

PLUME 3D: THREE-DIMENSIONAL PLUMES IN UNIFORM GROUND  
WATER FLOW

Oklahoma State University  
Stillwater, OK

Jun 85

U.S. DEPARTMENT OF COMMERCE  
National Technical Information Service

**NTIS**

EPA/600/2-85/067  
June 1985

PLUME3D :  
THREE-DIMENSIONAL PLUMES IN UNIFORM GROUND WATER FLOW

by

Jan Wagner and Stephanie A. Watts  
School of Chemical Engineering  
Oklahoma State University  
Stillwater, Oklahoma 74078

Douglas C. Kent  
Department of Geology  
Oklahoma State University  
Stillwater, Oklahoma 74078

CR811142

Project Officer

Carl G. Enfield  
Robert S. Kerr Environmental Research Laboratory  
U. S. Environmental Protection Agency  
Ada, Oklahoma 74820

ROBERT S. KERR ENVIRONMENTAL RESEARCH LABORATORY  
OFFICE OF RESEARCH AND DEVELOPMENT  
U.S. ENVIRONMENTAL PROTECTION AGENCY  
ADA, OK 74820

TECHNICAL REPORT DATA (Please read Instructions on the reverse before completing)		
1. REPORT NO. EPA/600/2-85/067	2.	3. RECIPIENT'S ACCESSION NO. P805 074443 /AS
4. TITLE AND SUBTITLE PLUME 3D: THREE-DIMENSIONAL PLUMES IN UNIFORM GROUND WATER FLOW.	5. REPORT DATE June 1985	
	6. PERFORMING ORGANIZATION CODE	
7. AUTHOR(S) Jan Wagner, Stephanie Watts, Douglas Kent	8. PERFORMING ORGANIZATION REPORT NO.	
9. PERFORMING ORGANIZATION NAME AND ADDRESS Oklahoma State University Stillwater, OK 74078	10. PROGRAM ELEMENT NO. ABRD1A	11. <del>CONTRACT NO.</del> Coop. Agr. CR-811142
12. SPONSORING AGENCY NAME AND ADDRESS Robert S. Kerr Environmental Research Laboratory Office of Research and Development U.S. Environmental Protection Agency Ada, OK 74820	13. TYPE OF REPORT AND PERIOD COVERED Final 9/83 - 2/85	14. SPONSORING AGENCY CODE EPA/600/15
15. SUPPLEMENTARY NOTES Carl G. Enfield, Project Officer		
16. ABSTRACT A closed-form analytical solution for three-dimensional plumes was incorporated in an interactive computer program. The assumption of an infinite aquifer depth and uniform source mass rate and source location was overcome by using the principle of superposition in space and time. The source code was written in a subset of FORTRAN 77 and can be compiled with FORTRAN IV, FORTRAN 66 as well as FORTRAN 77. As a result, the code is nearly independent of hardware and operating system.		
17. KEY WORDS AND DOCUMENT ANALYSIS		
a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS (This Report) UNCLASSIFIED	21. NO. OF PAGES 82
	20. SECURITY CLASS (This page) UNCLASSIFIED	22. PRICE

#### DISCLAIMER

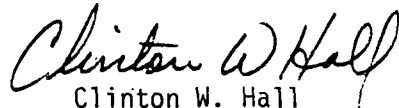
The information in this document has been funded wholly or in part by the United States Environmental Protection Agency under assistance agreement number CR-811142 to Oklahoma State University. It has been subject to the Agency's peer and administrative review, and it has been approved for publication as an EPA document.

## FOREWORD

EPA is charged by Congress to protect the Nation's land, air, and water systems. Under a mandate of national environmental laws focused on air and water quality, solid waste management and the control of toxic substances, pesticides, noise, and radiation, the Agency strives to formulate and implement actions which lead to a compatible balance between human activities and the ability of natural systems to support and nurture life.

The Robert S. Kerr Environmental Research Laboratory is the Agency's center of expertise for investigation of the soil and subsurface environment. Personnel at the Laboratory are responsible for management of research programs to: (a) determine the fate, transport and transformation rates of pollutants in the soil, the unsaturated zone and the saturated zones of the subsurface environment; (b) define the processes to be used in characterizing the soil and subsurface environment as a receptor of pollutants; (c) develop techniques for predicting the effect of pollutants on ground water, soil and indigenous organisms; and (d) define and demonstrate the applicability and limitations of using natural processes, indigenous to the soil and subsurface environment, for the protection of this resource.

This project was initiated to develop an interactive computer model which could be utilized to predict toxic chemical fate in homogeneous aquifers. The model should be useful in making comparisons, between chemicals, for idealized homogeneous aquifers. This model is not intended for addressing site specific problems where there is significant heterogeneity in the aquifer.



Clinton W. Hall

Director

Robert S. Kerr Environmental  
Research Laboratory

## ABSTRACT

A closed-form analytical solution for two dimensional plumes was incorporated in an interactive computer program. The assumption of an infinite aquifer depth and uniform source mass rate and source location was overcome by using the principal of superposition in space and time. The source code was written in a subset of FORTRAN 77 and can be compiled with FORTRAN IV, FORTRAN 66 as well as FORTRAN 77. As a result, the code is nearly independent of hardware and operating system.

## TABLE OF CONTENTS

INTRODUCTION.....	1
SECTION I - MATHEMATICAL DEVELOPMENT.....	2
Analytical Solution.....	3
Assumptions and Limitations.....	7
Superposition.....	8
SECTION II - COMPUTER PROGRAM.....	16
Basic Input Data.....	16
Edit Commands.....	20
SECTION III - APPLICATIONS.....	23
Site Location.....	23
Hydrogeology.....	23
Plating-Waste Contamination.....	24
Analytical Model.....	25
REFERENCES.....	32
APPENDIX A - Input Data Dialog and Results for Example Problem.....	A-1
APPENDIX B - Listing of Source Code for PLUME3D.....	B-1
APPENDIX C - Solute Transport in Uniform Ground-Water Flow Mathematical Development.....	C-1

## LIST OF TABLES

Table 1 - Edit Commands.....	22
Table 2 - Input Data Required for the Analytical Three-Dimensional Plume Model.....	26
Table 3 - Typical Values for Aquifer Properties.....	28
Table 4 - Model Input for Example Problem 1.....	30



## LIST OF FIGURES

Figure 1 - Decomposition of a variable rate using superposition in time.....	10
Figure 2 - Use of image sources to account for aquifers of finite depth.....	13
Figure 3 - Superposition in space to account for barrier boundaries.....	14

## 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

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

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	$L$
$\lambda$ = 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

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

where

$\rho_B$  = bulk density of the aquifer  $M/L^3$

$\theta$  = 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

$$\tau = t/R_d \quad (3)$$

and

$$X = x - V^* \tau \quad (4)$$

Then Equation 1 is transformed to

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

with boundary conditions

$$C(X, y, z, 0) = 0 \quad (6a)$$

$$C(X, y, \pm\infty, \tau) = 0 \quad (6b)$$

$$C(X, \pm\infty, z, \tau) = 0 \quad (6c)$$

$$C(\pm\infty, y, z, \tau) = 0 \quad (6d)$$

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  $M_0$  at the origin is

$$C_i = \frac{M_0}{8\theta \sqrt{\pi^3 t^3 D_x D_y D_z}} \exp \left( -\frac{x^2}{4D_x \tau} - \frac{y^2}{4D_y \tau} - \frac{z^2}{4D_z \tau} - R_d \lambda \tau \right) \quad (7)$$

In terms of the untransformed variables,

$$C_i = \frac{M_0}{8\theta \sqrt{\pi^3 t^3 D_x D_y D_z}} \exp \left( -\frac{(x - V^* t/R_d)^2}{4D_x t/R_d} - \frac{y^2}{4D_y t/R_d} - \frac{z^2}{4D_z t/R_d} - \lambda t \right) \quad (8)$$

The solution for a continuous point source is obtained by integrating Equation 8 with respect to time and letting  $C_0 Q = dM_0/dt$ , or

$$C_c = \frac{1}{8\theta \sqrt{\pi^3 D_x D_y D_z}} \int_0^t C_0 Q t^{-3/2} \exp \left( -\frac{(x - V^* t/R_d)^2}{4D_x t/R_d} - \frac{y^2}{4D_y t/R_d} - \frac{z^2}{4D_z t/R_d} - \lambda t \right) dt \quad (9)$$

Equation 9 can be rearranged slightly to

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

where

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

and

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

Turner (1972) gives the solution to Equation 10 as

$$C_c = \frac{C_o Q \exp \left( \frac{1}{2} \frac{V^* x}{D_x} \right)}{8\pi\theta R \sqrt{D_y D_z}} \left\{ 2 \cosh \left( \frac{1}{2} \frac{RU}{D_x} \right) \exp \left( \frac{1}{2} \frac{RU}{D_x} \right) \operatorname{erf} \left[ \frac{1}{2} \left( \frac{U^2 t}{D_x R_d} \right)^{1/2} \right. \right. \\ \left. \left. - \frac{1}{2} \left( \frac{R_d R^2}{D_x t} \right)^{1/2} \right] - \exp \left( -\frac{1}{2} \frac{RU}{D_x} \right) \operatorname{erf} \left[ \frac{1}{2} \left( \frac{U^2 t}{D_x R_d} \right)^{1/2} + \frac{1}{2} \left( \frac{R_d R^2}{D_x t} \right)^{1/2} \right] \right\} \quad (13)$$

which can be simplified somewhat to yield

$$C_c = \frac{C_o Q \exp\left(\frac{1}{2} \frac{V^* x}{D_x}\right)}{8\pi\theta R \sqrt{D_y D_z}} \left\{ \exp\left(\frac{1}{2} \frac{RU}{D_x}\right) \operatorname{erfc}\left(\frac{1}{2} \frac{R_d R + Ut}{\sqrt{R_d D_x t}}\right) \right. \\ \left. + \exp\left(-\frac{1}{2} \frac{RU}{D_x}\right) \operatorname{erfc}\left(\frac{1}{2} \frac{R_d R - Ut}{\sqrt{R_d D_x t}}\right) \right\} \quad (14a)$$

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

$$C_c = \frac{C_o Q \exp\left(-\frac{1}{2} \frac{V^* x}{D_x}\right)}{8\pi\theta R \sqrt{D_y D_z}} \left\{ \exp\left(-\frac{1}{2} \frac{RU}{D_x}\right) \operatorname{erfc}\left(\frac{1}{2} \frac{R_d R + Ut}{\sqrt{R_d D_x t}}\right) \right. \\ \left. + \exp\left(-\frac{1}{2} \frac{RU}{D_x}\right) \operatorname{erfc}\left(\frac{1}{2} \frac{R_d R - Ut}{\sqrt{R_d D_x t}}\right) \right\} \quad (14b)$$

for  $x < 0$ .

