarse material. Data from scattered well borings indicate that the lower 8 to 10 feet of the upper unit may consist of silty and sandy clays.

The principal direction of ground-water flow in the upper glacial unit is from north to south. The regional hydraulic gradient is approxmately 0.0025 ft/ft and the average coefficient of permeability is assumed to be 1,600 gal/day/ft^2 with an average total porosity of 0.35 (Perlmutter and Lieber, 1970). The ground-water movement is horizontal throughout the area of interest, with the exception of local recharge and discharge areas where vertical or oblique flow may be predominant.

Plating-Waste Contamination

The chromium contamination in the upper glacial unit was derived principally from the disposal of metal-plating and anodizing waste water to unlined basins. During World War II, and for several years thereafter, essentially untreated plating-water effluent was recharged to the aquifer through these disposal basins. Perlmutter and Lieber (1970) estimated that during the early 1940's as much as 200,000 to 300,000 gallons of effluent containing approximately 52 pounds of chromium was discharged daily into the upper glacial unit. At the end of World War II, the amount of plating-waste effluent was decreased substantially and a chromium removal unit was installed in 1949.

By 1949, or approximately 9 years after the start of plating-waste disposal, a plume of contaminated water had migrated southward approximately 3,900 feet with a maximum width of about 850 feet. Maximum observed chromium concentration was approximately 40 mg/l.

Since 1949 the chromium concentrations decreased substantially in nearly all sections of the sections of the plume. The maximum observed chromium concentration was about 10 mg/l in 1962. However, the plume of contaminated water had migrated further southward beyond Massapequa Creek, a small stream which serves as a natural drain for part of the contaminated ground water. The plume was approximately 4,300 feet long with a maximum width of almost 1000 feet in 1962.

Analytical Model

The data required for the analytical two-dimensional plume model are listed in Table 2. The following paragraphs will discuss the estimation of these model parameters based on the limited field data, judgement, and experience.

All input data for the computer program must be in consistent units. For the example problems, the following system of units will be selected: length in feet, time in days, and concentration in mg/l.

Assuming that the water table is located approximately at the ground surface, the average saturated thickness of the upper glacial unit can be estimated from the depth to the top of the deeper Magothy aquifer. Thus, the average saturated thickness, S_t, will be taken as:

$$S_t = \frac{80 + 140}{2} = 110 \text{ ft}$$

The superficial, or Darcy, velocity can be estimated from the average coefficient of permeability, K, and the regional hydraulic gradient, dh/dx. From Darcy's law

$$V = - K \frac{dh}{dx}$$

TABLE 2

Input Data Required for the Analytical Three-Dimensional Plume Model

Title - Units for length, time, and concentration

Saturated thickness (for aquifer of finite depth)

Effective porosity

Ground water interstitial velocity

Retardation coefficient

Longitudinal dispersion coefficient

Transverse dispersion coefficient

Vertical dispersion coefficient

First-order decay constant

Type of solution (transient or steady-state)

Number of sources

Location and rate schedules for each source

Coordinates of observation points

Observation times (for transient solution) where the minus sign indicates that the flow is in the direction of decreasing hydraulic head. Thus

$$V = \frac{1600 \text{ gal}}{\text{day ft}^2} \frac{\text{ft}^3}{7.48 \text{ gal}} \frac{0.0025 \text{ ft}}{\text{ft}}$$

and

$$V = 0.52 \text{ ft/day}$$

The average interstitial, or pore, velocity, V*, can be estimated by assuming that the areal porosity is equal to the volume porosity, Θ, and

$$V^* = \frac{V}{\Theta}$$

Using the estimated value of effective porosity

$$V^* = \frac{0.52 \text{ ft/day}}{0.35}$$

or

$$V^* = 1.5 \text{ ft/day}$$

The longitudinal, transverse and vertical dispersion coefficients are the most difficult parameters to estimate. Typical values for dispersivities, as well as hydraulic conductivity, are summarized in Table 3. Based on the results of a numerical model for the same site, Pinder (1973) estimated longitudinal and transverse dispersivities as α_x = 69.9 feet and α_y = 14.0 feet, respectively. Considering the interbedding of finer materials in the

TABLE 3

Typical Values of Aquifer Properties

(after Yeh, 1981)

Parameter	Material: Clay	Silt	Sand
Bulk density, lb/ft^3	87.36 - 137.2	80.50 - 112.3	73.63 - 98.59
Effective porosity	0.03 - 0.05	0.05 - 0.10	0.10 - 0.30
Hydraulic Conductivity, $gal/day/ft^2$	0.01 - 0.1	1 - 10	100 - 100,000
Dispersivity, ft			
Longitudinal	0.1 - 1.0	1 - 10	10 - 100
Transverse	0.01 - 0.1	0.1 - 1.0	1.0 - 10
Vertical	0.01 - 0.1	0.1 - 1.0	1 - 10

shallow upper unit together with the typical values of longitudinal and vertical dispersivities in Table 3, the vertical dispersivity will be assumed to be approximately two orders of magnitude smaller than the longitudinal dispersivity. Thus α_z = 0.7 ft, and the dispersion coefficients are evaluated as

$$D_x = \alpha_L V^* = (69.9 \text{ ft})(1.5 \text{ ft/day}) = 105 \text{ ft}^2\text{/day}$$

$$D_y = \alpha_y V^* = (14.0 \text{ ft})(1.5 \text{ ft/day}) = 21.0 \text{ ft}^2\text{/day}$$

and

$$D_z = \alpha_z V^* = (0.7 \text{ ft})(1.5 \text{ ft/day}) = 1.05 \text{ ft}^2\text{/day}$$

Chromium is believed to be a conservative material in this system (Perlmutter and Lieber, 1970), and both adsorption and chemical/biological decay can be neglected. Therefore, K_d = 0 (or R_d = 1) and λ = 0.

The last set of model input data to be specified is the source mass/rate schedule. A steady mass rate of 52 lb/day of chromium will be assumed from the time of initial injection to mid-1949, or approximately 2800/days. At this time, the actual extent of the contamination was estimated; and the chromium removal unit was installed. The actual volumetric rate and concentration of the source of chromium contamination are not required. However, the units of the source term must be consistent with other parameters in the model.

The mass rate of chromium can be converted to units of concentration times volume rate per unit width of aquifer as follows:

TABLE 4

Model Input Data for Example Problem 1.

Title:	Hexavalent Chromium Plume--Example 1
Units for length:	ft
Units for time:	dy
Units for concentration:	mg/l
Saturated thickness:	110 ft
Effective porosity:	0.35
Interstitial velocity:	1.5 ft/dy
Retardation coefficient:	1.0
x-dispersion coefficient	105 ft^2/dy
y-dispersion coefficient	21.0 ft^2/dy
z-dispersion coefficient	1.05 ft^2/dy
First-order decay constant:	0/dy
Source/rate schedule	
Number of sources:	1
Location of source:	x = 0, y = 0, z = 0
Number of rates:	1
Mass rate and time:	833,586 (mg/l)(ft^3/dy) from 0 to 2800 dy

$$\frac{52 \text{ lb}}{\text{day}} \; \frac{454 \times 10^3 \text{ mg}}{\text{lb}} \; \frac{\text{ft}^3}{28.321 \text{ liter}} = 833{,}586 \text{ (mg/liter)(ft}^3\text{/day)}$$

for 2800 days.

The model input data for this example problem are summarized in Table 4. The input data dialog for the example problem and the model results are included in Appendix A.

This example problem is not intended to serve as a verification of a model. The example illustrates the type of input data required, and some methods for estimating input data. The input data dialog and model results can be used to partially test the model code. The analytical model and the computer program are tools which can aid in the analysis of ground-water contamination problems. The user must select the best tools for the problem at hand based on a sound understanding of the principles of ground-water hydrology, the physical problems, and the limitations of the mathematical model(s).

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APPENDIX A

Input Data Dialog and Results for Example Problem

```
ENTER TITLE
?HEXAVALENT CHROMIUM PLUME -- EXAMPLE 1

ENTER UNITS FOR LENGTH (2 CHARACTERS)
?FT

ENTER UNITS FOR TIME (2 CHARACTERS)
?DY

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

ENTER SATURATED THICKNESS (Ø FOR INFINITE THICKNESS), FT
?11Ø.

ENTER AQUIFER POROSITY
?Ø.35

ENTER SEEPAGE VELOCITY, FT/DY
?1.5

ENTER RETARDATION COEFFICIENT
?1.Ø

ENTER X DISPERSION COEFFICIENT, SQ FT/DY
?1Ø5.

ENTER Y DISPERSION COEFFICIENT, SQ FT/DY
?21.

ENTER Z DISPERSION COEFFICIENT, SQ FT/DY
?1.Ø5

ENTER DECAY CONSTANT, 1/DY
?Ø.

SELECT TRANSIENT OR STEADY-STATE SOLUTION
   TR FOR TRANSIENT SOLUTION
   SS FOR STEADY-STATE SOLUTION
?TR
```

```
ENTER THE NUMBER OF SOURCES (MAXIMUM OF 10 )
?1

MASS RATES HAVE UNITS OF (MG/L  ) (CU FT/DY)
TIME HAS UNITS OF DY

ENTER X, Y, AND Z COORDINATES OF SOURCE 1 (FT)
?,?,?0.,0.,0.

ENTER THE NUMBER RATES FOR SOURCE 1 (MAXIMUM 0F 10)
?1

SOURCE  1, RATE  1 STARTS AT     0.0 DY
ENTER MASS RATE AND ENDING TIME
?,?833586.,2800.

ENTER XIRST, XLAST, DELTAX  (FT)
?,?,?600.,3600.,600.

ENTER YFIRST, YLAST, DELTAY  (FT)
?,?,?450.,-450.,150.

ENTER ZFIRST, ZLAST, DELTAZ  (FT)
?,?,?0.,110.,55.

ENTER PLANE FOR SECTIONING AQUIFER (XY,XZ,OR YZ)
?XY

ENTER TFIRST, TLAST, DELTAT  (DY)
?,?,?2800.,2800.,0.
```

PLUME3D
VERSION 2.Ø1
PAGE 1

HEXAVALENT CHROMIUM PLUME -- EXAMPLE 1

SATURATED THICKNESS, (FT)	11Ø.ØØØØ
SEEPAGE VELOCITY, (FT/DY)	1.5ØØØ
X DISPERSION COEFFICIENT (FT**2/DY)	1Ø5.ØØØØ
Y DISPERSION COEFFICIENT (FT**2/DY)	21.ØØØØ
Z DISPERSION COEFFICIENT (FT**2/DY)	1.Ø5ØØ
POROSITY	.35ØØ

RETARDATION COEFFICIENT	1.ØØØØ
FIRST ORDER DECAY CONSTANT (1/DY)	Ø.ØØØØ

SOURCE/RATE SCHEDULE (MG/L)(CU FT/DY)

	SOURCE			RATE	MASS	TIME (DY)	
NO	X (FT)	Y (FT)	Z (FT)	NO	RATE	START	END
1	Ø.ØØ	Ø.ØØ	Ø.ØØ				
				1	833586.ØØ	Ø.ØØ	28ØØ.ØØ

OBSERVATION POINTS (FT), AND TIMES (DY)

XFIRST =	6ØØ.ØØ	XLAST =	36ØØ.ØØ	DELX =	6ØØ.ØØØØ
YFIRST =	45Ø.ØØ	YLAST =	-45Ø.ØØ	DELY =	15Ø.ØØØØ
ZFIRST =	Ø.ØØ	ZLAST =	11Ø.ØØ	DELZ =	55.ØØØØ
TFIRST =	28ØØ.ØØ	TLAST =	28ØØ.ØØ	DELT =	Ø.ØØØØ

AQUIFER SECTIONED IN XY PLANE

MENU OF EDIT COMMANDS

SATURATED THICKNESS	ST	OBSERVATION POINTS	OB
POROSITY	PO	X COORDINATES	XC
SEEPAGE VELOCITY	VX	Y COORDINATES	YC
RETARDATION COEFFICIENT	RD	Z COORDINATES	ZC
X DISPERSION COEFFICIENT	DX	OBSERVATION TIMES	TC
Y DISPERSION COEFFICIENT	DY	AQUIFER SECTIONING	AS
Z DISPERSION COEFFICIENT	DZ	NEW PROBLEM	NP
DECAY CONSTANT	DE	MENU OF COMMANDS	MU
SOURCE/RATE SCHEDULE	RT	LIST INPUT DATA	LI
CHANGE SOLUTION/SOURCES	CS	RUN CALCULATIONS	RN
		DONE	DN

ENTER NEXT COMMAND
?RN

HEXAVALENT CHROMIUM PLUME -- EXAMPLE 1

CONCENTRATION DISTRIBUTION AT 2800.00 DY (MG/L)

Z = 0.00 FT

Y(FT) \ X(FT)	600.00	1200.00	1800.00	2400.00	3000.00	3600.00
450.00	1.1622	3.7737	6.0164	7.2392	7.3914	6.2020
300.00	10.5229	16.8523	17.7165	16.6967	14.7097	11.3227
150.00	62.9100	46.6486	35.3420	28.0852	22.4262	16.3152
0.00	134.5398	67.2738	44.8561	33.5146	25.8517	18.4413
-150.00	62.9100	46.6486	35.3420	28.0852	22.4262	16.3152
-300.00	10.5229	16.8523	17.7165	16.6967	14.7097	11.3227
-450.00	1.1622	3.7737	6.0164	7.2392	7.3914	6.2020

HEXAVALENT CHROMIUM PLUME -- EXAMPLE 1

CONCENTRATION DISTRIBUTION AT 2800.00 DY (MG/L)

Z = 55.00 FT

Y(FT) \ X(FT)	600.00	1200.00	1800.00	2400.00	3000.00	3600.00
450.00	.4395	1.8379	3.5409	4.8545	5.4148	4.8044
300.00	2.9774	7.3832	9.9691	10.9487	10.6514	8.7202
150.00	12.3888	18.7138	19.2646	18.1440	16.1159	12.5181
0.00	21.5268	26.0413	24.1684	21.5383	18.5286	14.1310
-150.00	12.3888	18.7138	19.2646	18.1440	16.1159	12.5181
-300.00	2.9774	7.3832	9.9691	10.9487	10.6514	8.7202
-450.00	.4395	1.8379	3.5409	4.8545	5.4148	4.8044

```
HEXAVALENT CHROMIUM PLUME -- EXAMPLE 1


             CONCENTRATION DISTRIBUTION AT     2800.00 DY (MG/L  )

             Z =     110.00 FT

*
  * X(FT)
    *          600.00    1200.00    1800.00    2400.00    3000.00    3600.00
Y(FT) *
       *
  450.00        .0755      .5147     1.4813     2.6624     3.5125     3.4326
  300.00        .3219     1.6706     3.7892     5.7406     6.7651     6.1702
  150.00        .8561     3.5798     6.8411     9.2287    10.0941     8.8018
    0.00       1.2145     4.6664     8.3725    10.8380    11.5486     9.9142
 -150.00        .8561     3.5798     6.8411     9.2287    10.0941     8.8018
 -300.00        .3219     1.6706     3.7892     5.7406     6.7651     6.1702
 -450.00        .0755      .5147     1.4813     2.6624     3.5125     3.4326

ENTER NEXT COMMAND
?YC

ENTER YFIRST, YLAST, DELTAY  (FT)
?,?,?0.,0.,0.


ENTER NEXT COMMAND
?ZC

ENTER ZFIRST, ZLAST, DELTAZ  (FT)
?,?,?0.,110.,20.


ENTER NEXT COMMAND
?AS

ENTER PLANE FOR SECTIONING AQUIFER (XY,XZ,OR YZ)
?XZ


ENTER NEXT COMMAND
?LI
```

HEXAVALENT CHROMIUM PLUME -- EXAMPLE 1

SATURATED THICKNESS, (FT)	110.0000
SEEPAGE VELOCITY, (FT/DY)	1.5000
X DISPERSION COEFFICIENT (FT**2/DY)	105.0000
Y DISPERSION COEFFICIENT (FT**2/DY)	21.0000
Z DISPERSION COEFFICIENT (FT**2/DY)	1.0500
POROSITY	.3500

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

SOURCE/RATE SCHEDULE (MG/L)(CU FT/DY)

NO	SOURCE X (FT)	Y (FT)	Z (FT)	RATE NO	MASS RATE	TIME (DY) START	END
1	0.00	0.00	0.00				
				1	833586.00	0.00	2800.00

OBSERVATION POINTS (FT), AND TIMES (DY)

XFIRST =	600.00	XLAST =	3600.00	DELX =	600.0000
YFIRST =	0.00	YLAST =	0.00	DELY =	0.0000
ZFIRST =	0.00	ZLAST =	110.00	DELZ =	20.0000
TFIRST =	2800.00	TLAST =	2800.00	DELT =	0.0000

AQUIFER SECTIONED IN XZ PLANE

ENTER NEXT COMMAND
?RN

HEXAVALENT CHROMIUM PLUME -- EXAMPLE 1

CONCENTRATION DISTRIBUTION AT 2800.00 DY (MG/L)

Y = 0.00 FT

Z(FT) \ X(FT)	600.00	1200.00	1800.00	2400.00	3000.00	3600.00
0.00	134.5398	67.2738	44.8561	33.5146	25.8517	18.4413
20.00	101.2264	58.9650	41.2153	31.5259	24.6661	17.7508
40.00	47.1345	40.1774	32.1269	26.3553	21.5287	15.9102
60.00	16.1375	22.0086	21.6384	19.9389	17.5144	13.5252
80.00	4.7086	10.3607	13.3152	14.3904	13.9192	11.3590
100.00	1.5140	5.2569	8.9261	11.2473	11.8248	10.0831
110.00	1.2145	4.6664	8.3725	10.8380	11.5486	9.9142