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

$$C_{c,\infty} = \int_0^\infty C_i \, dt \quad (15)$$

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

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

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 simpler 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

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

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

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

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

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

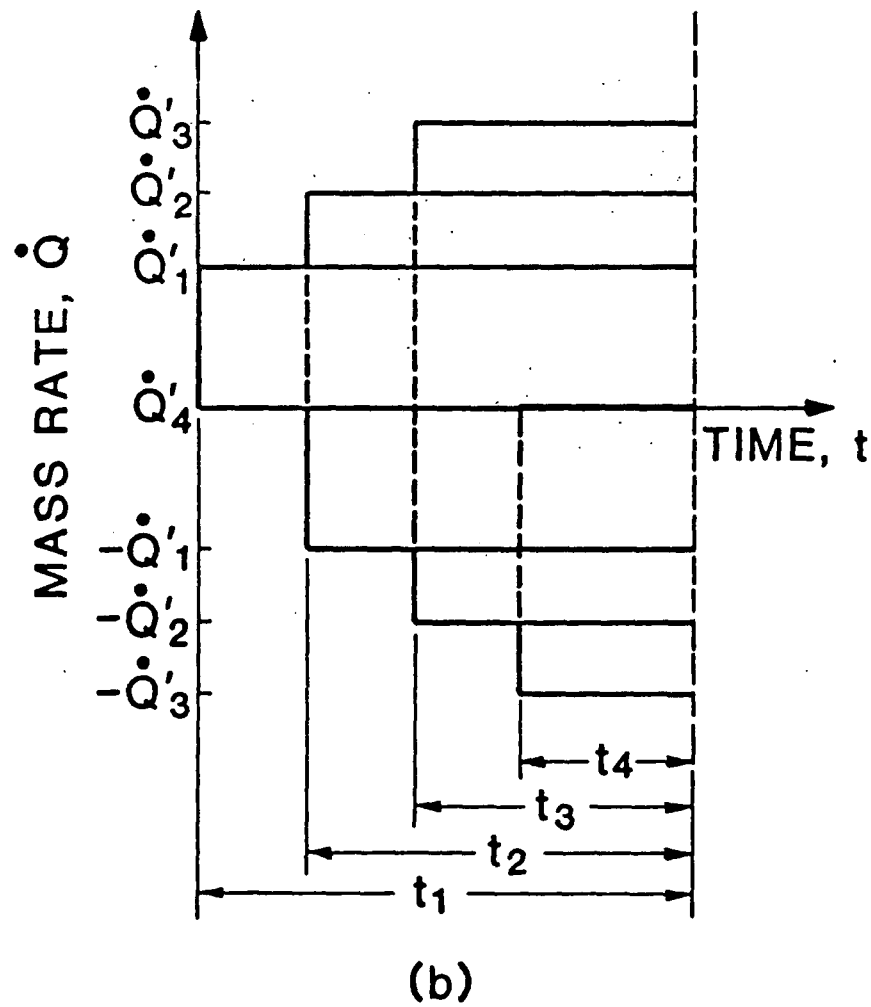
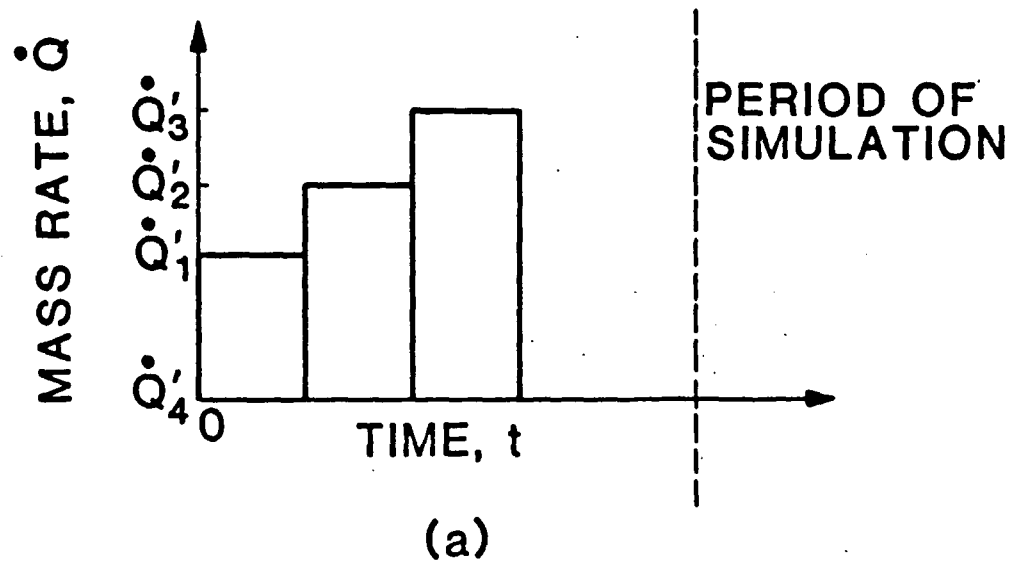


Figure 1. Decomposition of a variable source rate using superposition in time.

In general terms

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

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

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

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  $Q_0 = 0$  and  $t_0 = 0$ .

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.

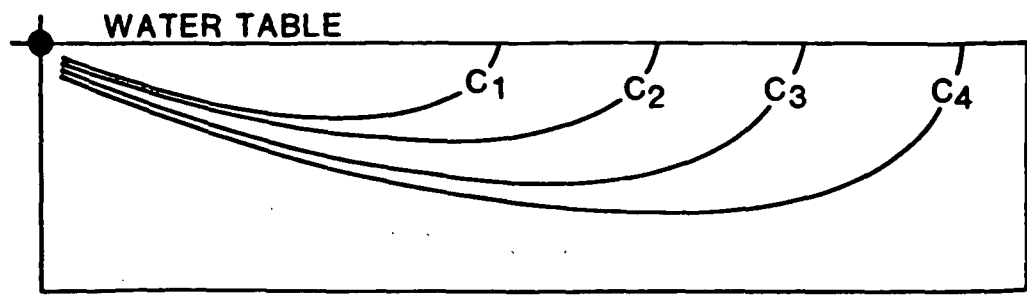
Consider the contaminant plume which would exist if the aquifer were of infinite depth as shown in Figure 2a. If the contaminant plume was to intersect an impermeable base of the aquifer as shown in Figure 2b, the vertical concentration gradient must change since there can be no transport of mass across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

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

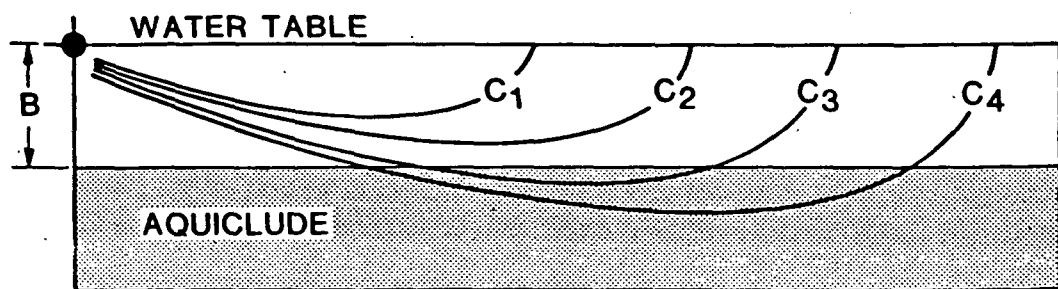
at  $z = B$ . Now, if an imaginary, or image, source were placed across the boundary at a distance equal to the depth of the aquifer, as shown in Figure 2c, this source would create a concentration gradient from the boundary to the image water table equal to the concentration gradient from the boundary 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.

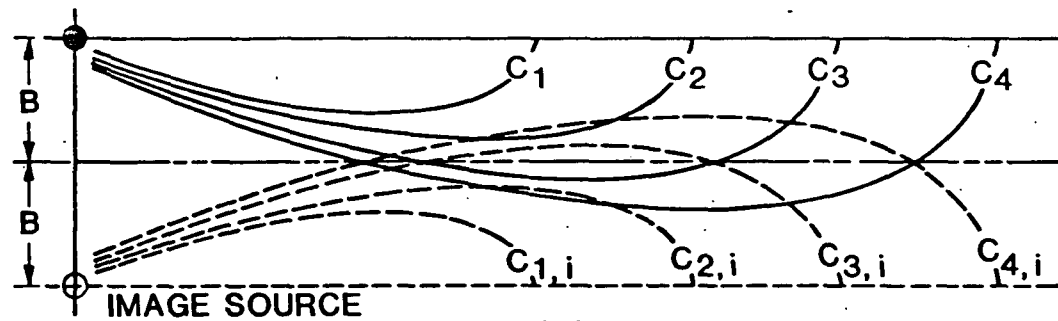
In theory an infinite number of image systems may be required. For example, if the plume in the infinite system intersects the water table in the image system a second no-transport boundary is encountered as shown in Figure 3. This boundary can be handled by introducing another image system across the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



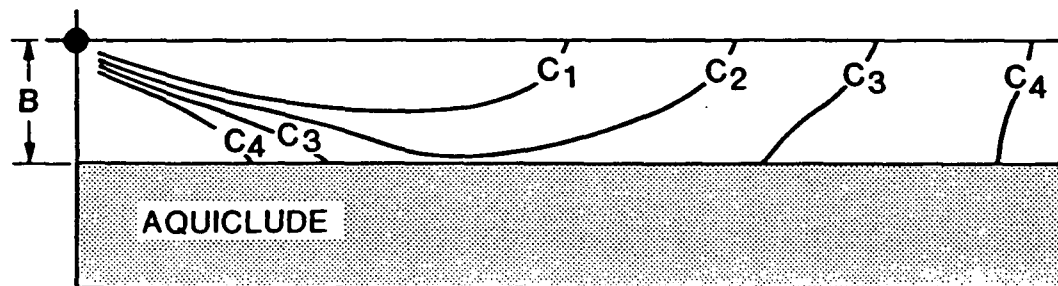
(a)



(b)

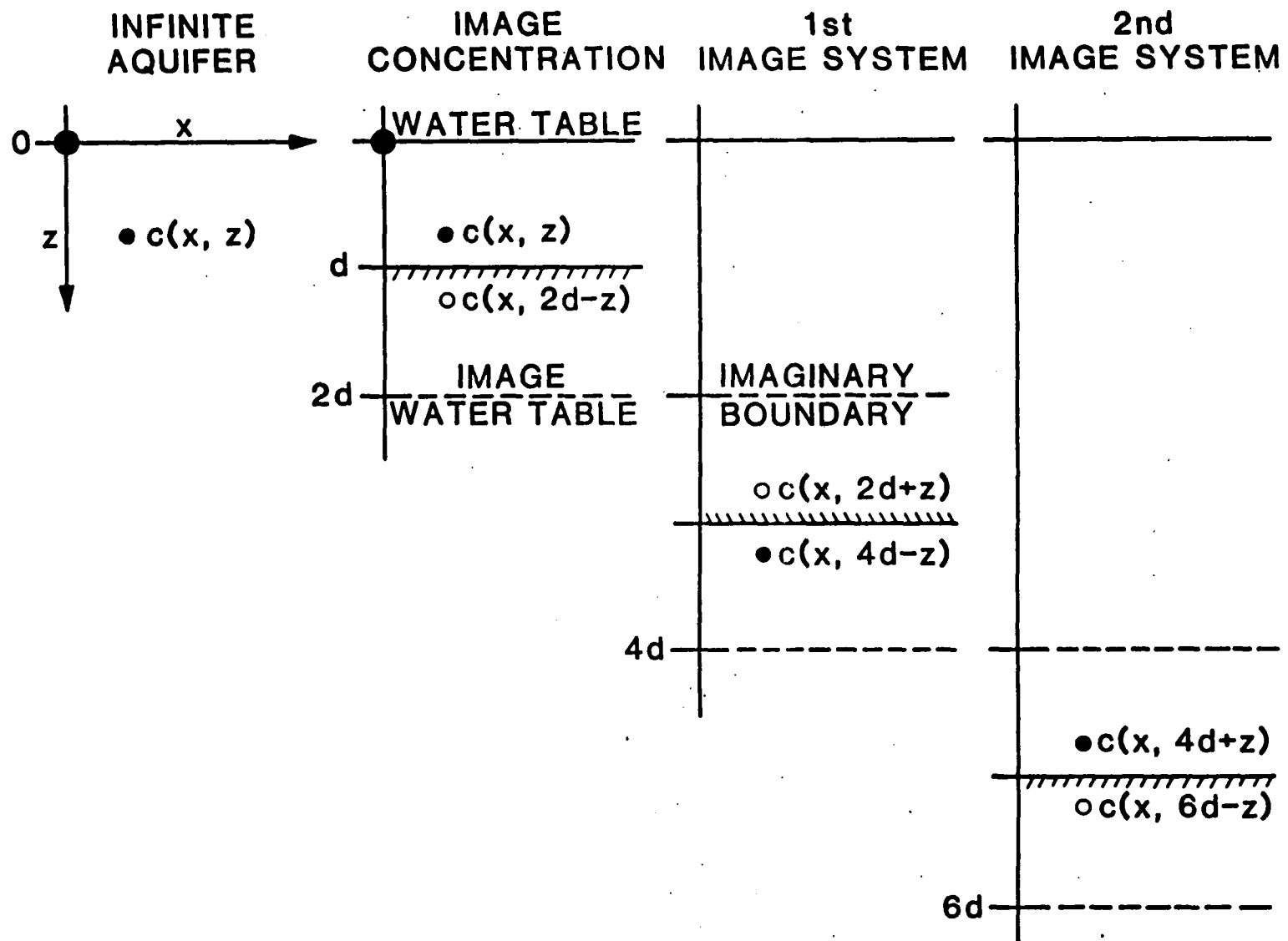


(c)



(d)

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



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

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 responses 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

<u>Command</u>	<u>Variable changed/Execution</u>
ST	Saturated Thickness
P0	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 approximately 0.0025 ft/ft and the average coefficient of permeability is assumed to be 1,600 gal/day/ft<sup>2</sup> 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,  $\theta$ , 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  $\alpha_x = 69.9$  feet and  $\alpha_y = 14.0$  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 <sup>3</sup>	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 <sup>2</sup>	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  $\alpha_z = 0.7$  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  $\lambda = 0$ .

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 <sup>2</sup> /dy
y-dispersion coefficient	21.0 ft <sup>2</sup> /dy
z-dispersion coefficient	1.05 ft <sup>2</sup> /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 <sup>3</sup> /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).



## REFERENCES

- Abramowitz, M. and I. A. Stegun, 1966, Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, National Bureau of Standards Applied Mathematics Series 55, U. S. Department of Commerce, 1046 pp.
- Carslaw, H. S. and J. C. Jaeger, 1959, Conduction of Heat in Solids, Oxford University Press, Oxford, England, 510 pp.
- Hunt, B., 1978, "Dispersive Sources in Uniform Ground-Water Flow, Jour. Hydraul. Div., ASCE, 104, No. HY1, January 1978, pp. 75-85.
- Perlmutter, N. M. and M. Lieber, 1970, "Dispersal of Plating Wastes and Sewage Contaminants in Ground Water and Surface Water, South Farmingdale-Massapequa Area, Nassau County, New York," U. S. Geological Survey Water-Supply Paper 1879-G, pp. G1-G67.
- Pinder, G. F., 1973, "A Galerkin Finite Element Simulation of Ground-water Contamination on Long Island," Water Resources Research, Vol. 9, No. 6, pp. 1657-1669.
- 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.
- Walton, W. C., 1970, Groundwater Resource Evaluation, Mc-Graw-Hill, New York, New York, 664 pp.
- Yeh, G. T., 1981, "AT123D: Analytical Transient One-, Two-, and Three-Dimensional Simulation of Waste Transport in the Aquifer System," Publication No. 1439, Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 83 pp.

## 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 (0 FOR INFINITE THICKNESS), FT  
?110.

ENTER AQUIFER POROSITY  
?0.35

ENTER SEEPAGE VELOCITY, FT/DY  
?1.5

ENTER RETARDATION COEFFICIENT  
?1.0

ENTER X DISPERSION COEFFICIENT, SQ FT/DY  
?105.

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

ENTER Z DISPERSION COEFFICIENT, SQ FT/DY  
?1.05

ENTER DECAY CONSTANT, 1/DY  
?0.

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 OF 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 2.01  
 PAGE 1

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	X (FT)	SOURCE		Z (FT)	RATE NO	MASS RATE	TIME (DY)	
		Y (FT)					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 =	450.00	YLAST =	-450.00	DELY =	150.0000
ZFIRST =	0.00	ZLAST =	110.00	DELZ =	55.0000
TFIRST =	2800.00	TLAST =	2800.00	DELT =	0.0000

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

PLUME3D  
 VERSION 2.01  
 PAGE 2

HEXAVALENT CHROMIUM PLUME -- EXAMPLE 1

CONCENTRATION DISTRIBUTION AT 2800.00 DY (MG/L )

Z = 0.00 FT

*						
* X(FT)						
	*					
Y(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

PLUME3D  
 VERSION 2.01  
 PAGE 3

HEXAVALENT CHROMIUM PLUME -- EXAMPLE 1

CONCENTRATION DISTRIBUTION AT 2800.00 DY (MG/L )

Z = 55.00 FT

*							
* X(FT)							
* 600.00 1200.00 1800.00 2400.00 3000.00 3600.00							
Y(FT) *							
*							
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	



PLUME3D  
 VERSION 2.01  
 PAGE 4

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

PLUME3D  
 VERSION 2.01  
 PAGE 5

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	X (FT)	SOURCE		Z (FT)	RATE NO	MASS RATE	TIME (DY)	
		Y (FT)					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

PLUME3D  
 VERSION 2.01  
 PAGE 6

HEXAVALENT CHROMIUM PLUME -- EXAMPLE 1

CONCENTRATION DISTRIBUTION AT 2800.00 DY (MG/L )

Y = 0.00 FT

*							
* X(FT)							
* 600.00 1200.00 1800.00 2400.00 3000.00 3600.00							
Z(FT) *							
*							
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	PL3D001
C	VERSION 2.02	PL3D002
C	THREE-DIMENSIONAL PLUMES IN UNIFORM GROUND-WATER FLOW	PL3D003
C	JAN WAGNER	PL3D004
C	SCHOOL OF CHEMICAL ENGINEERING	PL3D005
C	OKLAHOMA STATE UNIVERSITY	PL3D006
C	STILLWATER, OK. 74078	PL3D007
C	PHONE (405) 624-5280	PL3D008
C	MARCH, 1984	PL3D009
C		PL3D010
C	REVISIONS: 2.01 23 NOV 84	PL3D011
C	2.02 9 DEC 84	PL3D012
C		PL3D013
C	DIMENSION COL(7),CON(7),D(3),DEL(3),XF(3),XL(3),XS(10),YS(10),	PL3D014
C	ZS(10)	PL3D015
C	DIMENSION IC(21),IS(4),KSEC(3),LBL(2,6),NP(3),NR(10),TITLE(30)	PL3D016
C	REAL LAMBDA	PL3D017
C	INTEGER TITLE	PL3D018
C	COMMON/IO/NI,NO	PL3D019
C	COMMON/RATE/Q(10,12),T(10,12)	PL3D020
C	COMMON/PHYPRO/ALPHA,BETA,GAMMA,DX,LAMBDA,PE,RD,V	PL3D021
C	DATA IC/'NP','ST','PO','VX','RD','DX','DY','DZ','DE','CS','XC',	PL3D022
C	1'YC','ZC','AS','TC','LI','RN','OB','RT','MU','DN'//	PL3D023
C	DATA IS/'R','M','A','D'//	PL3D024
C	DATA KAR1,KAR2,KAR3/'X','Y','Z'//	PL3D025
C	DATA KSEC/'XY','XZ','YZ'//	PL3D026
C	DATA LBL/' ','(C',' ','ON',' ','TI',' ','NU',' ','ED',	PL3D027
C	1' ','')//	PL3D028
C	DATA IY/'Y'//	PL3D029
C	DATA KSOL1,KSOL2/'TR','SS'//	PL3D030
C		PL3D031
C	READ DEVICE: NI WRITE DEVICE: NO	PL3D032
C	NI=1	PL3D033
C	NO=1	PL3D034
C		PL3D035
C	MAXIMUM NUMBER OF PRINTED COLUMNS PER PAGE IS SET TO MAXCOL	PL3D036
C	DIMENSION COL(MAXCOL),CON(MAXCOL)	PL3D037
C	MAXCOL = 7	PL3D038
C		PL3D039
C	MAXIMUM NUMBER OF PRINTED ROWS PER PAGE IS SET TO MAXROW	PL3D040
C	MAXROW = 40	PL3D041
C		PL3D042
C	MAXIMUM NUMBER OF SOURCES IS SET TO MAXSOR	PL3D043
C	DIMENSION XS(MAXSOR),YS(MAXSOR),ZS(MAXSOR),NR(MAXSOR)	PL3D044
C	MAXSOR = 10	PL3D045
C		PL3D046
C	MAXIMUM NUMBER OF SOURCE RATES FOR SUPERPOSITION IN TIME	PL3D047
C	IS SET TO MAXRT	PL3D048
C	COMMON/RATE/ Q(MAXSOR,MAXRT+2),T(MAXSOR,MAXRT+2)	PL3D049
C	MAXRT = 10	PL3D050
C		PL3D051
C	MAXIMUM NUMBER OF IMAGE WELLS FOR SUPERPOSITION IN SPACE	PL3D052
C	IS SET TO MAXIMG	PL3D053
C	MAXIMG = 20	PL3D054
C		PL3D055
C		PL3D056
C		PL3D057
C	INITIALIZE PROGRAM FLOW CONTROL VARIABLES	PL3D058
C	10 IEDIT = 1	PL3D059
C	KNTL = 1	PL3D060
C	NPAGE = 1	PL3D061
C		PL3D062
C		PL3D063
C	***** SECTION I -- BASIC INPUT DATA	PL3D064
C		PL3D065
C	READ TITLE	PL3D066
C	WRITE(NO,15)	PL3D067
C	15 FORMAT(1H1,2X,'ENTER TITLE',/' ?')	PL3D068
C	READ(NI,25) (TITLE(I), I=1,30)	PL3D069
C	25 FORMAT(30A2)	PL3D070