ENTER NEXT COMMAND
?DN

STOP

APPENDIX B

Listing of Source Code for PLUME3D

```
C     PLUME3D
C     VERSION 2.02
C     THREE-DIMENSIONAL PLUMES 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        MARCH, 1984
C
C        REVISIONS:   2.01    23 NOV 84
C                     2.02     9 DEC 84
C
      DIMENSION COL(7),CON(7),D(3),DEL(3),XF(3),XL(3),XS(10),YS(10),
     1ZS(10)
      DIMENSION IC(21),IS(4),KSEC(3),LBL(2,6),NP(3),NR(10),TITLE(30)
      REAL LAMBDA
      INTEGER TITLE
      COMMON/IO/NI,NO
      COMMON/RATE/Q(10,12),T(10,12)
      COMMON/PHYPRO/ALPHA,BETA,GAMMA,DX,LAMBDA,PE,RD,V
      DATA IC/'NP','ST','PO','VX','RD','DX','DY','DZ','DE','CS','XC',
     1'YC','ZC','AS','TC','LI','RN','OB','RT','MU','DN'/
      DATA IS/'R','M','A','D'/
      DATA KAR1,KAR2,KAR3/'X','Y','Z'/
      DATA KSEC/'XY','XZ','YZ'/
      DATA LBL/'  ','(C','  ','ON','  ','TI','  ','NU','  ','ED',
     1'  ',') '/
      DATA IY/'Y'/
      DATA KSOL1,KSOL2/'TR','SS'/
C
C     READ DEVICE: NI      WRITE DEVICE: NO
      NI=1
      NO=1
C
C     MAXIMUM NUMBER OF PRINTED COLUMNS PER PAGE IS SET TO MAXCOL
C        DIMENSION COL(MAXCOL),CON(MAXCOL)
      MAXCOL = 7
C
C     MAXIMUM NUMBER OF PRINTED ROWS PER PAGE IS SET TO MAXROW
      MAXROW = 40
C
C     MAXIMUM NUMBER OF SOURCES IS SET TO MAXSOR
C        DIMENSION XS(MAXSOR),YS(MAXSOR),ZS(MAXSOR),NR(MAXSOR)
      MAXSOR = 10
C
C     MAXIMUM NUMBER OF SOURCE RATES FOR SUPERPOSITION IN TIME
C     IS SET TO MAXRT
C        COMMON/RATE/ Q(MAXSOR,MAXRT+2),T(MAXSOR,MAXRT+2)
      MAXRT = 10
C
C     MAXIMUM NUMBER OF IMAGE WELLS FOR SUPERPOSITION IN SPACE
C     IS SET TO MAXIMG
      MAXIMG = 20
C
C
C
C     INITIALIZE PROGRAM FLOW CONTROL VARIABLES
   10 IEDIT = 1
      KNTL = 1
      NPAGE = 1
C
C
C ***** SECTION I -- BASIC INPUT DATA
C
C     READ TITLE
      WRITE(NO,15)
   15 FORMAT(1H1,2X,'ENTER TITLE',/'    ?')
      READ(NI,25) (TITLE(I), I=1,30)
   25 FORMAT(30A2)
```

```
C
C     DEFINE UNITS
      WRITE(NO,35)
   35 FORMAT(3X,'ENTER UNITS FOR LENGTH (2 CHARACTERS)',/,'   ?')
      READ(NI,45) IL
   45 FORMAT(A2)
      WRITE(NO,55)
   55 FORMAT(3X,'ENTER UNITS FOR TIME (2 CHARACTERS)',/,'   ?')
      READ(NI,45) IT
      WRITE(NO,65)
   65 FORMAT(3X,'ENTER UNITS FOR CONCENTRATION (6 CHARACTERS)',/,'   ?')
      READ(NI,75) IM1,IM2,IM3
   75 FORMAT(3A2)
C
C     ENTER DATA FOR FIRST PROBLEM
C
C     SATURATED THICKNESS
   80 IMAGE = MAXIMG/2
   84 WRITE(NO,85) IL
   85 FORMAT(3X,'ENTER SATURATED THICKNESS (0 FOR INFINITE THICKNESS), '
     1A2,/,'   ?')
      READ(NI,95,ERR=84) ST
   95 FORMAT(F10.0)
      IF(ST.GT.0.0) GO TO 100
      IMAGE = 1
      ST = 1.0E32
  100 CONTINUE
      GO TO (120,110),IEDIT
  110 IF(XF(3).LE.ST.AND.XL(3).LE.ST) GO TO 3000
      WRITE(NO,115) ST,IL
  115 FORMAT(3X,'RANGE OF Z-COORDINATES IS OUTSIDE UPPER LIMIT OF',/,
     13X,'SATURATED THICKNESS = ',F10.4,A3)
      GO TO 590
C
C     POROSITY
  120 WRITE(NO,125)
  125 FORMAT(3X,'ENTER AQUIFER POROSITY',/,'   ?')
  130 READ(NI,95,ERR=120) P
      IF(P.GT.0.0.AND.P.LT.1.0) GO TO 150
      WRITE(NO,145)
  145 FORMAT(3X,'POROSITY MUST BE GREATER THAN ZERO',
     1' AND LESS THAN ONE -- REENTER',/,'   ?')
      GO TO 130
  150 GO TO (160,3000),IEDIT
C
C     SEEPAGE VELOCITY
  160 WRITE(NO,165) IL,IT
  165 FORMAT(3X,'ENTER SEEPAGE VELOCITY, 'A2,'/',A2,/,'   ?')
  170 READ(NI,95,ERR=160) V
      IF(V.GT.0.0) GO TO 180
      WRITE(NO,175)
  175 FORMAT(3X,'SEEPAGE VELOCITY MUST BE GREATER THAN ZERO',
     1' -- REENTER',/,'   ?')
      GO TO 170
  180 GO TO (190,3000),IEDIT
C
C     RETARDATION COEFFICIENT
  190 WRITE(NO,195)
  195 FORMAT(3X,'ENTER RETARDATION COEFFICIENT',/,'   ?')
  200 READ(NI,95,ERR=190) RD
      IF(RD.GE.1.0) GO TO 210
      WRITE(NO,205)
  205 FORMAT(3X,'RETARDATION COEFFICIENT MUST BE GREATER THAN OR',
     1' EQUAL TO ONE',/,3X,' -- REENTER',/,'   ?')
      GO TO 200
  210 GO TO (220,3000),IEDIT
C
C     X DISPERSION COEFFICIENT
  220 WRITE(NO,225) IL,IT
  225 FORMAT(3X,'ENTER X DISPERSION COEFFICIENT, SQ ',A2,
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```
     1'/',A2,/,'    ?')
  230 READ(NI,95,ERR=220) DX
      IF(DX.GT.0.0) GO TO 240
      WRITE(NO,235)
  235 FORMAT(3X,'X DISPERSION COEFFICIENT MUST BE GREATER THAN ZERO',
     1' -- REENTER',/,'    ?')
      GO TO 230
  240 GO TO (250,3000),IEDIT
C
C     Y DISPERSION COEFFICIENT
  250 WRITE(NO,255) IL,IT
  255 FORMAT(3X,'ENTER Y DISPERSION COEFFICIENT, SQ ',A2,
     1'/',A2,/,'    ?')
  260 READ(NI,95,ERR=250) DY
      IF(DY.GT.0.0) GO TO 270
      WRITE(NO,265)
  265 FORMAT(3X,'Y  DISPERSION COEFFICIENT MUST BE GREATER THAN ZERO',
     1' -- REENTER',/,'    ?')
      GO TO 260
  270 GO TO (280,3000),IEDIT
C
C     Z DISPERSION COEFFICIENT
  280 WRITE(NO,285) IL,IT
  285 FORMAT(3X,'ENTER Z DISPERSION COEFFICIENT, SQ ',A2,
     1'/',A2,/,'    ?')
  290 READ(NI,95,ERR=280) DZ
      IF(DZ.GT.0.0) GO TO 300
      WRITE(NO,295)
  295 FORMAT(3X,'Z  DISPERSION COEFFICIENT MUST BE GREATER THAN ZERO',
     1' -- REENTER',/,'    ?')
      GO TO 290
  300 GO TO (310,3000),IEDIT
C
C     FIRST-ORDER DECAY CONSTANT
  310 WRITE(NO,315) IT
  315 FORMAT(3X,'ENTER DECAY CONSTANT, 1/',A2,/,'    ?')
      READ(NI,95,ERR=310) DECAY
      GO TO (320,3000),IEDIT
C
C     DEFINE LOCATIONS AND RATES OF SOURCES
C     INITIALIZE SOURCE/RATE ARRAYS
  320 MAXRT2 = MAXRT + 2
      DO 330  I=1,MAXSOR
        DO 330  J=1,MAXRT2
            Q(I,J) = 0.0
            T(I,J) = 0.0
  330 CONTINUE
      JFLOW = 3
  340 WRITE(NO,345)
  345 FORMAT(3X,'SELECT TRANSIENT OR STEADY-STATE SOLUTION',/,
     16X,'TR FOR TRANSIENT SOLUTION',/,
     26X,'SS FOR STEADY-STATE SOLUTION',/,'    ?')
  350 READ(NI,45) KSOL
      IF(KSOL.EQ.KSOL1) JFLOW=1
      IF(KSOL.EQ.KSOL2) JFLOW=2
      GO TO (370,370,360), JFLOW
  360 WRITE(NO,365)
  365 FORMAT(3X,'ERROR IN SELECTION -- REENTER'/,'    ?')
      GO TO 350
C
  370 WRITE(NO,375) MAXSOR
  375 FORMAT(3X,'ENTER THE NUMBER OF SOURCES (MAXIMUM OF',I3,' )',/,
     1'   ?')
  380 READ(NI,385,ERR=370) FDUM
  385 FORMAT(F10.0)
      NS=FDUM
      IF(NS.GT.0.AND.NS.LE.MAXSOR) GO TO 400
      WRITE(NO,395) MAXSOR
  395 FORMAT(3X,'NUMBER OF SOURCES MUST BE GREATER THAN ZERO '
     1'AND LESS THAN',I3,' -- REENTER',/,'    ?')
```

```
      GO TO 380
  400 WRITE (NO,405) IM1,IM2,IM3,IL,IT,IT
  405 FORMAT(3X,'MASS RATES HAVE UNITS OF (',3A2,') (CU ',A2,'/',A2,
     1 ')',/,3X,'TIME HAS UNITS OF ',A2,/)
      DO 540  I=1,NS
  414 WRITE(NO,415) I,IL
  415 FORMAT(3X,'ENTER X, Y, AND Z COORDINATES OF SOURCE',I2,
     1' (',A2,')',/,'    ?,?,?')
      READ(NI,425,ERR=414) XS(I),YS(I),ZS(I)
  425 FORMAT(3F10.0)
  430 IF(ZS(I).GE.0.0.AND.ZS(I).LE.ST) GO TO 440
  434 WRITE(NO,435) ST,IL
  435 FORMAT(3X,'Z-COORDINATE MUST BE GREATER THAN OR EQUAL TO ZERO',
     1' AND',/,3X,'LESS THAN OR EQUAL TO SATURATED THICKNESS (',
     2F10.4,A3,')',/,3X,' -- REENTER',/,'    ?')
      READ(NI,95,ERR=434) ZS(I)
      GO TO 430
  440 IF(JFLOW.EQ.2) GO TO 530
      Q(I,1) = 0.0
      T(I,1) = 0.0
  450 WRITE(NO,455) I,MAXRT
  455 FORMAT(3X,'ENTER THE NUMBER RATES FOR SOURCE',I2,
     1' (MAXIMUM OF',I3,')',/,'    ?')
  460 READ(NI,465,ERR=450) FDUM
  465 FORMAT(F10.0)
      NR(I)=FDUM
      IF(NR(I).GT.0.AND.NR(I).LE.MAXRT) GO TO 480
      WRITE(NO,475) MAXRT
  475 FORMAT(3X,'NUMBER OF RATES MUST BE GREATER THAN ZERO AND ',
     1'LESS THAN',I3,'  -- REENTER',/,'    ?')
      GO TO 460
  480 CONTINUE
      NRT = NR(I)
      DO 520  J=1,NRT
         M = J + 1
  484    WRITE(NO,485) I,J,T(I,M-1),IT
  485    FORMAT(3X,'SOURCE ',I2,', RATE ',I2,' STARTS AT',F8.1,A3,/,
     1   3X,'ENTER MASS RATE AND ENDING TIME ',/,'    ?,?')
         READ(NI,495,ERR=484) Q(I,M),T(I,M)
  495    FORMAT(2F10.0)
  500    IF(T(I,M).GT.T(I,M-1)) GO TO 510
  504    WRITE(NO,505)
  505    FORMAT(3X,'ENDING TIME MUST BE GREATER THAN STARTING TIME '
     1   ' -- REENTER',/,'    ?')
         READ(NI,95,ERR=504) T(I,M)
         GO TO 500
  510    CONTINUE
  520 CONTINUE
      GO TO 540
  530 WRITE(NO,535) I
  535 FORMAT(3X,'ENTER STEADY-STATE MASS RATE',I2,/,'    ?')
      READ(NI,95,ERR=530) Q(I,1)
      NR(I) = 0
  540 CONTINUE
      IF(IEDIT.EQ.2.AND.JFLOW.EQ.1.AND.TF.LE.1.0E-06) GO TO 720
  550 GO TO (560,3000),IEDIT
C
C     COORDINATES OF THE OBSERVATION POINTS
  560 WRITE(NO,565) IL
  565 FORMAT(3X,'ENTER XIRST, XLAST, DELTAX  (',A2,')' ,/,'    ?,?,?')
      READ(NI,575,ERR=560) XF(1),XL(1),DEL(1)
  575 FORMAT(3F10.0)
      DEL(1) = ABS(DEL(1))
      IF(DEL(1).LE.1.0E-06) XL(1)=XF(1)
      GO TO (580,3000),KNTL
C