C		PL3D071
C	DEFINE UNITS	PL3D072
	WRITE(N0,35)	PL3D073
	35 FORMAT(3X,'ENTER UNITS FOR LENGTH (2 CHARACTERS)',/, ' ?')	PL3D074
	READ(NI,45) IL	PL3D075
	45 FORMAT(A2)	PL3D076
	WRITE(N0,55)	PL3D077
	55 FORMAT(3X,'ENTER UNITS FOR TIME (2 CHARACTERS)',/, ' ?')	PL3D078
	READ(NI,45) IT	PL3D079
	WRITE(N0,65)	PL3D080
	65 FORMAT(3X,'ENTER UNITS FOR CONCENTRATION (6 CHARACTERS)',/, ' ?')	PL3D081
	READ(NI,75) IM1,IM2,IM3	PL3D082
	75 FORMAT(3A2)	PL3D083
C		PL3D084
C	ENTER DATA FOR FIRST PROBLEM	PL3D085
C		PL3D086
C	SATURATED THICKNESS	PL3D087
	80 IMAGE = MAXIMG/2	PL3D088
	84 WRITE(N0,85) IL	PL3D089
	85 FORMAT(3X,'ENTER SATURATED THICKNESS (0 FOR INFINITE THICKNESS),	PL3D090
	1A2,/, ' ?')	PL3D091
	READ(NI,95,ERR=84) ST	PL3D092
	95 FORMAT(F10.0)	PL3D093
	IF(ST.GT.0.0) GO TO 100	PL3D094
	IMAGE = 1	PL3D095
	ST = 1.OE32	PL3D096
	100 CONTINUE	PL3D097
	GO TO (120,110),IEDIT	PL3D098
	110 IF(XF(3).LE.ST.AND.XL(3).LE.ST) GO TO 3000	PL3D099
	WRITE(N0,115) ST,IL	PL3D100
	115 FORMAT(3X,'RANGE OF Z-COORDINATES IS OUTSIDE UPPER LIMIT OF',/.	PL3D101
	13X,'SATURATED THICKNESS = ',F10.4,A3).	PL3D102
	GO TO 590	PL3D103
C		PL3D104
C	POROSITY	PL3D105
	120 WRITE(N0,125)	PL3D106
	125 FORMAT(3X,'ENTER AQUIFER POROSITY',/, ' ?')	PL3D107
	130 READ(NI,95,ERR=120) P	PL3D108
	IF(P.GT.0.0.AND.P.LT.1.0) GO TO 150	PL3D109
	WRITE(N0,145)	PL3D110
	145 FORMAT(3X,'POROSITY MUST BE GREATER THAN ZERO',	PL3D111
	1' AND LESS THAN ONE -- REENTER',/, ' ?')	PL3D112
	GO TO 130	PL3D113
	150 GO TO (160,3000),IEDIT	PL3D114
C		PL3D115
C	SEEPAGE VELOCITY	PL3D116
	160 WRITE(N0,165) IL,IT	PL3D117
	165 FORMAT(3X,'ENTER SEEPAGE VELOCITY, 'A2,/,',A2,/, ' ?')	PL3D118
	170 READ(NI,95,ERR=160) V	PL3D119
	IF(V.GT.0.0) GO TO 180	PL3D120
	WRITE(N0,175)	PL3D121
	175 FORMAT(3X,'SEEPAGE VELOCITY MUST BE GREATER THAN ZERO',	PL3D122
	1' -- REENTER',/, ' ?')	PL3D123
	GO TO 170	PL3D124
	180 GO TO (190,3000),IEDIT	PL3D125
C		PL3D126
C	RETARDATION COEFFICIENT	PL3D127
	190 WRITE(N0,195)	PL3D128
	195 FORMAT(3X,'ENTER RETARDATION COEFFICIENT',/, ' ?')	PL3D129
	200 READ(NI,95,ERR=190) RD	PL3D130
	IF(RD.GE.1.0) GO TO 210	PL3D131
	WRITE(N0,205)	PL3D132
	205 FORMAT(3X,'RETARDATION COEFFICIENT MUST BE GREATER THAN OR',	PL3D133
	1' EQUAL TO ONE',/,3X,' -- REENTER',/, ' ?')	PL3D134
	GO TO 200	PL3D135
	210 GO TO (220,3000),IEDIT	PL3D136
C		PL3D137
C	X DISPERSION COEFFICIENT	PL3D138
	220 WRITE(N0,225) IL,IT	PL3D139
	225 FORMAT(3X,'ENTER X DISPERSION COEFFICIENT, SQ ',A2,	PL3D140

1'/',A2,/,', ?')	PL3D141
230 READ(NI,95,ERR=220) DX	PL3D142
IF(DX.GT.O.O) GO TO 240	PL3D143
WRITE(NO,235)	PL3D144
235 FORMAT(3X,'X DISPERSION COEFFICIENT MUST BE GREATER THAN ZERO',	PL3D145
1' -- REENTER',/,', ?')	PL3D146
GO TO 230	PL3D147
240 GO TO (250,3000),IEDIT	PL3D148
C	PL3D149
C Y DISPERSION COEFFICIENT	PL3D150
250 WRITE(NO,255) IL,IT	PL3D151
255 FORMAT(3X,'ENTER Y DISPERSION COEFFICIENT, SQ ',A2,	PL3D152
1'/',A2,/,', ?')	PL3D153
260 READ(NI,95,ERR=250) DY	PL3D154
IF(DY.GT.O.O) GO TO 270	PL3D155
WRITE(NO,265)	PL3D156
265 FORMAT(3X,'Y DISPERSION COEFFICIENT MUST BE GREATER THAN ZERO',	PL3D157
1' -- REENTER',/,', ?')	PL3D158
GO TO 260	PL3D159
270 GO TO (280,3000),IEDIT	PL3D160
C	PL3D161
C Z DISPERSION COEFFICIENT	PL3D162
280 WRITE(NO,285) IL,IT	PL3D163
285 FORMAT(3X,'ENTER Z DISPERSION COEFFICIENT, SQ ',A2,	PL3D164
1'/',A2,/,', ?')	PL3D165
290 READ(NI,95,ERR=280) DZ	PL3D166
IF(DZ.GT.O.O) GO TO 300	PL3D167
WRITE(NO,295)	PL3D168
295 FORMAT(3X,'Z DISPERSION COEFFICIENT MUST BE GREATER THAN ZERO',	PL3D169
1' -- REENTER',/,', ?')	PL3D170
GO TO 290	PL3D171
300 GO TO (310,3000),IEDIT	PL3D172
C	PL3D173
C FIRST-ORDER DECAY CONSTANT	PL3D174
310 WRITE(NO,315) IT	PL3D175
315 FORMAT(3X,'ENTER DECAY CONSTANT, 1'/',A2,/,', ?')	PL3D176
READ(NI,95,ERR=310) DECAY	PL3D177
GO TO (320,3000),IEDIT	PL3D178
C	PL3D179
C DEFINE LOCATIONS AND RATES OF SOURCES	PL3D180
C INITIALIZE SOURCE/RATE ARRAYS	PL3D181
320 MAXRT2 = MAXRT + 2	PL3D182
DO 330 I=1,MAXSOR	PL3D183
DO 330 J=1,MAXRT2	PL3D184
Q(I,J) = 0.0	PL3D185
T(I,J) = 0.0	PL3D186
330 CONTINUE	PL3D187
JFLOW = 3	PL3D188
340 WRITE(NO,345)	PL3D189
345 FORMAT(3X,'SELECT TRANSIENT OR STEADY-STATE SOLUTION',/,	PL3D190
16X,'TR FOR TRANSIENT SOLUTION',/,	PL3D191
26X,'SS FOR STEADY-STATE SOLUTION',/,', ?')	PL3D192
350 READ(NI,45) KSOL	PL3D193
IF(KSOL.EQ.KSOL1) JFLOW=1	PL3D194
IF(KSOL.EQ.KSOL2) JFLOW=2	PL3D195
GO TO (370,370,360), JFLOW	PL3D196
360 WRITE(NO,365)	PL3D197
365 FORMAT(3X,'ERROR IN SELECTION -- REENTER',/,', ?')	PL3D198
GO TO 350	PL3D199
C	PL3D200
370 WRITE(NO,375) MAXSOR	PL3D201
375 FORMAT(3X,'ENTER THE NUMBER OF SOURCES (MAXIMUM OF',I3,', )',/,	PL3D202
1' ', ?')	PL3D203
380 READ(NI,385,ERR=370) FDUM	PL3D204
385 FORMAT(F10.0)	PL3D205
NS=FDUM	PL3D206
IF(NS.GT.O.AND.NS.LE.MAXSOR) GO TO 400	PL3D207
WRITE(NO,395) MAXSOR	PL3D208
395 FORMAT(3X,'NUMBER OF SOURCES MUST BE GREATER THAN ZERO '	PL3D209
1'AND LESS THAN',I3,' -- REENTER',/,', ?')	PL3D210

GO TO 380	PL3D211
400 WRITE (NO,405) IM1,IM2,IM3,IL,IT,IT	PL3D212
405 FORMAT(3X,'MASS RATES HAVE UNITS OF ('',3A2,') (CU ',A2,'/',A2,	PL3D213
1 ' '),'',/3X,'TIME HAS UNITS OF ',A2,/) )	PL3D214
DO 540 I=1,NS	PL3D215
414 WRITE(NO,415) I,IL	PL3D216
415 FORMAT(3X,'ENTER X, Y, AND Z COORDINATES OF SOURCE',I2,	PL3D217
1 ' ('',A2,')',/,' ' ? ,? ,? ')	PL3D218
READ(NI,425,ERR=414) XS(I),YS(I),ZS(I)	PL3D219
425 FORMAT(3F10.0)	PL3D220
430 IF(ZS(I).GE.O.O.AND.ZS(I).LE.ST) GO TO 440	PL3D221
434 WRITE(NO,435) ST,IL	PL3D222
435 FORMAT(3X,'Z-COORDINATE MUST BE GREATER THAN OR EQUAL TO ZERO',	PL3D223
1 ' AND',/3X,'LESS THAN OR EQUAL TO SATURATED THICKNESS ('',	PL3D224
2F10.4,A3,')',/3X,' -- REENTER',/,' ' ? ')	PL3D225
READ(NI,95,ERR=434) ZS(I)	PL3D226
GO TO 430	PL3D227
440 IF(JFLOW.EQ.2) GO TO 530	PL3D228
Q(I,1) = O.O	PL3D229
T(I,1) = O.O	PL3D230
450 WRITE(NO,455) I,MAXRT	PL3D231
455 FORMAT(3X,'ENTER THE NUMBER RATES FOR SOURCE',I2,	PL3D232
1 ' (MAXIMUM OF',I3,')',/,' ' ? ')	PL3D233
460 READ(NI,465,ERR=450) FDUM	PL3D234
465 FORMAT(F10.0)	PL3D235
NR(I)=FDUM	PL3D236
IF(NR(I).GT.O.O.AND.NR(I).LE.MAXRT) GO TO 480	PL3D237
WRITE(NO,475) MAXRT	PL3D238
475 FORMAT(3X,'NUMBER OF RATES MUST BE GREATER THAN ZERO AND ',	PL3D239
1 ' LESS THAN',I3,' -- REENTER',/,' ' ? ')	PL3D240
GO TO 460	PL3D241
480 CONTINUE	PL3D242
NRT = NR(I)	PL3D243
DO 520 J=1,NRT	PL3D244
M = J + 1	PL3D245
484 WRITE(NO,485) I,J,T(I,M-1),IT	PL3D246
485 FORMAT(3X,'SOURCE ',I2,'. RATE ',I2,' STARTS AT',F8.1,A3,/,	PL3D247
1 3X,'ENTER MASS RATE AND ENDING TIME ',/,' ' ? ,? ')	PL3D248
READ(NI,495,ERR=484) Q(I,M),T(I,M)	PL3D249
495 FORMAT(2F10.0)	PL3D250
500 IF(T(I,M).GT.T(I,M-1)) GO TO 510	PL3D251
504 WRITE(NO,505)	PL3D252
505 FORMAT(3X,'ENDING TIME MUST BE GREATER THAN STARTING TIME '	PL3D253
1 ' -- REENTER',/,' ' ? ')	PL3D254
READ(NI,95,ERR=504) T(I,M)	PL3D255
GO TO 500	PL3D256
510 CONTINUE	PL3D257
520 CONTINUE	PL3D258
GO TO 540	PL3D259
530 WRITE(NO,535) I	PL3D260
535 FORMAT(3X,'ENTER STEADY-STATE MASS RATE',I2,/, ' ? ')	PL3D261
READ(NI,95,ERR=530) Q(I,1)	PL3D262
NR(I) = O	PL3D263
540 CONTINUE	PL3D264
IF(IEDIT.EQ.2.AND.JFLOW.EQ.1.AND.TF.LE.1.OE-06) GO TO 720	PL3D265
550 GO TO (560,3000),IEDIT	PL3D266
C	PL3D267
COORDINATES OF THE OBSERVATION POINTS	PL3D268
560 WRITE(NO,565) IL	PL3D269
565 FORMAT(3X,'ENTER XIRST, XLAST, DELTAX ('',A2,')',/,' ' ? ,? ,? ')	PL3D270
READ(NI,575,ERR=560) XF(1),XL(1),DEL(1)	PL3D271
575 FORMAT(3F10.0)	PL3D272
DEL(1) = ABS(DEL(1))	PL3D273
IF(DEL(1).LE.1.OE-06) XL(1)=XF(1)	PL3D274
GO TO (580,3000),KNTL	PL3D275
C	PL3D276
580 WRITE(NO,585) IL	PL3D277
585 FORMAT(3X,'ENTER YFIRST, YLAST, DELTAY ('',A2,')',/,' ' ? ,? ,? ')	PL3D278
READ(NI,575,ERR=580) XF(2),XL(2),DEL(2)	PL3D279
DEL(2) = ABS(DEL(2))	PL3D280



IF(DEL(2).LE.1.OE-06) XL(2)=XF(2)	PL3D281
GO TO (590,3000),KNTL	PL3D282
C	PL3D283
590 WRITE(NO,595) IL	PL3D284
595 FORMAT(3X,'ENTER ZFIRST, ZLAST, DELTAZ ('',A2,'')',/, ' ', '?', '?', '?')	PL3D285
READ(NI,575,ERR=590) XF(3),XL(3),DEL(3)	PL3D286
DEL(3) = ABS(DEL(3))	PL3D287
600 IF(XF(3).GE.O.O.AND.XF(3).LE.ST.AND.DEL(3).LE.1.OE-06) GO TO 620	PL3D288
IF(XF(3).GE.O.O.AND.XF(3).LE.ST) GO TO 610	PL3D289
604 WRITE(NO,605) ST,IL	PL3D290
605 FORMAT(3X,'ZFIRST MUST BE GREATER THAN OR EQUAL TO ZERO AND',/,	PL3D291
13X,' LESS THAN OR EQUAL TO SATURATED THICKNESS ('',F10.4,A3,'')',/,	PL3D292
2' -- REENTER',/, ' ' ?')	PL3D293
READ(NI,95,ERR=604) XF(3)	PL3D294
GO TO 600	PL3D295
610 IF(XL(3).GE.O.O.AND.XL(3).LE.ST) GO TO 630	PL3D296
614 WRITE(NO,615) ST,IL	PL3D297
615 FORMAT(3X,'ZLAST MUST BE GREATER THAN OR EQUAL TO ZERO AND',/,	PL3D298
13X,' LESS THAN OR EQUAL TO SATURATED THICKNESS ('',F10.4,A3,'')',/,	PL3D299
23X,' -- REENTER',/, ' ' ?')	PL3D300
READ(NI,95,ERR=614) XL(3)	PL3D301
GO TO 630	PL3D302
620 XL(3) = XF(3)	PL3D303
630 GO TO (640,3000), IEDIT	PL3D304
C	PL3D305
C PLANE FOR SECTIONING AQUIFER	PL3D306
640 WRITE(NO,645)	PL3D307
645 FORMAT(3X,'ENTER PLANE FOR SECTIONING AQUIFER (XY,XZ,OR YZ)',	PL3D308
1/, ' ' ?')	PL3D309
650 READ(NI,45) ISEC	PL3D310
DO 660 LSEC=1,3	PL3D311
IF(ISEC.EQ.KSEC(LSEC)) GO TO 670	PL3D312
660 CONTINUE	PL3D313
WRITE(NO,665)	PL3D314
665 FORMAT(3X,'INVALID SECTION -- REENTER',/, ' ' ?')	PL3D315
GO TO 650	PL3D316
670 GO TO (680,690,700), LSEC	PL3D317
680 KHAR1 = KAR3	PL3D318
KHAR2 = KAR1	PL3D319
KHAR3 = KAR2	PL3D320
GO TO 710	PL3D321
690 KHAR1 = KAR2	PL3D322
KHAR2 = KAR1	PL3D323
KHAR3 = KAR3	PL3D324
GO TO 710	PL3D325
700 KHAR1 = KAR1	PL3D326
KHAR2 = KAR2	PL3D327
KHAR3 = KAR3	PL3D328
710 GO TO (720,3000),IEDIT	PL3D329
C	PL3D330
C OBSERVATION TIMES	PL3D331
720 IF(JFLOW.EQ.2) GO TO 770	PL3D332
724 WRITE(NO,725) IT	PL3D333
725 FORMAT(3X,'ENTER TFIRST, TLAST, DELTAT ('',A2,'')',/, ' ', '?', '?', '?')	PL3D334
730 READ(NI,575,ERR=724) TF,TL,DELT	PL3D335
DELT = ABS(DELT)	PL3D336
740 IF(TF.GT.O.O.AND.DELT.LE.1.OE-06) GO TO 760	PL3D337
IF(TF.GT.O.O) GO TO 750	PL3D338
744 WRITE(NO,745)	PL3D339
745 FORMAT(3X,'TFIRST MUST BE GREATER THAN ZERO -- REENTER',/, ' ' ?')	PL3D340
READ(NI,95,ERR=744) TF	PL3D341
GO TO 740	PL3D342
750 IF(TL.GT.O.O) GO TO 770	PL3D343
754 WRITE(NO,755)	PL3D344
755 FORMAT(3X,'TLAST MUST BE GREATER THAN ZERO -- REENTER',/, ' ' ?')	PL3D345
READ(NI,95,ERR=754) TL	PL3D346
GO TO 750	PL3D347
760 TL = TF	PL3D348
770 GO TO (1000,780),IEDIT	PL3D349
780 IF(JFLOW.EQ.2) WRITE(NO,785)	PL3D350

785	FORMAT(3X,'TIME IS NOT A PARAMETER IN STEADY-STATE SOLUTION')	PL3D351
	GO TO 3000	PL3D352
C		PL3D353
C		PL3D354
C	LIST PROBLEM DEFINITION	PL3D355
1000	WRITE(NO,1005) NPAGE,(TITLE(I),I=1,30)	PL3D356
1005	FORMAT(1H1,/,3X,'PLUME3D',/,3X,'VERSION 2.02',	PL3D357
	1/,3X,'PAGE ',I3,///,3X,30A2,///)	PL3D358
	NPAGE = NPAGE + 1	PL3D359
	IF(ST.LE.O.9E32) WRITE(NO,1015) IL,ST	PL3D360
1015	FORMAT(1H0,2X,'SATURATED THICKNESS, ('',A2,'')',.26X,F10.4)	PL3D361
	WRITE(NO,1025) IL,IT,V,IL,IT,DX,IL,IT,DY,IL,IT,DZ,P	PL3D362
1025	FORMAT(3X,'SEEPAGE VELOCITY, ('',A2,'/'',A2,'')',.27X,F10.4,/,	PL3D363
	13X,'X DISPERSION COEFFICIENT ('',A2,'**2/'',A2,'')',.15X,F10.4,/,	PL3D364
	23X,'Y DISPERSION COEFFICIENT ('',A2,'**2/'',A2,'')',.15X,F10.4,/,	PL3D365
	33X,'Z DISPERSION COEFFICIENT ('',A2,'**2/'',A2,'')',.15X,F10.4,/,	PL3D366
	43X,'POROSITY ',.44X,F10.4)	PL3D367
	WRITE(NO,1035) RD,IT,DECAY	PL3D368
1035	FORMAT(///,3X,'RETARDATION COEFFICIENT',.30X,F10.4,/,	PL3D369
	13X,'FIRST ORDER DECAY CONSTANT (1/'',A2,'')',.20X,F10.4)	PL3D370
	GO TO (1070,1040), JFLOW	PL3D371
1040	WRITE(NO,1045) IL,IL,IL,IM1,IM2,IM3,IL,IT	PL3D372
1045	FORMAT(///,3X,'STEADY-STATE SOURCE RATES',///,	PL3D373
	13X,'SOURCE',.6X,'X',.11X,'Y',.11X,'Z',.17X,'RATE',/,	PL3D374
	25X,'ND',.6X,'('',A2,'')',.8X,'('',A2,'')',.8X,'('',A2,'')',.6X,'('',3A2,	PL3D375
	3')'(CU ',A2,'/'',A2,'')',/)	PL3D376
	DO 1060 I=1,NS	PL3D377
	WRITE(NO,1055) I,XS(I),YS(I),ZS(I),Q(I,1)	PL3D378
1055	FORMAT(5X,I2,F10.2,2X,F10.2,2X,F10.2,6X,F16.4)	PL3D379
1060	CONTINUE	PL3D380
	GO TO 1110	PL3D381
1070	WRITE(NO,1075) IM1,IM2,IM3,IL,IT,IT,IL,IL,IL	PL3D382
1075	FORMAT(///,3X,'SOURCE/RATE SCHEDULE ('',3A2,'')(CU ',A2,'/'',A2,	PL3D383
	1')'///,15X,'SOURCE',.13X,'RATE',.4X,'MASS',.8X,'TIME ('',A2,'')',	PL3D384
	2/,3X,'NO X ('',A2,'') Y ('',A2,'') Z ('',A2,'') NO',.5X,'RATE',	PL3D385
	35X,'START',.6X,'END',/)	PL3D386
	DO 1100 I=1,NS	PL3D387
	WRITE(NO,1085) I,XS(I),YS(I),ZS(I)	PL3D388
1085	FORMAT(/,3X,I2,3F9.2)	PL3D389
	NRT = NR(I)	PL3D390
	DO 1100 J=1,NRT	PL3D391
	M = J + 1	PL3D392
	WRITE(NO,1095) J,Q(I,M),T(I,M-1),T(I,M)	PL3D393
1095	FORMAT(34X,I2,.F12.2,2F9.2)	PL3D394
1100	CONTINUE	PL3D395
1110	WRITE(NO,1115) IL,IT,XF(1),XL(1),DEL(1),XF(2),XL(2),DEL(2),	PL3D396
	1 XF(3),XL(3),DEL(3)	PL3D397
1115	FORMAT(///,3X,'OBSERVATION POINTS ('',A2,''), AND TIMES ('',A2,'')'///,	PL3D398
	15X,'XFIRST =',F10.2,5X,'XLAST =',F10.2,5X,'DELX =',F10.4,/,	PL3D399
	25X,'YFIRST =',F10.2,5X,'YLAST =',F10.2,5X,'DELY =',F10.4,/,	PL3D400
	35X,'ZFIRST =',F10.2,5X,'ZLAST =',F10.2,5X,'DELZ =',F10.4)	PL3D401
	IF(JFLOW.EQ.1) WRITE(NO,1125) TF,TL,DELT	PL3D402
1125	FORMAT(/,5X,'TFIRST =',F10.2,5X,'TLAST =',F10.2,5X,'DELT =',F10.4)	PL3D403
	WRITE(NO,1135) KSEC(LSEC)	PL3D404
1135	FORMAT(///,3X,'AQUIFER SECTIONED IN ',A2,' PLANE')	PL3D405
	GO TO 3000	PL3D406
C		PL3D407
C		PL3D408
C		PL3D409
C	***** SECTION II -- NUMERICAL EVALUATION OF CONCENTRATION AT	PL3D410
C	SPECIFIED GRID COORDINATES	PL3D411
C		PL3D412
C		PL3D413
C	NUMBER OF OBSERVATION POINTS IN EACH COORDINATE DIRECTION	PL3D414
2000	CONTINUE	PL3D415
	DO 2020 L=1,3	PL3D416
	NP(L) = 1	PL3D417
	DEL(L) = ABS(DEL(L))	PL3D418
	IF(DEL(L).LE.1.OE-03) GO TO 2020	PL3D419
	DIF = XL(L) - XF(L)	PL3D420