  580 WRITE(NO,585) IL
  585 FORMAT(3X,'ENTER YFIRST, YLAST, DELTAY  (',A2,')',/,'    ?,?,?')
      READ(NI,575,ERR=580) XF(2),XL(2),DEL(2)
      DEL(2) = ABS(DEL(2))
```

```
      IF(DEL(2).LE.1.0E-06) XL(2)=XF(2)
      GO TO (590,3000),KNTL
C
  590 WRITE(NO,595) IL
  595 FORMAT(3X,'ENTER ZFIRST, ZLAST, DELTAZ  (',A2,')',/,'    ?,?,?')
      READ(NI,575,ERR=590) XF(3),XL(3),DEL(3)
      DEL(3) = ABS(DEL(3))
  600 IF(XF(3).GE.0.0.AND.XF(3).LE.ST.AND.DEL(3).LE.1.0E-06) GO TO 620
      IF(XF(3).GE.0.0.AND.XF(3).LE.ST) GO TO 610
  604 WRITE(NO,605) ST,IL
  605 FORMAT(3X,'ZFIRST MUST BE GREATER THAN OR EQUAL TO ZERO AND',/,
     13X,' LESS THAN OR EQUAL TO SATURATED THICKNESS (',F10.4,A3,')',/,
     2' -- REENTER',/,'    ?')
      READ(NI,95,ERR=604) XF(3)
      GO TO 600
  610 IF(XL(3).GE.0.0.AND.XL(3).LE.ST) GO TO 630
  614 WRITE(NO,615) ST,IL
  615 FORMAT(3X,'ZLAST MUST BE GREATER THAN OR EQUAL TO ZERO AND',/,
     13X,' LESS THAN OR EQUAL TO SATURATED THICKNESS (',F10.4,A3,')',/,
     23X,' -- REENTER',/,'    ?')
      READ(NI,95,ERR=614) XL(3)
      GO TO 630
  620 XL(3) = XF(3)
  630 GO TO (640,3000), IEDIT
C
C     PLANE FOR SECTIONING AQUIFER
  640 WRITE(NO,645)
  645 FORMAT(3X,'ENTER PLANE FOR SECTIONING AQUIFER (XY,XZ,OR YZ)',
     1/,'    ?')
  650 READ(NI,45) ISEC
      DO 660 LSEC=1,3
         IF(ISEC.EQ.KSEC(LSEC)) GO TO 670
  660 CONTINUE
      WRITE(NO,665)
  665 FORMAT(3X,'INVALID SECTION -- REENTER',/,'    ?')
      GO TO 650
  670 GO TO (680,690,700), LSEC
  680 KHAR1 = KAR3
      KHAR2 = KAR1
      KHAR3 = KAR2
      GO TO 710
  690 KHAR1 = KAR2
      KHAR2 = KAR1
      KHAR3 = KAR3
      GO TO 710
  700 KHAR1 = KAR1
      KHAR2 = KAR2
      KHAR3 = KAR3
  710 GO TO (720,3000),IEDIT
C
C     OBSERVATION TIMES
  720 IF(JFLOW.EQ.2) GO TO 770
  724 WRITE(NO,725) IT
  725 FORMAT(3X,'ENTER TFIRST, TLAST, DELTAT  (',A2,')',/,'    ?,?,?')
  730 READ(NI,575,ERR=724) TF,TL,DELT
      DELT = ABS(DELT)
  740 IF(TF.GT.0.0.AND.DELT.LE.1.0E-06) GO TO 760
      IF(TF.GT.0.0) GO TO 750
  744 WRITE(NO,745)
  745 FORMAT(3X,'TFIRST MUST BE GREATER THAN ZERO -- REENTER',/,'    ?')
      READ(NI,95,ERR=744) TF
      GO TO 740
  750 IF(TL.GT.0.0) GO TO 770
  754 WRITE(NO,755)
  755 FORMAT(3X,'TLAST MUST BE GREATER THAN ZERO -- REENTER',/,'    ?')
      READ(NI,95,ERR=754) TL
      GO TO 750
  760 TL = TF
  770 GO TO (1000,780),IEDIT
  780 IF(JFLOW.EQ.2) WRITE(NO,785)
```

```
  785 FORMAT(3X,'TIME IS NOT A PARAMETER IN STEADY-STATE SOLUTION')
      GO TO 3000
C
C
C     LIST PROBLEM DEFINITION
 1000 WRITE(NO,1005) NPAGE,(TITLE(I),I=1,30)
 1005 FORMAT(1H1,/,3X,'PLUME3D',/,3X,'VERSION 2.02',
     1/,3X,'PAGE ',I3,///,3X,30A2,///)
      NPAGE = NPAGE + 1
      IF(ST.LE.0.9E32) WRITE(NO,1015) IL,ST
 1015 FORMAT(1H0,2X,'SATURATED THICKNESS, (',A2,')  ',26X,F10.4)
      WRITE(NO,1025) IL,IT,V,IL,IT,DX,IL,IT,DY,IL,IT,DZ,P
 1025 FORMAT(3X,'SEEPAGE VELOCITY, (',A2,'/',A2,') ',27X,F10.4,/,
     13X,'X DISPERSION COEFFICIENT (',A2,'**2/',A2,')   ',15X,F10.4,/,
     23X,'Y DISPERSION COEFFICIENT (',A2,'**2/',A2,')   ',15X,F10.4,/,
     33X,'Z DISPERSION COEFFICIENT (',A2,'**2/',A2,')   ',15X,F10.4,/,
     43X,'POROSITY ',44X,F10.4)
      WRITE(NO,1035) RD,IT,DECAY
 1035 FORMAT(//,3X,'RETARDATION COEFFICIENT',30X,F10.4,/,
     13X,'FIRST ORDER DECAY CONSTANT (1/',A2,')',20X,F10.4)
      GO TO (1070,1040), JFLOW
 1040 WRITE(NO,1045) IL,IL,IL,IM1,IM2,IM3,IL,IT
 1045 FORMAT(//,3X,'STEADY-STATE SOURCE RATES',//,
     13X,'SOURCE',6X,'X',11X,'Y',11X,'Z',17X,'RATE',/,
     25X,'NO',6X,'(',A2,')',8X,'(',A2,')',8X,'(',A2,')',6X,'(',3A2,
     3')(CU ',A2,'/',A2,')',/)
      DO 1060 I=1,NS
         WRITE(NO,1055) I,XS(I),YS(I),ZS(I),Q(I,1)
 1055    FORMAT(5X,I2,F10.2,2X,F10.2,2X,F10.2,6X,F16.4)
 1060 CONTINUE
      GO TO 1110
 1070 WRITE(NO,1075) IM1,IM2,IM3,IL,IT,IT,IL,IL,IL
 1075 FORMAT(//,3X,'SOURCE/RATE SCHEDULE  (',3A2,')(CU ',A2,'/',A2,
     1')'//,15X,'SOURCE',13X,'RATE',4X,'MASS',8X,'TIME (',A2,')',
     2/,3X,'NO    X (',A2,')    Y (',A2,')    Z (',A2,')    NO',5X,'RATE',
     35X,'START',6X,'END',/)
      DO 1100  I=1,NS
      WRITE(NO,1085) I,XS(I),YS(I),ZS(I)
 1085 FORMAT(/,3X,I2,3F9.2)
      NRT = NR(I)
      DO 1100  J=1,NRT
         M = J + 1
         WRITE(NO,1095) J,Q(I,M),T(I,M-1),T(I,M)
 1095    FORMAT(34X,I2,F12.2,2F9.2)
 1100 CONTINUE
 1110 WRITE(NO,1115) IL,IT,XF(1),XL(1),DEL(1),XF(2),XL(2),DEL(2),
     1 XF(3),XL(3),DEL(3)
 1115 FORMAT(//,3X,'OBSERVATION POINTS (',A2,'), AND TIMES (',A2,')',//,
     15X,'XFIRST =',F10.2,5X,'XLAST =',F10.2,5X,'DELX =',F10.4,/,
     25X,'YFIRST =',F10.2,5X,'YLAST =',F10.2,5X,'DELY =',F10.4,/,
     35X,'ZFIRST =',F10.2,5X,'ZLAST =',F10.2,5X,'DELZ =',F10.4)
      IF(JFLOW.EQ.1) WRITE(NO,1125) TF,TL,DELT
 1125 FORMAT(/,5X,'TFIRST =',F10.2,5X,'TLAST =',F10.2,5X,'DELT =',F10.4)
      WRITE(NO,1135) KSEC(LSEC)
 1135 FORMAT(//,3X,'AQUIFER SECTIONED IN ',A2,' PLANE')
      GO TO 3000
C
C
C
C ***** SECTION II -- NUMERICAL EVALUATION OF CONCENTRATION AT
C                     SPECIFIED GRID COORDINATES
C
C
C     NUMBER OF OBSERVATION POINTS IN EACH COORDINATE DIRECTION
 2000 CONTINUE
      DO 2020 L=1,3
         NP(L) = 1
         DEL(L) = ABS(DEL(L))
         IF(DEL(L).LE.1.0E-03) GO TO 2020
         DIF = XL(L) - XF(L)
```

```
        IF(ABS(DIF).LE.1.0E-03) GO TO 2020
        IF(DIF.LE.0.0) DEL(L)=-DEL(L)
        NPTS = ABS(DIF/DEL(L))
        REM = DIF - DEL(L)*FLOAT(NPTS)
        NPTS = NPTS + 1
        NP(L) = NPTS
        IF(ABS(REM).LT.1.0E-03) GO TO 2020
        NP(L) = NP(L) + 1
 2020 CONTINUE
      GO TO (2040,2060,2080),LSEC
 2040 MAXSC = NP(3)
      MAXRW = NP(2)
      MAXCL = NP(1)
      GO TO 2100
 2060 MAXSC = NP(2)
      MAXRW = NP(3)
      MAXCL = NP(1)
      GO TO 2100
 2080 MAXSC = NP(1)
      MAXRW = NP(3)
      MAXCL = NP(2)
 2100 CONTINUE
C
C     TIME COORDINATES
      NTIME = 1
      IF(DELT.LE.1.0E-06) GO TO 2110
      NTIME = ABS(TL-TF)/DELT + 1.0
      IF(TF.GT.TL) DELT=-DELT
 2110 TSOL = TF
      MTIME = NTIME
C
C
      DAMK = DX*DECAY*RD/(V*V)
      ALPHA=SQRT(1.0+4.0*DAMK)
      PE=V/DX
      BETA = DX/DY
      GAMMA = DX/DZ
      LAMBDA = 1.0/(25.132741*P*SQRT(DY*DZ))
C
C
      DO 2660  NT=1,NTIME
C
      NSEC = 1
 2120 LPRT = 1
      LP = 1
      NCFLG = 1
 2140 NROW1 = 1
      NROW2 = MAXROW
 2160 IF(NROW2.GT.MAXRW) NROW2=MAXRW
      DO 2580  NROW=NROW1,NROW2
      GO TO (2180,2220,2200),NCFLG
 2180 NCOL1 = 1
      NCOL2 = MAXCOL
 2200 IF(NCOL2.GT.MAXCL) NCOL2=MAXCL
      NCOL = MAXCOL
      IF(NCOL2.EQ.MAXCL) NCOL=NCOL2-NCOL1+1
 2220 GO TO (2240,2260,2280), LSEC
 2240 IX1 = NCOL1
      IX2 = NCOL2
      JY1 = NROW
      JY2 = NROW
      KZ1 = NSEC
      KZ2 = NSEC
      GO TO 2290
 2260 IX1 = NCOL1
      IX2 = NCOL2
      JY1 = NSEC
      JY2 = NSEC
      KZ1 = NROW
      KZ2 = NROW
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```
      GO TO 2290
 2280 IX1 = NSEC
      IX2 = NSEC
      JY1 = NCOL1
      JY2 = NCOL2
      KZ1 = NROW
      KZ2 = NROW
 2290 CONTINUE
C
      DO 2300  L=1,MAXCOL
         CON(L) = 0.0
 2300 CONTINUE
C
      DO 2440   N=1,NS
         D(1) = ST - ZS(N)
         IF(ST.GE.0.9E32) D(1)=0.0
         D(2) = ZS(N)
         D(3) = D(1)
         COEF = 1.0
         IF(D(1).LT.1.0E-03.OR.D(2).LT.1.0E-03) COEF=2.0
         DO 2440  I=IX1,IX2
            X = XF(1) + FLOAT(I-1)*DEL(1)
            IF(I.EQ.NP(1)) X=XL(1)
            XXS = X - XS(N)
            PEX = PE*XXS
            DO 2440  J=JY1,JY2
               Y = XF(2) + FLOAT(J-1)*DEL(2)
               IF(J.EQ.NP(2)) Y=XL(2)
               YYS = Y - YS(N)
               PEY = PE*YYS
               DO 2430  K=KZ1,KZ2
                  L = I-IX1 + J-JY1 + K-KZ1 + 1
                  IF(CON(L).LT.0.0) GO TO 2430
                  Z = XF(3) + FLOAT(K-1)*DEL(3)
                  IF(K.EQ.NP(3)) Z=XL(3)
                  ZM = Z - ZS(N)
                  IF(ABS(XXS).LT.1.0.AND.ABS(YYS).LT.1.0.AND.
     1               ABS(ZM).LT.1.0) GO TO 2330
                  PEZ = PE*ZM
                  CALL SOL3D(C,PEX,PEY,PEZ,TSOL,N,NR(N))
                  CXYZT = COEF*C
                  IF(IMAGE.EQ.1) GO TO 2325
C
                  DO 2320  LM=1,2
                     ZM = ((-1.0)**(LM+1))*ZM
                     IF(D(LM).LT.1.0E-03) GO TO 2320
                     ZIMAGE = 2.0*D(LM) - ZM
                     PEZ = PE*ZIMAGE
                     CALL SOL3D(C,PEX,PEY,PEZ,TSOL,N,NR(N))
                     CXYZT = CXYZT + COEF*C
                     DO 2310  IM = 1,IMAGE
                        ZIMAGE = (2.0*D(LM)+ZM) + 2.0*FLOAT(IM)*D(LM+1)