IF(ABS(DIF).LE.1.OE-03) GO TO 2020	PL3D421
IF(DIF.LE.0.0) DEL(L)=-DEL(L)	PL3D422
NPTS = ABS(DIF/DEL(L))	PL3D423
REM = DIF - DEL(L)*FLOAT(NPTS)	PL3D424
NPTS = NPTS + 1	PL3D425
NP(L) = NPTS	PL3D426
IF(ABS(REM).LT.1.OE-03) GO TO 2020	PL3D427
NP(L) = NP(L) + 1	PL3D428
2020 CONTINUE	PL3D429
GO TO (2040,2060,2080),LSEC	PL3D430
2040 MAXSC = NP(3)	PL3D431
MAXRW = NP(2)	PL3D432
MAXCL = NP(1)	PL3D433
GO TO 2100	PL3D434
2060 MAXSC = NP(2)	PL3D435
MAXRW = NP(3)	PL3D436
MAXCL = NP(1)	PL3D437
GO TO 2100	PL3D438
2080 MAXSC = NP(1)	PL3D439
MAXRW = NP(3)	PL3D440
MAXCL = NP(2)	PL3D441
2100 CONTINUE	PL3D442
C	PL3D443
C TIME COORDINATES	PL3D444
NTIME = 1	PL3D445
IF(DELT.LE.1.OE-06) GO TO 2110	PL3D446
NTIME = ABS(TL-TF)/DELT + 1.0	PL3D447
IF(TF.GT.TL) DELT=-DELT	PL3D448
2110 TSOL = TF	PL3D449
MTIME = NTIME	PL3D450
C	PL3D451
C	PL3D452
DAMK = DX*DECAY*RD/(V*V)	PL3D453
ALPHA=SQRT(1.0+4.0*DAMK)	PL3D454
PE=V/DX	PL3D455
BETA = DX/DY	PL3D456
GAMMA = DX/DZ	PL3D457
LAMBDA = 1.0/(25.132741*P*SQRT(DY*DZ))	PL3D458
C	PL3D459
C	PL3D460
DO 2660 NT=1,NTIME	PL3D461
C	PL3D462
NSEC = 1	PL3D463
2120 LPRT = 1	PL3D464
LP = 1	PL3D465
NCFLG = 1	PL3D466
2140 NROW1 = 1	PL3D467
NROW2 = MAXROW	PL3D468
2160 IF(NROW2.GT.MAXRW) NROW2=MAXRW	PL3D469
DO 2580 NROW=NROW1,NROW2	PL3D470
GO TO (2180,2220,2200),NCFLG	PL3D471
2180 NCOL1 = 1	PL3D472
NCOL2 = MAXCOL	PL3D473
2200 IF(NCOL2.GT.MAXCL) NCOL2=MAXCL	PL3D474
NCOL = MAXCOL	PL3D475
IF(NCOL2.EQ.MAXCL) NCOL=NCOL2-NCOL1+1	PL3D476
2220 GO TO (2240,2260,2280), LSEC	PL3D477
2240 IX1 = NCOL1	PL3D478
IX2 = NCOL2	PL3D479
JY1 = NROW	PL3D480
JY2 = NROW	PL3D481
KZ1 = NSEC	PL3D482
KZ2 = NSEC	PL3D483
GO TO 2290	PL3D484
2260 IX1 = NCOL1	PL3D485
IX2 = NCOL2	PL3D486
JY1 = NSEC	PL3D487
JY2 = NSEC	PL3D488
KZ1 = NROW	PL3D489
KZ2 = NROW	PL3D490

	GO TO 2290	PL3D491
2280	IX1 = NSEC	PL3D492
	IX2 = NSEC	PL3D493
	JY1 = NCOL1	PL3D494
	JY2 = NCOL2	PL3D495
	KZ1 = NROW	PL3D496
	KZ2 = NROW	PL3D497
2290	CONTINUE	PL3D498
C		PL3D499
	DO 2300 L=1,MAXCOL	PL3D500
	CON(L) = 0.0	PL3D501
2300	CONTINUE	PL3D502
C		PL3D503
	DO 2440 N=1,NS	PL3D504
	D(1) = ST - ZS(N)	PL3D505
	IF(ST.GE.0.9E32) D(1)=0.0	PL3D506
	D(2) = ZS(N)	PL3D507
	D(3) = D(1)	PL3D508
	COEF = 1.0	PL3D509
	IF(D(1).LT.1.0E-03.OR.D(2).LT.1.0E-03) COEF=2.0	PL3D510
	DO 2440 I=IX1,IX2	PL3D511
	X = XF(1) + FLOAT(I-1)*DEL(1)	PL3D512
	IF(I.EQ.NP(1)) X=XL(1)	PL3D513
	XXS = X - XS(N)	PL3D514
	PEX = PE*XXS	PL3D515
	DO 2440 J=JY1,JY2	PL3D516
	Y = XF(2) + FLOAT(J-1)*DEL(2)	PL3D517
	IF(J.EQ.NP(2)) Y=XL(2)	PL3D518
	YYS = Y - YS(N)	PL3D519
	PEY = PE*YYS	PL3D520
	DO 2430 K=KZ1,KZ2	PL3D521
	L = I-IX1 + J-JY1 + K-KZ1 + 1	PL3D522
	IF(CON(L).LT.0.0) GO TO 2430	PL3D523
	Z = XF(3) + FLOAT(K-1)*DEL(3)	PL3D524
	IF(K.EQ.NP(3)) Z=XL(3)	PL3D525
	ZM = Z - ZS(N)	PL3D526
	IF(ABS(XXS).LT.1.0.AND.ABS(YYS).LT.1.0.AND.	PL3D527
1	ABS(ZM).LT.1.0) GO TO 2330	PL3D528
	PEZ = PE*ZM	PL3D529
	CALL SOL3D(C,PEX,PEY,PEZ,TSOL,N,NR(N))	PL3D530
	CXYZT = COEF*C	PL3D531
	IF(IMAGE.EQ.1) GO TO 2325	PL3D532
C		PL3D533
	DO 2320 LM=1,2	PL3D534
	ZM = ((-1.0)**(LM+1))*ZM	PL3D535
	IF(D(LM).LT.1.0E-03) GO TO 2320	PL3D536
	ZIMAGE = 2.0*D(LM) - ZM	PL3D537
	PEZ = PE*ZIMAGE	PL3D538
	CALL SOL3D(C,PEX,PEY,PEZ,TSOL,N,NR(N))	PL3D539
	CXYZT = CXYZT + COEF*C	PL3D540
	DO 2310 IM = 1,IMAGE	PL3D541
	ZIMAGE = (2.0*D(LM)+ZM) + 2.0*FLOAT(IM)*D(LM+1)	PL3D542
1	+ FLOAT(2*IM-2)*D(LM)	PL3D543
	PEZ = PE*ZIMAGE	PL3D544
	CALL SOL3D(C,PEX,PEY,PEZ,TSOL,N,NR(N))	PL3D545
	IF(C.LT.1.0E-06) GO TO 2312	PL3D546
	CXYZT = CXYZT + COEF*C	PL3D547
2310	CONTINUE	PL3D548
2312	CONTINUE	PL3D549
	DO 2314 IM=1,IMAGE	PL3D550
	ZIMAGE = (2.0*D(LM)-ZM) + 2.0*FLOAT(IM)*D(LM+1)	PL3D551
1	+ FLOAT(2*IM)*D(LM)	PL3D552
	PEZ = PE*ZIMAGE	PL3D553
	CALL SOL3D(C,PEX,PEY,PEZ,TSOL,N,NR(N))	PL3D554
	IF(C.LT.1.0E-06) GO TO 2320	PL3D555
	CXYZT = CXYZT + COEF*C	PL3D556
2314	CONTINUE	PL3D557
	WRITE(NO,2315) MAXIMG,X,Y,Z	PL3D558
2315	FORMAT(3X,'***** WARNING -- SOLUTION DID NOT',	PL3D559
1	' CONVERGE USING',/,9X,I2,' IMAGE WELLS AT X =',	PL3D560

2	F10.4,' Y =',F10.4,' Z =',F10.4)	PL3D561
2320	CONTINUE	PL3D562
2325	CON(L) = CON(L) + CXYZT	PL3D563
	GO TO 2340	PL3D564
2330	CON(L) = -9.9999	PL3D565
2340	GO TO (2360,2380,2400), LSEC	PL3D566
2360	SEC = Z	PL3D567
	ROW = Y	PL3D568
	COL(L) = X	PL3D569
	GO TO 2420	PL3D570
2380	SEC = Y	PL3D571
	ROW = Z	PL3D572
	COL(L) = X	PL3D573
	GO TO 2420	PL3D574
2400	SEC = X	PL3D575
	ROW = Z	PL3D576
	COL(L) = Y	PL3D577
2420	CONTINUE	PL3D578
2430	CONTINUE	PL3D579
2440	CONTINUE	PL3D580
C		PL3D581
C	PRINT CONCENTRATION DISTRIBUTION	PL3D582
	GO TO (2460,2560), LPRT	PL3D583
2460	WRITE(NO,1005) NPAGE, (TITLE(I),I=1,30)	PL3D584
	NPAGE = NPAGE + 1	PL3D585
	IF(JFLOW.EQ.2) GO TO 2500	PL3D586
	WRITE(NO,2465) TSOL,IT,IM1,IM2,IM3,KHAR1,SEC,IL,	PL3D587
	1(LBL(LP,L),L=1,6),KHAR2,IL	PL3D588
2465	FORMAT(13X,'CONCENTRATION DISTRIBUTION AT ',F10.2,	PL3D589
	11X,A2,' ('.3A2,') ',//,13X,A1,' =',F10.2,1X,A2,3X,6A2,/,	PL3D590
	2' *',/, ' * ',A1,' ('.A2,')')	PL3D591
	GO TO 2520	PL3D592
2500	WRITE(NO,2505) IM1,IM2,IM3,KHAR1,SEC,IL,(LBL(LP,L),L=1,6),	PL3D593
	1KHAR2,IL	PL3D594
2505	FORMAT(13X,'CONCENTRATION DISTRIBUTION AT STEADY STATE',	PL3D595
	1' ('.3A2,') ',//,13X,A1,' =',F10.2,1X,A2,3X,6A2,/,	PL3D596
	2' *',/, ' * ',A1,' ('.A2,')')	PL3D597
2520	CONTINUE	PL3D598
	WRITE(NO,2525) (COL(L),L=1,NCOL)	PL3D599
2525	FORMAT(' *',4X,7F10.2)	PL3D600
	WRITE(NO,2545) KHAR3,IL	PL3D601
2545	FORMAT(1X,A1,' ('.A2,') *',/,9X,'*')	PL3D602
C		PL3D603
2560	WRITE(NO,2565) ROW,(CON(L),L=1,NCOL)	PL3D604
2565	FORMAT(2X,F8.2,7F10.4)	PL3D605
	LPRT = 2	PL3D606
2580	CONTINUE	PL3D607
	IF(NROW2.EQ.MAXRW) GO TO 2600	PL3D608
	NROW1 = NROW1 + MAXROW	PL3D609
	NROW2 = NROW2 + MAXROW	PL3D610
	LPRT = 1	PL3D611
	LP = 2	PL3D612
	NCFLG = 2	PL3D613
	GO TO 2160	PL3D614
2600	IF(NCOL2.EQ.MAXCL) GO TO 2620	PL3D615
	NCOL1 = NCOL1 + MAXCOL	PL3D616
	NCOL2 = NCOL2 + MAXCOL	PL3D617
	LPRT = 1	PL3D618
	LP = 2	PL3D619
	NCFLG = 3	PL3D620
	GO TO 2140	PL3D621
2620	IF(NSEC.EQ.MAXSC) GO TO 2640	PL3D622
	NSEC = NSEC + 1	PL3D623
	GO TO 2120	PL3D624
2640	CONTINUE	PL3D625
	TSOL = TSOL + DELT	PL3D626
	IF(NT.EQ.MTIME) TSOL=TL	PL3D627
2660	CONTINUE	PL3D628
C		PL3D629
C		PL3D630

C ***** SECTION III -- PROBLEM REDEFINITION AND CONTROL OF EXECUTION	PL3D631
C	PL3D632
C	PL3D633
3000 CONTINUE	PL3D634
IF(IEDIT.EQ.2) GO TO 3010	PL3D635
WRITE(NO,3705)	PL3D636
IEDIT = 2	PL3D637
3010 KNTL = 2	PL3D638
WRITE(NO,3015)	PL3D639
3015 FORMAT(//,3X,'ENTER NEXT COMMAND',/, ' ?')	PL3D640
3020 READ(NI,3025) NEXT	PL3D641
3025 FORMAT(A2)	PL3D642
C	PL3D643
DO 3030 I=1,21	PL3D644
IF(NEXT.EQ.IC(I)) GO TO 3040	PL3D645
3030 CONTINUE	PL3D646
WRITE(NO,3035)	PL3D647
3035 FORMAT(3X,'ERROR IN LAST COMMAND -- REENTER',/, ' ?')	PL3D648
GO TO 3020	PL3D649
3040 GO TO (10,80,120,160,190,220,250,280,310,320,560,580,590,640,	PL3D650
1 720,1000,2000,3050,3060,3700,4000),I	PL3D651
C	PL3D652
C NEW SET OF X, Y, AND Z OBSERVATIONS	PL3D653
3050 KNTL = 1	PL3D654
GO TO 560.	PL3D655
C	PL3D656
C	PL3D657
C	PL3D658
C NEW SOURCE/RATE SCHEDULE	PL3D659
3060 WRITE(NO,3065)	PL3D660
3065 FORMAT(3X,'ADD(A),DELETE(D),MODIFY(M) A SOURCE OR RETURN(R)'	PL3D661
1' TO EDIT ?')	PL3D662
3070 READ(NI,3075) ISK	PL3D663
3075 FORMAT(A1)	PL3D664
DO 3080 I=1,4	PL3D665
IF(ISK.EQ.IS(I)) GO TO 3090	PL3D666
3080 CONTINUE	PL3D667
WRITE(NO,3085)	PL3D668
3085 FORMAT(3X,'ERROR IN SELECTION -- REENTER ?')	PL3D669
GO TO 3070	PL3D670
3090 GO TO (3000,3100,3450,3490),I	PL3D671
C	PL3D672
C MODIFY SOURCE	PL3D673
C	PL3D674
3100 WRITE(NO,3105) NS	PL3D675
3105 FORMAT(3X,I2,' SOURCES IN CURRENT SCHEDULE',/,	PL3D676
13X,'ENTER SOURCE TO MODIFY',/, ' ?')	PL3D677
READ(NI,465,ERR=3100) FDUM	PL3D678
JS=FDUM	PL3D679
IF(JS.GT.O.AND.JS.LE.NS) GO TO 3220	PL3D680
WRITE(NO,3215) JS	PL3D681
3215 FORMAT(3X,'SOURCE',I4,' NOT IN SCHEDULE')	PL3D682
GO TO 3060	PL3D683
3220 GO TO (3230,3260),JFLOW	PL3D684
3230 WRITE(NO,3235) JS,XS(JS),IL,YS(JS),IL,ZS(JS),IL,IT,	PL3D685
1IM1,IM2,IM3,IL,IT	PL3D686
3235 FORMAT(3X,'SOURCE ',I2,': X =',F8.2,A3,', Y =',F8.2,A3,	PL3D687
1', Z =',F8.2,A3,/,3X,'RATE',7X,'MASS RATE',14X,'TIME (',	PL3D688
2A2,')',/,4X,'NO',3X,'('',3A2,')(CU ',A2,/'',A2,')',	PL3D689
38X,'START',7X,'END',/)	PL3D690
NRT = NR(JS)	PL3D691
DO 3250 J=1,NRT	PL3D692
M = J + 1	PL3D693
WRITE(NO,3245) J,Q(JS,M),T(JS,M-1),T(JS,M)	PL3D694
3245 FORMAT(4X,I2,5X,F14.2,7X,F8.3,3X,F8.2)	PL3D695
3250 CONTINUE	PL3D696
GO TO 3270	PL3D697
3260 WRITE(NO,3265) JS,XS(JS),IL,YS(JS),IL,ZS(JS),IL,Q(JS,1),	PL3D698
1IM1,IM2,IM3,IL,IT	PL3D699
3265 FORMAT(3X,'SOURCE ',I2,': X =',F8.2,A3,', Y =',F8.2,A3,	PL3D700

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.O.O.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
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 O TO CHANGE ALL RATES)',/, ' ?')	PL3D722
READ(NI,465,ERR=3310) FDUM	PL3D723
JR=FDUM	PL3D724
IF(JR.LE.O) 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.O)	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) = O.O	PL3D741
T(JS,M) = O.O	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.O.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
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
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' ?')	PL3D771
READ(NI,3345,ERR=3444) Q(JS,1)	PL3D772
GO TO 3060	PL3D773
C	PL3D774
C ADD A NEW SOURCE	PL3D775
C	PL3D776
3450 NS = NS + 1	PL3D777
JS = NS	PL3D778
3454 WRITE(NO,415) JS,IL	PL3D779
READ(NI,425,ERR=3454) XS(JS),YS(JS),ZS(JS)	PL3D780
3460 IF(ZS(JS).GE.O.O.AND.ZS(JS).LE.ST) GO TO 3470	PL3D781
3464 WRITE(NO,435) ST,IL	PL3D782
READ(NI,95,ERR=3464) ZS(JS)	PL3D783
GO TO 3460	PL3D784
3470 GO TO (3370,3480),JFLOW	PL3D785
C	PL3D786
C STEADY-STATE SOURCES	PL3D787
3480 WRITE(NO,3485) JS	PL3D788
3485 FORMAT(3X,'ENTER STEADY-STATE MASS RATE FOR SOURCE ',I2,	PL3D789
1/,' ?')	PL3D790
READ(NI,3345,ERR=3480) Q(JS,1)	PL3D791
NR(JS) = 0	PL3D792
GO TO 3060	PL3D793
C	PL3D794
C DELETE A SOURCE	PL3D795
C	PL3D796
3490 IF(NS.GT.1) GO TO 3500	PL3D797
WRITE(NO,3495)	PL3D798
3495 FORMAT(3X,'ONLY ONE SOURCE IN SCHEDULE -- CAN NOT DELETE',/)	PL3D799
GO TO 3060	PL3D800
3500 WRITE(NO,3505) IL,IL,IL	PL3D801
3505 FORMAT(3X,'SOURCE ',6X,'X (',A2,')',3X,'Y (',A2,')',3X,	PL3D802
1'Z (',A2,')',/)	PL3D803
DO 3520 I=1,NS	PL3D804
WRITE(NO,3515) I,XS(I),YS(I),ZS(I)	PL3D805
3515 FORMAT(5X,I2,3X,F8.2,3X,F8.2,3X,F8.2)	PL3D806
3520 CONTINUE	PL3D807
3530 WRITE(NO,3535)	PL3D808
3535 FORMAT(3X,'ENTER SOURCE TO DELETE',/,	PL3D809
13X,'(ENTER O TO CANCEL)',/,' ?')	PL3D810
READ(NI,465,ERR=3530) FDUM	PL3D811
JS=FDUM	PL3D812
IF(JS.LE.O) GO TO 3060	PL3D813
IF(JS.LE.NS) GO TO 3550	PL3D814
WRITE(NO,3545) JS	PL3D815
3545 FORMAT(3X,'SOURCE ',I2,' NOT IN CURRENT SCHEDULE')	PL3D816
GO TO 3530	PL3D817
3550 WRITE(NO,3555) JS	PL3D818
3555 FORMAT(3X,'DELETE SOURCE ',I2,' (Y/N)?')	PL3D819
READ(NI,3075) JC	PL3D820
IF(JC.NE.IY) GO TO 3530	PL3D821
NSD = NS - 1	PL3D822
GO TO (3560,3590),JFLOW	PL3D823
C	PL3D824
C TRANSIENT SOURCES	PL3D825
3560 IF(JS.EQ.NS) GO TO 3575	PL3D826
DO 3570 J=JS,NSD	PL3D827
XS(J) = XS(J+1)	PL3D828
YS(J) = YS(J+1)	PL3D829
ZS(J) = ZS(J+1)	PL3D830
NR(J) = NR(J+1)	PL3D831
NRT = NR(J)	PL3D832
DO 3570 K=1,NRT	PL3D833
M = K + 1	PL3D834
Q(J,M) = Q(J+1,M)	PL3D835
T(J,M) = T(J+1,M)	PL3D836
3570 CONTINUE	PL3D837
3575 NRT = NR(NS)	PL3D838
DO 3580 K=1,NRT	PL3D839
M = K + 1	PL3D840



Q(NS,M) = 0.0			PL3D841
T(NS,M) = 0.0			PL3D842
3580 CONTINUE			PL3D843
NR(NS) = 0			PL3D844
NS = NSD			PL3D845
GO TO 3060			PL3D846
C			PL3D847
C	STEADY-STATE SOURCES		PL3D848
3590 IF(JS.EQ.NS) GO TO 3605			PL3D849
DO 3600 J=JS,NSD			PL3D850
Q(J,1) = Q(J+1,1)			PL3D851
XS(J) = XS(J+1)			PL3D852
YS(J) = YS(J+1)			PL3D853
ZS(J) = ZS(J+1)			PL3D854
3600 CONTINUE			PL3D855
3605 Q(NS,1) = 0.0			PL3D856
NS = NSD			PL3D857
GO TO 3060			PL3D858
C			PL3D859
C			PL3D860
C	MENU OF EDIT COMMANDS FOR PLUME3D VERSION 2.02		PL3D861
3700 WRITE(NO,3705)			PL3D862
3705 FORMAT(1H1,/,3X,'MENU OF EDIT COMMANDS',/,/,			PL3D863
13X,'SATURATED THICKNESS	ST	OBSERVATION POINTS	OB',/, PL3D864
23X,'POROSITY	PO	X COORDINATES	XC',/, PL3D865
33X,'SEEPAGE VELOCITY	VX	Y COORDINATES	YC',/, PL3D866
43X,'RETARDATION COEFFICIENT	RD	Z COORDINATES	ZC',/, PL3D867
53X,'X DISPERSION COEFFICIENT	DX	OBSERVATION TIMES	TC',/, PL3D868
53X,'Y DISPERSION COEFFICIENT	DY	AQUIFER SECTIONING	AS',/, PL3D869
63X,'Z DISPERSION COEFFICIENT	DZ	NEW PROBLEM	NP',/, PL3D870
73X,'DECAY CONSTANT	DE	MENU OF COMMANDS	MU',/, PL3D871
83X,'SOURCE/RATE SCHEDULE	RT	LIST INPUT DATA	LI',/, PL3D872
93X,'CHANGE SOLUTION/SOURCES	CS	RUN CALCULATIONS	RN',/, PL3D873
13X,'		DONE	DN') PL3D874
GO TO 3000			PL3D875
C			PL3D876
4000 STOP			PL3D877
END			PL3D878