     1                           + FLOAT(2*IM-2)*D(LM)
                        PEZ = PE*ZIMAGE
                        CALL SOL3D(C,PEX,PEY,PEZ,TSOL,N,NR(N))
                        IF(C.LT.1.0E-06) GO TO 2312
                        CXYZT = CXYZT + COEF*C
  2310               CONTINUE
  2312               CONTINUE
                     DO 2314  IM=1,IMAGE
                        ZIMAGE = (2.0*D(LM)-ZM) + 2.0*FLOAT(IM)*D(LM+1)
     1                           + FLOAT(2*IM)*D(LM)
                        PEZ = PE*ZIMAGE
                        CALL SOL3D(C,PEX,PEY,PEZ,TSOL,N,NR(N))
                        IF(C.LT.1.0E-06) GO TO 2320
                        CXYZT = CXYZT + COEF*C
  2314               CONTINUE
                     WRITE(NO,2315) MAXIMG,X,Y,Z
  2315               FORMAT(3X,'****** WARNING -- SOLUTION DID NOT',
     1               ' CONVERGE USING',/,9X,I2,' IMAGE WELLS AT X =',
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     2               F10.4,'  Y =',F10.4,'  Z =',F10.4)
 2320          CONTINUE
 2325          CON(L) = CON(L) + CXYZT
               GO TO 2340
 2330          CON(L) = -9.9999
 2340          GO TO (2360,2380,2400), LSEC
 2360          SEC = Z
               ROW = Y
               COL(L) = X
               GO TO 2420
 2380          SEC = Y
               ROW = Z
               COL(L) = X
               GO TO 2420
 2400          SEC = X
               ROW = Z
               COL(L) = Y
 2420          CONTINUE
 2430       CONTINUE
 2440 CONTINUE
C
C     PRINT CONCENTRATION DISTRIBUTION
      GO TO (2460,2560), LPRT
 2460 WRITE(NO,1005) NPAGE, (TITLE(I),I=1,30)
      NPAGE = NPAGE + 1
      IF(JFLOW.EQ.2) GO TO 2500
      WRITE(NO,2465) TSOL,IT,IM1,IM2,IM3,KHAR1,SEC,IL,
     1(LBL(LP,L),L=1,6),KHAR2,IL
 2465 FORMAT(13X,'CONCENTRATION DISTRIBUTION AT ',F10.2,
     11X,A2,' (',3A2,') ',//,13X,A1,' =',F10.2,1X,A2,3X,6A2,//,
     2' *',/,'    * ',A1,'(',A2,')')
      GO TO 2520
 2500 WRITE(NO,2505) IM1,IM2,IM3,KHAR1,SEC,IL,(LBL(LP,L),L=1,6),
     1KHAR2,IL
 2505 FORMAT(13X,'CONCENTRATION DISTRIBUTION AT STEADY STATE',
     1' (',3A2,') ',//13X,A1,' =',F10.2,1X,A2,3X,6A2,//,
     2' *',/,'    * ',A1,'(',A2,')')
 2520 CONTINUE
      WRITE(NO,2525) (COL(L),L=1,NCOL)
 2525 FORMAT('      *',4X,7F10.2)
      WRITE(NO,2545) KHAR3,IL
 2545 FORMAT(1X,A1,'(',A2,') *',/,9X,'*')
C
 2560 WRITE(NO,2565) ROW,(CON(L),L=1,NCOL)
 2565 FORMAT(2X,F8.2,7F10.4)
      LPRT = 2
 2580 CONTINUE
      IF(NROW2.EQ.MAXRW) GO TO 2600
      NROW1 = NROW1 + MAXROW
      NROW2 = NROW2 + MAXROW
      LPRT = 1
      LP = 2
      NCFLG = 2
      GO TO 2160
 2600 IF(NCOL2.EQ.MAXCL) GO TO 2620
      NCOL1 = NCOL1 + MAXCOL
      NCOL2 = NCOL2 + MAXCOL
      LPRT = 1
      LP = 2
      NCFLG = 3
      GO TO 2140
 2620 IF(NSEC.EQ.MAXSC) GO TO 2640
      NSEC = NSEC + 1
      GO TO 2120
 2640 CONTINUE
      TSOL = TSOL + DELT
      IF(NT.EQ.MTIME) TSOL=TL
 2660 CONTINUE
C
C
```

```
C ***** SECTION III -- PROBLEM REDEFINITION AND CONTROL OF EXECUTION
C
C
 3000 CONTINUE
      IF(IEDIT.EQ.2) GO TO 3010
      WRITE(NO,3705)
      IEDIT = 2
 3010 KNTL = 2
      WRITE(NO,3015)
 3015 FORMAT(//,3X,'ENTER NEXT COMMAND',/,'   ?')
 3020 READ(NI,3025) NEXT
 3025 FORMAT(A2)
C
      DO 3030  I=1,21
         IF(NEXT.EQ.IC(I)) GO TO 3040
 3030 CONTINUE
      WRITE(NO,3035)
 3035 FORMAT(3X,'ERROR IN LAST COMMAND -- REENTER',/,'   ?')
      GO TO 3020
 3040 GO TO (10,80,120,160,190,220,250,280,310,320,560,580,590,640,
     1        720,1000,2000,3050,3060,3700,4000),I
C
C     NEW SET OF X, Y, AND Z OBSERVATIONS
 3050 KNTL = 1
      GO TO 560
C
C
C
C     NEW SOURCE/RATE SCHEDULE
 3060 WRITE(NO,3065)
 3065 FORMAT(3X,'ADD(A),DELETE(D),MODIFY(M) A SOURCE OR RETURN(R)'
     1' TO EDIT ?')
 3070 READ(NI,3075) ISK
 3075 FORMAT(A1)
      DO 3080  I=1,4
         IF(ISK.EQ.IS(I)) GO TO 3090
 3080 CONTINUE
      WRITE(NO,3085)
 3085 FORMAT(3X,'ERROR IN SELECTION -- REENTER ?')
      GO TO 3070
 3090 GO TO (3000,3100,3450,3490),I
C
C     MODIFY SOURCE
C
 3100 WRITE(NO,3105) NS
 3105 FORMAT(3X,I2,' SOURCES IN CURRENT SCHEDULE',/,
     13X,'ENTER SOURCE TO MODIFY',/,'   ?')
      READ(NI,465,ERR=3100) FDUM
      JS=FDUM
      IF(JS.GT.0.AND.JS.LE.NS) GO TO 3220
      WRITE(NO,3215) JS
 3215 FORMAT(3X,'SOURCE',I4,' NOT IN SCHEDULE')
      GO TO 3060
 3220 GO TO (3230,3260),JFLOW
 3230 WRITE(NO,3235) JS,XS(JS),IL,YS(JS),IL,ZS(JS),IL,IT,
     1IM1,IM2,IM3,IL,IT
 3235 FORMAT(3X,'SOURCE ',I2,':    X =',F8.2,A3,',   Y =',F8.2,A3,
     1',   Z =',F8.2,A3,//,3X,'RATE',7X,'MASS RATE',14X,'TIME (',
     2A2,')',/,4X,'NO',3X,'(',3A2,')(CU ',A2,'/',A2,')',
     38X,'START',7X,'END',/)
      NRT = NR(JS)
      DO 3250  J=1,NRT
         M = J + 1
         WRITE(NO,3245) J,Q(JS,M),T(JS,M-1),T(JS,M)
 3245    FORMAT(4X,I2,5X,F14.2,7X,F8.3,3X,F8.2)
 3250 CONTINUE
      GO TO 3270
 3260 WRITE(NO,3265) JS,XS(JS),IL,YS(JS),IL,ZS(JS),IL,Q(JS,1),
     1IM1,IM2,IM3,IL,IT
 3265 FORMAT(3X,'SOURCE ',I2,':    X =',F8.2,A3,',   Y =',F8.2,A3,
```

```
     1',  Z=',F8.2,A3,/,3X,'STEADY-STATE MASS RATE =',F16.4,             PL3D701
     2' (',3A3,')(CU ',A2,'/',A2,')',/)                                   PL3D702
 3270 WRITE(NO,3275)                                                      PL3D703
 3275 FORMAT(3X,'CHANGE COORDINATES (Y/N)?')                              PL3D704
      READ(NI,3075) JC                                                    PL3D705
      IF(JC.NE.IY) GO TO 3290                                             PL3D706
 3276 WRITE(NO,415) JS,IL                                                 PL3D707
      READ(NI,425,ERR=3276) XS(JS),YS(JS),ZS(JS)                          PL3D708
 3280 IF(ZS(JS).GE.0.0.AND.ZS(JS).LE.ST) GO TO 3290                       PL3D709
 3284 WRITE(NO,435) ST,IL                                                 PL3D710
      READ(NI,95,ERR=3284) ZS(JS)                                         PL3D711
      GO TO 3280                                                          PL3D712
 3290 GO TO (3300,3430),JFLOW                                             PL3D713
C                                                                         PL3D714
C     TRANSIENT SOURCES                                                   PL3D715
 3300 WRITE(NO,3305) JS                                                   PL3D716
 3305 FORMAT(3X,'MODIFY RATE SCHEDULE FOR SOURCE',I3,' (Y/N) ?')          PL3D717
      READ(NI,3075) JY                                                    PL3D718
      IF(JY.NE.IY) GO TO 3060                                             PL3D719
 3310 WRITE(NO,3315)                                                      PL3D720
 3315 FORMAT(3X,'ENTER RATE TO BE CHANGED',/,                             PL3D721
     13X,'(ENTER 0 TO CHANGE ALL RATES)',/,'   ?')                        PL3D722
      READ(NI,465,ERR=3310) FDUM                                          PL3D723
      JR=FDUM                                                             PL3D724
      IF(JR.LE.0) GO TO 3350                                              PL3D725
      IF(JR.LE.NR(JS)) GO TO 3330                                         PL3D726
      WRITE(NO,3325) JR                                                   PL3D727
 3325 FORMAT(3X,'RATE ',I2,' NOT IN CURRENT SCHEDULE')                    PL3D728
      GO TO 3300                                                          PL3D729
 3330 WRITE(NO,3335) JS,JR,T(JS,JR),T(JS,JR+1),IT                         PL3D730
 3335 FORMAT(3X,'SOURCE ',I2,', RATE ',I2,' STARTS AT',F8.2,              PL3D731
     1' AND ENDS AT',F8.2,A3,/,3X,'ENTER NEW MASS RATE',/,'   ?')         PL3D732
      M = JR + 1                                                          PL3D733
      READ(NI,3345,ERR=3330) Q(JS,M)                                      PL3D734
 3345 FORMAT(F10.0)                                                       PL3D735
      GO TO 3300                                                          PL3D736
C                                                                         PL3D737
 3350 NRT = NR(JS)                                                        PL3D738
      DO 3360  J=1,NRT                                                    PL3D739
         M = J + 1                                                        PL3D740
         Q(JS,M) = 0.0                                                    PL3D741
         T(JS,M) = 0.0                                                    PL3D742
 3360 CONTINUE                                                            PL3D743
 3370 WRITE(NO,455) JS,MAXRT                                              PL3D744
 3380 READ(NI,465,ERR=3370) FDUM                                          PL3D745
      NR(JS)=FDUM                                                         PL3D746
      IF(NR(JS).GT.0.AND.NR(JS).LE.MAXRT) GO TO 3390                      PL3D747
      WRITE(NO,475) MAXRT                                                 PL3D748
      GO TO 3380                                                          PL3D749
 3390 CONTINUE                                                            PL3D750
      NRT = NR(JS)                                                        PL3D751
      DO  3420  J=1,NRT                                                   PL3D752
         M = J + 1                                                        PL3D753
 3394    WRITE(NO,485) JS,J,T(JS,M-1),IT                                  PL3D754
         READ(NI,495,ERR=3394) Q(JS,M),T(JS,M)                            PL3D755
 3400    IF(T(JS,M).GT.T(JS,M-1)) GO TO 3410                              PL3D756
 3404    WRITE(NO,505)                                                    PL3D757
         READ(NI,95,ERR=3404) T(JS,M)                                     PL3D758
         GO TO 3400                                                       PL3D759
 3410    CONTINUE                                                         PL3D760
 3420 CONTINUE                                                            PL3D761
      GO TO 3060                                                          PL3D762
C                                                                         PL3D763
C     STEADY-STATE SOURCES                                                PL3D764
 3430 WRITE(NO,3435) JS                                                   PL3D765
 3435 FORMAT(3X,'CHANGE STEADY-STATE RATE FOR SOURCE ',I2,' (Y/N) ?')     PL3D766
      READ(NI,3075) JC                                                    PL3D767
      IF(JC.NE.IY) GO TO 3060                                             PL3D768
 3444 WRITE(NO,3445) JS                                                   PL3D769
 3445 FORMAT(3X,'ENTER NEW STEADY-STATE MASS RATE FOR SOURCE ',I2,/,      PL3D770
```

```
     1'    ?')
      READ(NI,3345,ERR=3444) Q(JS,1)
      GO TO 3060
C
C     ADD A NEW SOURCE
C
 3450 NS = NS + 1
      JS = NS
 3454 WRITE(NO,415) JS,IL
      READ(NI,425,ERR=3454) XS(JS),YS(JS),ZS(JS)
 3460 IF(ZS(JS).GE.0.0.AND.ZS(JS).LE.ST) GO TO 3470
 3464 WRITE(NO,435) ST,IL
      READ(NI,95,ERR=3464) ZS(JS)
      GO TO 3460
 3470 GO TO (3370,3480),JFLOW
C
C     STEADY-STATE SOURCES
 3480 WRITE(NO,3485) JS
 3485 FORMAT(3X,'ENTER STEADY-STATE MASS RATE FOR SOURCE ',I2,
     1/,'    ?')
      READ(NI,3345,ERR=3480) Q(JS,1)
      NR(JS) = 0
      GO TO 3060
C
C     DELETE A SOURCE
C
 3490 IF(NS.GT.1) GO TO 3500
      WRITE(NO,3495)
 3495 FORMAT(3X,'ONLY ONE SOURCE IN SCHEDULE -- CAN NOT DELETE',/)
      GO TO 3060
 3500 WRITE(NO,3505) IL,IL,IL
 3505 FORMAT(3X,'SOURCE',6X,'X (',A2,')',3X,'Y (',A2,')',3X,
     1'Z (',A2,')',/)
      DO 3520  I=1,NS
         WRITE(NO,3515) I,XS(I),YS(I),ZS(I)
 3515    FORMAT(5X,I2,3X,F8.2,3X,F8.2,3X,F8.2)
 3520 CONTINUE
 3530 WRITE(NO,3535)
 3535 FORMAT(3X,'ENTER SOURCE TO DELETE',/,
     13X,'(ENTER 0 TO CANCEL)',/,'    ?')
      READ(NI,465,ERR=3530) FDUM
      JS=FDUM
      IF(JS.LE.0) GO TO 3060
      IF(JS.LE.NS) GO TO 3550
      WRITE(NO,3545) JS
 3545 FORMAT(3X,'SOURCE ',I2,' NOT IN CURRENT SCHEDULE')
      GO TO 3530
 3550 WRITE(NO,3555) JS
 3555 FORMAT(3X,'DELETE SOURCE ',I2,' (Y/N)?')
      READ(NI,3075) JC
      IF(JC.NE.IY) GO TO 3530
      NSD = NS - 1
      GO TO (3560,3590),JFLOW
C
C     TRANSIENT SOURCES
 3560 IF(JS.EQ.NS) GO TO 3575
      DO  3570  J=JS,NSD
         XS(J) = XS(J+1)
         YS(J) = YS(J+1)
         ZS(J) = ZS(J+1)
         NR(J) = NR(J+1)
         NRT = NR(J)
            DO 3570  K=1,NRT
            M = K + 1
            Q(J,M) = Q(J+1,M)
            T(J,M) = T(J+1,M)
 3570 CONTINUE
 3575 NRT = NR(NS)
      DO 3580  K=1,NRT
         M = K + 1
```

```
         Q(NS,M) = 0.0
         T(NS,M) = 0.0
 3580 CONTINUE
      NR(NS) = 0
      NS = NSD
      GO TO 3060
C
C     STEADY-STATE SOURCES
 3590 IF(JS.EQ.NS) GO TO 3605
      DO 3600  J=JS,NSD
         Q(J,1) = Q(J+1,1)
         XS(J) = XS(J+1)
         YS(J) = YS(J+1)
         ZS(J) = ZS(J+1)
 3600 CONTINUE
 3605 Q(NS,1) = 0.0
      NS = NSD
      GO TO 3060
C
C
C     MENU OF EDIT COMMANDS FOR PLUME3D VERSION 2.02
 3700 WRITE(NO,3705)
 3705 FORMAT(1H1,/,3X,'MENU OF EDIT COMMANDS',//,
     13X,'SATURATED THICKNESS        ST       OBSERVATION POINTS    OB',/,
     23X,'POROSITY                   PO       X COORDINATES         XC',/,
     33X,'SEEPAGE VELOCITY           VX       Y COORDINATES         YC',/,
     43X,'RETARDATION COEFFICIENT    RD       Z COORDINATES         ZC',/,
     53X,'X DISPERSION COEFFICIENT   DX       OBSERVATION TIMES     TC',/,
     53X,'Y DISPERSION COEFFICIENT   DY       AQUIFER SECTIONING    AS',/,
     63X,'Z DISPERSION COEFFICIENT   DZ       NEW PROBLEM           NP',/,
     73X,'DECAY CONSTANT             DE       MENU OF COMMANDS      MU',/,
     83X,'SOURCE/RATE SCHEDULE       RT       LIST INPUT DATA       LI',/,
     93X,'CHANGE SOLUTION/SOURCES    CS       RUN CALCULATIONS      RN',/,
     13X,'                                    DONE                  DN')
      GO TO 3000
C
 4000 STOP
      END
```

```
      FUNCTION ERFCLG(Z)
C     RATIONAL APPROXIMATION OF THE COMPLIMENTARY ERROR FUNCTION
C     SEE SECTION 7.1 OF ABRAMOWITZ AND STEGUN (1966)
C     THE FOLLOWING IDENTITIES ARE USED TO HANDLE NEGATIVE ARGUMENTS
C        ERFC( Z) = 1 - ERF(Z)
C        ERF (-Z) = -ERF (Z)
C
      REAL*8 COEFLG,DERFC,DI,FX,TERMI,TERMO,SUM,X
      COMMON/IO/NI,NO
C
      X = ABS(Z)
      IF (X.GT.3.0D00) GO TO 50
C
C     FOR X<3 A RATIONAL APPROXIMATION OF THE COMPLIMENTARY ERROR
C     FUNCTION IS USED.
C
      DERFC = 1.0D00/((1.0D00 + 7.05230784D-02*X + 4.22820123D-02*(X**2)
     1                  + 9.2705272D-03*(X**3) + 1.520143D-04*(X**4)
     2                  + 2.76572D-04*(X**5) + 4.30638D-05*(X**6))**16)
      ERFCLG = DLOG(DERFC)
      GO TO 100
C
C     FOR X>3 AN ASYMPTOTCI EXPANSION OF THE COMPLIMENTARY ERROR
C     FUNCTION IS USED.
   50 COEFLG = X*X + DLOG(X) + 0.57236494D00
      FX = 2.0D00*X*X
      SUM = 1.0D00
      TERMO = 1.0D00
      DO 60 I=2,50
      DI = I
      TERMI = -TERMO*(2.0D00*DI - 3.0D00)/FX
      IF(DABS(TERMI).GT.DABS(TERMO)) GO TO 70
      SUM = SUM + TERMI
      TEST = TERMI/SUM
      IF(ABS(TEST).LT.1.0E-16) GO TO 70
      TERMO = TERMI
   60 CONTINUE
      WRITE(NO,65)
   65 FORMAT(6X,'*** WARNING -- ASYMPTOTIC EXPANSION FOR ERFC DID NOT',
     1'                CONVERGE WITH 50 TERMS IN THE SUMMATION')
   70 SUM = DLOG(SUM) - COEFLG
      ERFCLG = SUM
  100 CONTINUE
C
C     FOR Z<0. ERFC(-Z) = 2-ERFC(Z)
      IF(Z.LT.0.0) GO TO 200
      RETURN
  200 ERFC = 2.0 - EXP(ERFCLG)
      ERFCLG = ALOG(ERFC)
      RETURN
      END
```

```
      SUBROUTINE SOL3D(C,PEX,PEY,PEZ,TSOL,N,NR)
C     NUMERICAL EVALUATION OF ANALYTICAL SOLUTION
C
      REAL LAMBDA
      COMMON/RATE/Q(10,12),T(10,12)
      COMMON/PHYPRO/ALPHA,BETA,GAMMA,DX,LAMBDA,PE,RD,V
C
      PEXYZ = SQRT(PEX*PEX + BETA*(PEY*PEY) + GAMMA*(PEZ*PEZ))
      R = PEXYZ/PE
      PEL = PEXYZ*ALPHA
      PEX12 = PEX/2.0
      PEL12 = PEL/2.0
      COEF = LAMBDA/R
      MT = NR + 1
      IF(MT.GT.1) GO TO 10
C
C     STEADY-STATE SOLUTION
C
      S = Q(N,1)
      IF(CLG.LT.-72.0) CLG = -72.0
      IF(CLG.GT. 72.0) CLG =  72.0
      C = 2.0*EXP(CLG)
      GO TO 50
C
C     TRANSIENT SOLUTION
   10 C = 0.0
      IF(T(N,MT).LT.TSOL) MT=MT+1
      DO 40  K=2,MT
         IF(T(N,K-1).GT.TSOL) GO TO 50
         S = Q(N,K) - Q(N,K-1)
         SGN = 1.0
         IF(S.LT.0.0) SGN = -1.0
         SA = ABS(S)
         IF(SA.LT.1.0E-3) GO TO 40
         COEFLG = ALOG(COEF*SA)
         PINJ = V*V*(TSOL-T(N,K-1))/(DX*RD)
         PINJL = PINJ*ALPHA*ALPHA
         TAU = PINJ/(PEXYZ*PEXYZ)
         Z1 = 0.5/SQRT(TAU)
         Z2 = 0.5*SQRT(PINJL)
         Z = Z1 + Z2
         T1 = ERFCLG(Z)
         C1LG = T1 + PEL12 + PEX12 + COEFLG
         Z = Z1 - Z2
         T2 = ERFCLG(Z)
         C2LG = T2 - PEL12 + PEX12 + COEFLG
         IF(C1LG.GT. 72.0) C1LG= 72.0
         IF(C1LG.LT.-72.0) C1LG=-72.0
         IF(C2LG.GT. 72.0) C2LG= 72.0
         IF(C2LG.LT.-72.0) C2LG=-72.0
         CK = EXP(C1LG) + EXP(C2LG)
         C = C + SGN*CK
   40 CONTINUE
   50 RETURN
      END
```

APPENDIX C

Solute Transport in Uniform Ground-Water Flow Mathematical Development

SOLUTE TRANSPORT IN UNIFORM GROUND-WATER FLOW

MATHEMATICAL DEVELOPMENT

Analytical solute-transport models are highly idealized mathematical approximations of complex physical phenomena. However, if applied properly this class of models represents a useful tool for analyzing the transport and fate of substances under both field and laboratory conditions.

This mathematical derivation of a governing differential equation for solute transport in uniform ground-water flow is developed in an effort to show the relationship between physical processes in the aquifer and terms in the mathematical model. In this context, the "mathematical manipulations" of the derivation are not as important as the simplifying assumptions which are required to obtain a mathematical description of the problem.

The resulting differential equation serves as the basis of many analytical solute-transport models. Solutions of the differential equation which would provide the actual concentration distributions in time and space are not addressed in this document. However, the simplifying assumptions which are incorporated in the formulation of the mathematical model must be considered in both the application of the model and in the interpretation of modeling results, regardless of how the model is solved.

Derivation or the Governing Differential Equation.

Consider a differential element of homogeneous aquifer as shown in Figure 1. A material balance for any tracer can be written as

$$\text{Rate of Mass In} - \text{Rate of Mass Out} + \text{Rate of Mass Generation} = \text{Rate of Mass Accumulation} \qquad (1)$$

Each of the terms in this expression are developed in the following paragraphs.

Rate of Mass In:

The tracer can enter the differential control volume by two mechanisms. The first is convection, or bulk flow, of tracer in solution. This mechanism can be expressed as

$$Q_x C|_x + Q_y C|_y + Q_z C|_z$$

where Q_x, Q_y and Q_z are the volumetric flow rates in the x, y and z directions, respectively, and C is the concentration of tracer in the fluid.

Tracer can also enter the control volume by molecular diffusion and hydrodynamic dispersion. For the time being these processes can be combined as a "dispersion flux" term, q", with dimensions of mass input per unit time per unit area. Thus,

$$q''_x|_x \, \Delta y \Delta z + q''_y|_y \, \Delta z \Delta z + q''_z|_z \, \Delta z \Delta y$$

represents the rate of mass entering the control volume by "dispersion."

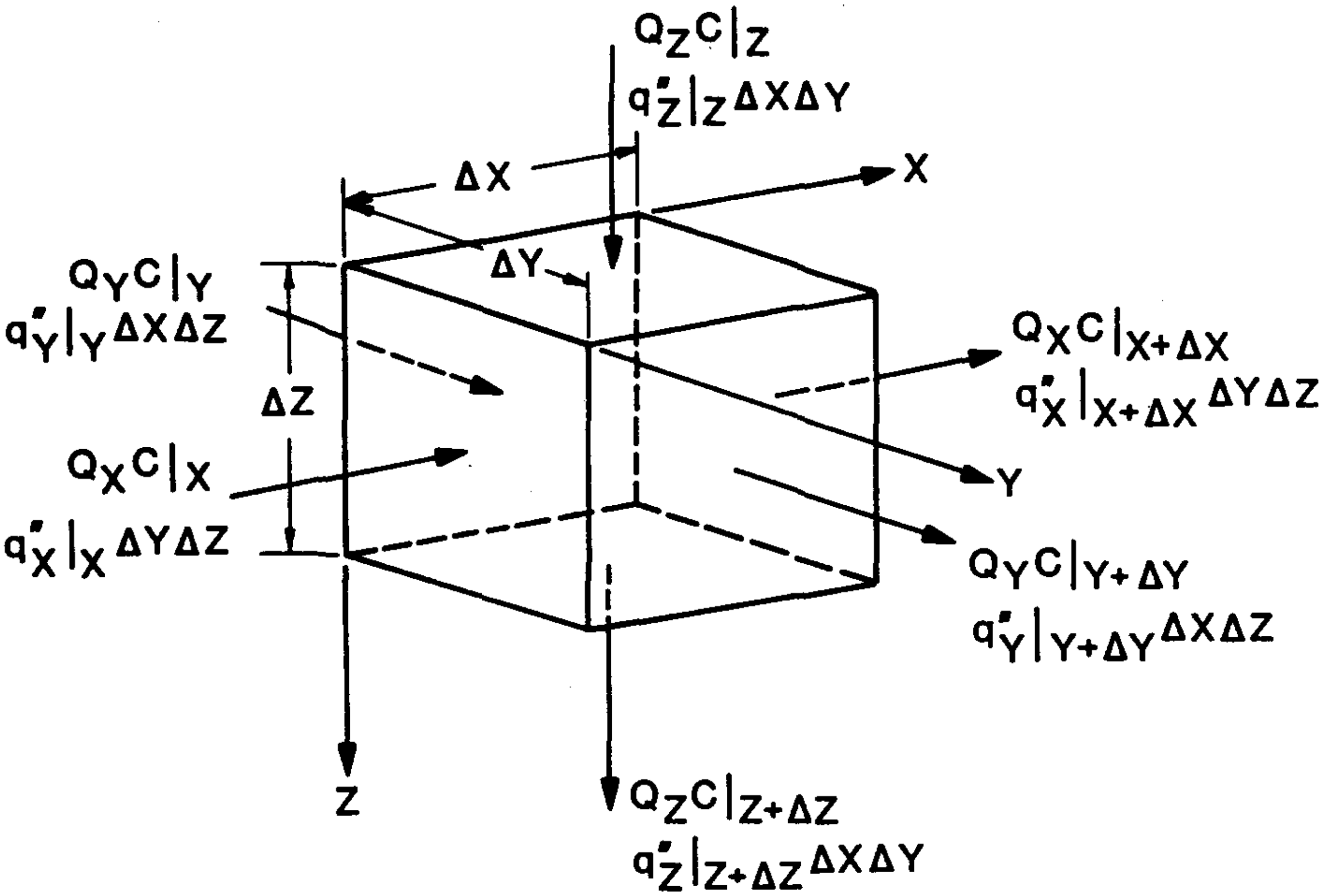

Figure 1 - Differential Control Volume for Mass Balance

Rate of Mass Out:

Tracer can leave the control volume by the same mechanisms described for the input terms. Thus, the rates of mass leaving by convection and dispersion can be written as

$$Q_x C|_{x+\Delta x} + Q_y C|_{y+\Delta y} + Q_z C|_{z+\Delta z}$$

and

$$q''_x|_{x+\Delta x}\ \Delta y \Delta z + q''_y|_{y+\Delta y}\ \Delta x \Delta z + q''_z|_{z+\Delta z}\ \Delta x \Delta y$$

respectively

Rate of Mass Generation:

Tracer can be generated (or degraded) in the control volume by physical, chemical, and/or biological reaction. A general relationship can be written as

$$r_T\ \Delta x \Delta y \Delta z$$

where r_T is the total, or overall, rate of generation per unit volume of aquifer.

Rate of Mass Accumulation:

The total rate of mass accumulated in the control volume during a differential period of time is

$$\frac{C_T|_{t+\Delta t} - C_T|_t}{\Delta t} (\Delta x \Delta y \Delta z)$$

where C_T is the total mass of trace per unit volume of aquifer.

Substituting the expressions for the various terms into Equation 1, and dividing by $(\Delta x \Delta y \Delta z)$ yields

$$- \frac{Q_x C|_{x+\Delta x} - Q_x C|_x}{\Delta x \ (\Delta y \Delta z)} - \frac{Q_y C|_{y+\Delta y} - Q_y C|_y}{\Delta y \ (\Delta x \Delta z)} - \frac{Q_z C|_{z+\Delta z} - Q_z C|_z}{\Delta z \ (\Delta x \Delta y)}$$

$$- \frac{q''_x|_{x+\Delta x} - q''_x|_x}{\Delta x} - \frac{q''_y|_{y+\Delta y} - q''_y|_y}{\Delta y} - \frac{q''_z|_{z+\Delta z} - q''_z|_z}{\Delta z} + r_T$$

$$= \frac{(C_T)_{t+\Delta t} - (C_T)_t}{\Delta t} \qquad (2)$$

Now

$$V_x \equiv \frac{Q_x}{\Delta y \Delta z} \qquad (3a)$$

$$V_y \equiv \frac{Q_y}{\Delta z \Delta x} \qquad (3b)$$

and

$$V_z \equiv \frac{Q_z}{\Delta x \Delta y} \qquad (3c)$$

where V is the superficial, or Darcy, velocity. Taking the limit of Equation 2 as Δx, Δy, Δz, and Δt go to zero yields

$$- \frac{\partial(V_x C)}{\partial_x} - \frac{\partial(V_y C)}{\partial_y} - \frac{\partial(V_z C)}{\partial_z} - \frac{\partial q''_x}{\partial_x} - \frac{\partial q''_y}{\partial_y} - \frac{\partial q''_z}{\partial_z} + r_T = \frac{\partial C_T}{\partial_t} \quad (4)$$

Equation 4 is the differential mass balance for a tracer in a porous medium.

If a Fickian model is assumed for the dispersion flux, these fluxes can be expressed in terms of concentration gradients. Neglecting surface diffusion of tracer which may be adsorbed on the solid matrix,

$$q''_n = - D_n \frac{\partial(\Theta C)}{\partial_n} \quad (5)$$

where n is the coordinate direction, D_n is a dispersion coefficient, and Θ is the effective porosity or fractional void volume. The concentration gradient in the liquid phase is the driving force for mass tranport by dispersion. The porosity has been included since the mass balance has been formulated for a unit volume of aquifer, which includes the solid matrix as well as the fluid-filled pores. Substituting an expression of the form of Equation 5 for each of the dispersion flux terms in Equation 4 yields

$$\frac{\partial C_T}{\partial_x} + \frac{\partial(V_x C)}{\partial_x} + \frac{\partial(V_y C)}{\partial_y} + \frac{\partial(V_z C)}{\partial_z}$$

$$= \frac{\partial}{\partial_x} D_x \frac{\partial(\Theta C)}{\partial_x} + \frac{\partial}{\partial_y} D_y \frac{\partial(\Theta C)}{\partial_y} + \frac{\partial}{\partial_z} D_z \frac{\partial(\Theta C)}{\partial_z} + r_T \quad (6)$$

Two assumptions will be made at this point. The first is that the aquifer is homogeneous, which implies that the porosity and dispersion coefficients are not functions of position. The second assumption is that the ground-water flow is uniform and directed along the x-axis, i.e., V_x = constant and $V_y = V_z = 0$. With these assumptions, Equation 6 reduces to

$$\frac{\partial C_T}{\partial t} + V_x \frac{\partial C}{\partial x} = \Theta D_x \frac{\partial^2 C}{\partial x^2} + \Theta D_y \frac{\partial^2 C}{\partial y^2} + \Theta D_z \frac{\partial^2 C}{\partial z^2} + r_T \qquad (7)$$

This equation is a statement of conservation of tracer in homogeneous aquifer with uniform ground-water flow. The accumulation and reaction terms are developed in the following paragraphs.

Accumulation. In general, the total mass of tracer per unit volume of aquifer, C_T, can be distributed as dissolved solute in the fluid-filled pore volume and as adsorbed solute on the solid matrix, or

$$\frac{\text{mass of tracer}}{\text{bulk volume}} = \frac{\text{mass of tracer}}{\text{volume of solution}} \; \frac{\text{volume of solution}}{\text{bulk volume}} + \frac{\text{mass of tracer}}{\text{mass of solids}} \; \frac{\text{mass of solids}}{\text{bulk volume}} \qquad (8)$$

Equation 8 can be written in terms of aquifer properties as

$$C_T = \Theta C + \rho_B C_s \qquad (9)$$

where ρ_B is the bulk density of the solid matrix and C_s is the adsorbed mass concentration (mass of tracer per unit mass of solids). For a homogeneous aquifer, the accumulation term in Equation 7 can be written as

$$\frac{\partial C_T}{\partial t} = \Theta \frac{\partial C}{\partial t} + \rho_B \frac{\partial C_s}{\partial t} \qquad (10)$$

In general, the concentration of absorbed solute, C_s, is a function of the concentration of solute in solution, C, and

$$\frac{\partial C_s}{\partial t} = \frac{dC_s}{dC} \frac{\partial C}{\partial t} \tag{11}$$

For a linear adsorption isotherm,

$$C_s = K_d C \tag{12}$$

or

$$\frac{dC_s}{dC} = K_d \tag{13}$$

where K_d is a constant commonly referred to as an adsorption, or distribution, coefficient. The rate of accumulation of tracer per unit volume of aquifer can be expressed in terms of the concentration in solution by combining Equations 10, 11 and 13 as follows:

$$\frac{\partial C_T}{\partial t} = \Theta \frac{\partial C}{\partial t} + \rho_B K_d \frac{\partial C}{\partial t} \tag{14}$$

The coefficients of $\partial C/\partial t$ are often combined as

$$R_d \equiv 1 + \frac{K_d \rho_B}{\Theta} \tag{15}$$

where R_d is referred to as a "retardation coefficient." Rewriting Equation 14 as

$$\frac{\partial C_T}{\partial t} = \Theta R_d \frac{\partial C}{\partial t} \qquad (14)$$

or

$$\frac{\partial C_T}{\partial t} = \Theta \frac{\partial C}{\partial (t/R_d)} \qquad (15)$$

gives some insight into the effect of adsorption on accumulation of tracer in the homogeneous aquifer. The apparent effect is a distortion or "retardation" of the time dimension.

Reaction. Only first-order reactions will be considered in formulating the rate of reaction term, r_T, in Equation 7. The kinetic models for reaction of tracer in solution and adsorbed tracer are

$$\frac{\partial C}{\partial t} = - \lambda_f C \qquad (16)$$

and

$$\frac{\partial C_s}{\partial t} = - \lambda_s C_s \qquad (17)$$

where λ_f and λ_s are the fluid phase and solid phase rate coefficients, respectively. Equations 16 and 17 have been written for degradation of tracer, i.e. negative generation. The overall rate of reaction can be written as

$$r_T \equiv \frac{\partial C_T}{\partial t} = - \Theta \lambda_f C - \rho_B \lambda_s C_s \qquad (18)$$

Including the linear adsorption isotherm developed above

$$C_s = K_d C$$

and

$$r_T = -\theta\left(\lambda_f + \frac{\rho_B K_d}{\theta}\lambda_s\right) C \qquad (19)$$

or

$$r_T = -\theta\lambda_T C \quad . \qquad (20)$$

where λ_T is an apparent overall first-order rate constant defined as

$$\lambda_T \equiv \lambda_f + \frac{\rho_B K_d}{\theta}\lambda_s \qquad (21)$$

For radioactive decay, the rate of reaction is usually expressed in terms of the "half-life" or the time required for the concentration to be reduced to one-half of the initial concentration, $t_{1/2}$. Integrating Equation 16 or 17 from $t = 0$ to $t = t_{1/2}$

$$\int_{C_o}^{C_o/2} \frac{dC}{C} = -\lambda \int_0^{t_{1/2}} dt$$

or

$$\ln C \Big|_{C_o}^{C_o/2} = -\lambda\, t_{1/2}$$

Solving for the rate constant,

$$\lambda = \frac{\ln 2}{t_{1/2}}$$

which is an expression for evaluating a first-order rate constant from the half-life of the reaction.

In the case of radioactive decay, the rate constants are independent of the phase in which the reaction is occuring, and

$$\lambda = \lambda_f = \lambda_s$$

Equation 21 can then be written as

$$\lambda_T = R_d \lambda$$

and Equation 19 becomes

$$r_T = - \Theta R_d \lambda C \qquad (22)$$

Equation 22 applies to all cases where the first-order reaction rate constants are the same for both fluid and solid phase reactions.

Differential Equation in Terms of Fluid Phase Concentrations.

The differential mass balance for a tracer in a homogeneous aquifer with uniform ground-water flow, Equation 7, can be written in terms of fluid-phase concentrations by incorporating Equation 14 for linear adsorption and Equation 19 for first-order reactions. Making these substitutions and rearranging yields

$$R_d \frac{\partial C}{\partial t} + V^* \frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - \lambda_T C \qquad (23)$$

where V^* is the average interstitial, or pore, velocity defined as

$$V^* \equiv \frac{V}{\Theta} \qquad (24)$$

Integration of Equation 23 with appropriate initial and boundary conditions yields the temporal and spacial distribution of a tracer in a homogeneous aquifer with uniform ground-water flow.

Closed-form analytical solutions to Equation 23 can be obtained by making a change of variables. Let

$$\tau = t/R_d \qquad (25)$$

and

$$X = x - V^*\tau \qquad (26)$$

Now, $C = C(x,y,z,t)$, and holding y and z constant

$$\left(\frac{\partial C}{\partial \tau}\right)_X = \left(\frac{\partial C}{\partial X}\right)_\tau \left(\frac{\partial x}{\partial \tau}\right)_X + \left(\frac{\partial C}{\partial \tau}\right)_x \left(\frac{\partial \tau}{\partial \tau}\right)_X \qquad (27)$$

Also,

$$\left(\frac{\partial x}{\partial \tau}\right)_X = \left(\frac{\partial X}{\partial \tau}\right)_X + V^* \left(\frac{\partial \tau}{\partial \tau}\right)_X \qquad (28)$$

Substituting Equation 28 into Equation 27 yields

$$\left(\frac{\partial C}{\partial \tau}\right)_x = \left(\frac{\partial C}{\partial \tau}\right)_X - V^* \left(\frac{\partial C}{\partial X}\right)_\tau \tag{29}$$

For the second derivative term in x,

$$\left(\frac{\partial^2 C}{\partial X^2}\right)_\tau = \frac{\partial}{\partial X}\left(\frac{\partial X}{\partial X}\right)_\tau \left[\left(\frac{\partial C}{\partial X}\right)_\tau \left(\frac{\partial x}{\partial X}\right)_\tau\right] = \frac{\partial^2 C}{\partial x^2} \tag{30}$$

Substituting Equations 25, 29 and 30 into Equation 23 yields

$$\frac{\partial C}{\partial \tau} = D_x \frac{\partial^2 C}{\partial X^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - \lambda_T C \tag{31}$$

which is a special form of the heat conduction equation. Closed-form analytical solutions for this equation are available in the literature for a variety of boundary conditions.

Summary.

Equation 23 provides the basis for many of the analytical solutions for solute transport in uniform ground-water flow. This equation is a mathematical model of complex physical phenomena and incorporates many simplyfying assumptions which are required to obtain a solution to the problem. Assumptions incorporated in the formulation of the differential equation are also present in the solution and must be considered in interpreting any numerical results.

The assumption that the aquifer is homogeneous is seldom satisfied in practical field problems. Also, the use of an equilibrium adsorption isotherm implies that adsorption of solute on the solid matrix is both reversible and instantaneous. Although these assumptions are seldom met in either field or laboratory problems, the approximations to the physical system may be reasonable for initial estimates of concentration distributions.

Solutions to Equation 23 with a continuous source of tracer are often encountered in the literature. The assumption of a uniform velocity in the x-direction makes no provision for the effects of a high volumetric source rate on the flow-field in the region of the source. For most problems, this assumption is probably reasonable at moderate distances from either sources or sinks of fluid, or on a regional basis.

The use of a Fickian model for the dispersive flux is probably the most frequently misinterpreted or incorrectly applied portion of the mathematical model. Hydrodynamic dispersion is an observed effect of one or more physical phenomena which are difficult to define and cannot be measured. A discussion of the topic is beyond the scope of this brief treatise. However, the mathematical formulation of the problem as developed in this paper treats dispersion as a potential flow problem. Analogous mechanism are conduction in heat transfer and molecular diffusion in mass transfer. Thus, the model does not distinguish between hydrodynamic dispersion in the direction of ground-water flow or opposite to the direction of ground-water flow. The model is a statement of conservation of tracer, and solutions of the governing differential equation can lead to higher concentrations upgradient of sources (and thus lower concentrations downgradient) than would be observed in practice.

Analytical solutions to the solute transport equation present viable and valuable alternatives for analyzing fairly complex problems, even with the simplifying assumptions which have been incorporated. Interpretation of the results of an analytical solution to the problem must be based on an understanding of both the physical system and the mathematical model.