	FUNCTION ERFC(Z)	EFLG001
C	RATIONAL APPROXIMATION OF THE COMPLIMENTARY ERROR FUNCTION	EFLG002
C	SEE SECTION 7.1 OF ABRAMOWITZ AND STEGUN (1966)	EFLG003
C	THE FOLLOWING IDENTITIES ARE USED TO HANDLE NEGATIVE ARGUMENTS	EFLG004
C	ERFC(Z) = 1 - ERF(Z)	EFLG005
C	ERF(-Z) = -ERF(Z)	EFLG006
C		EFLG007
	REAL*8 COEFLG,DERFC,DI,FX,TERMI,TERMO,SUM,X	EFLG008
	COMMON/IO/NI,NO	EFLG009
C		EFLG010
	X = ABS(Z)	EFLG011
	IF (X.GT.3.0DOO) GO TO 50	EFLG012
C		EFLG013
C	FOR X<3 A RATIONAL APPROXIMATION OF THE COMPLIMENTARY ERROR	EFLG014
C	FUNCTION IS USED.	EFLG015
C		EFLG016
	DERFC = 1.0DOO/((1.0DOO + 7.05230784D-02*X + 4.22820123D-02*(X**2)	EFLG017
1	+ 9.2705272D-03*(X**3) + 1.520143D-04*(X**4)	EFLG018
2	+ 2.76572D-04*(X**5) + 4.30638D-05*(X**6))**16)	EFLG019
	ERFCLG = DLOG(DERFC)	EFLG020
	GO TO 100	EFLG021
C		EFLG022
C	FOR X>3 AN ASYMPTOTIC EXPANSION OF THE COMPLIMENTARY ERROR	EFLG023
C	FUNCTION IS USED.	EFLG024
50	COEFLG = X*X + DLOG(X) + 0.57236494DOO	EFLG025
	FX = 2.0DOO*X*X	EFLG026
	SUM = 1.0DOO	EFLG027
	TERMO = 1.0DOO	EFLG028
	DO 60 I=2,50	EFLG029
	DI = I	EFLG030
	TERMI = -TERMO*(2.0DOO*DI - 3.0DOO)/FX	EFLG031
	IF(DABS(TERMI).GT.DABS(TERMO)) GO TO 70	EFLG032
	SUM = SUM + TERMI	EFLG033
	TEST = TERMI/SUM	EFLG034
	IF(ABS(TEST).LT.1.0E-16) GO TO 70	EFLG035
	TERMO = TERMI	EFLG036
60	CONTINUE	EFLG037
	WRITE(NO,65)	EFLG038
65	FORMAT(6X,'*** WARNING -- ASYMPTOTIC EXPANSION FOR ERFC DID NOT'	EFLG039
1	CONVERGE WITH 50 TERMS IN THE SUMMATION')	EFLG040
70	SUM = DLOG(SUM) - COEFLG	EFLG041
	ERFCLG = SUM	EFLG042
100	CONTINUE	EFLG043
C		EFLG044
C	FOR Z<0. ERFC(-Z) = 2-ERFC(Z)	EFLG045
	IF(Z.LT.0.0) GO TO 200	EFLG046
	RETURN	EFLG047
200	ERFC = 2.0 - EXP(ERFCLG)	EFLG048
	ERFCLG = ALOG(ERFC)	EFLG049
	RETURN	EFLG050
	END	EFLG051

C	SUBROUTINE SOL3D(C,PEX,PEY,PEZ,TSOL,N,NR)	SOL3001
C	NUMERICAL EVALUATION OF ANALYTICAL SOLUTION	SOL3002
	REAL LAMBDA	SOL3003
	COMMON/RATE/Q(10,12),T(10,12)	SOL3004
	COMMON/PHYPRO/ALPHA,BETA,GAMMA,DX,LAMBDA,PE,RD,V	SOL3005
C	PEXYZ = SQRT(PEX*PEX + BETA*(PEY*PEY) + GAMMA*(PEZ*PEZ))	SOL3006
	R = PEXYZ/PE	SOL3007
	PEL = PEXYZ*ALPHA	SOL3008
	PEX12 = PEX/2.0	SOL3009
	PEL12 = PEL/2.0	SOL3010
	COEF = LAMBDA/R	SOL3011
	MT = NR + 1	SOL3012
	IF(MT.GT.1) GO TO 10	SOL3013
C	STEADY-STATE SOLUTION	SOL3014
C	S = Q(N,1)	SOL3015
C	IF(CLG.LT.-72.0) CLG = -72.0	SOL3016
	IF(CLG.GT. 72.0) CLG = 72.0	SOL3017
	C = 2.0*EXP(CLG)	SOL3018
	GO TO 50	SOL3019
C	TRANSIENT SOLUTION	SOL3020
10	C = 0.0	SOL3021
	IF(T(N,MT).LT.TSOL) MT=MT+1	SOL3022
	DO 40 K=2,MT	SOL3023
	IF(T(N,K-1).GT.TSOL) GO TO 50	SOL3024
	S = Q(N,K) - Q(N,K-1)	SOL3025
	SGN = 1.0	SOL3026
	IF(S.LT.0.0) SGN = -1.0	SOL3027
	SA = ABS(S)	SOL3028
	IF(SA.LT.1.0E-3) GO TO 40	SOL3029
	COEFLG = ALOG(COEF*SA)	SOL3030
	PINJ = V*V*(TSOL-T(N,K-1))/(DX*RD)	SOL3031
	PINJL = PINJ*ALPHA*ALPHA	SOL3032
	TAU = PINJ/(PEXYZ*PEXYZ)	SOL3033
	Z1 = 0.5/SQRT(TAU)	SOL3034
	Z2 = 0.5*SQRT(PINJL)	SOL3035
	Z = Z1 + Z2	SOL3036
	T1 = ERFCLG(Z)	SOL3037
	C1LG = T1 + PEL12 + PEX12 + COEFLG	SOL3038
	Z = Z1 - Z2	SOL3039
	T2 = ERFCLG(Z)	SOL3040
	C2LG = T2 - PEL12 + PEX12 + COEFLG	SOL3041
	IF(C1LG.GT. 72.0) C1LG= 72.0	SOL3042
	IF(C1LG.LT.-72.0) C1LG=-72.0	SOL3043
	IF(C2LG.GT. 72.0) C2LG= 72.0	SOL3044
	IF(C2LG.LT.-72.0) C2LG=-72.0	SOL3045
	CK = EXP(C1LG) + EXP(C2LG)	SOL3046
	C = C + SGN*CK	SOL3047
40	CONTINUE	SOL3048
50	RETURN	SOL3049
	END	SOL3050
		SOL3051
		SOL3052
		SOL3053
		SOL3054
		SOL3055

## 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 of 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

$$\begin{array}{l} \text{Rate of} \\ \text{Mass In} \end{array} - \begin{array}{l} \text{Rate of} \\ \text{Mass Out} \end{array} + \begin{array}{l} \text{Rate of Mass} \\ \text{Generation} \end{array} = \begin{array}{l} \text{Rate of Mass} \\ \text{Accumulation} \end{array} \quad (1)$$

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,

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

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

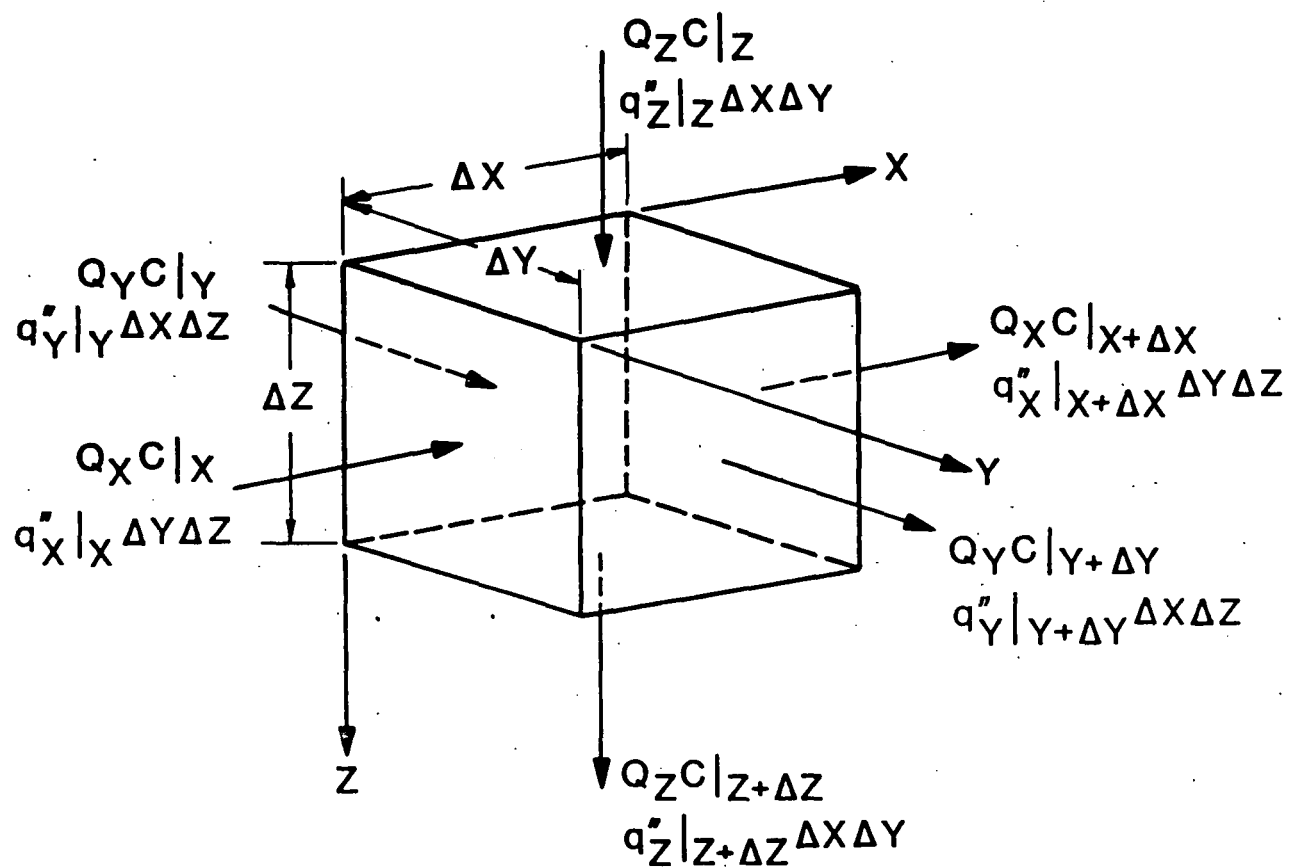


Figure 1 - Differential Control Volume for Mass Balance

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

$$\begin{aligned} & - \frac{Q_x C|_{x+\Delta x} - Q_x C|_x}{\Delta x (\Delta y \Delta z)} - \frac{Q_y C|_{y+\Delta y} - Q_y C|_y}{\Delta y (\Delta x \Delta z)} - \frac{Q_z C|_{z+\Delta z} - Q_z C|_z}{\Delta z (\Delta x \Delta y)} \\ & - \frac{q_x''|_{x+\Delta x} - q_x''|_x}{\Delta x} - \frac{q_y''|_{y+\Delta y} - q_y''|_y}{\Delta y} - \frac{q_z''|_{z+\Delta z} - q_z''|_z}{\Delta z} + r_T \\ & = \frac{(C_T)_{t+\Delta t} - (C_T)_t}{\Delta t} \end{aligned} \quad (2)$$

Now

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

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

and

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

where  $V$  is the superficial, or Darcy, velocity. Taking the limit of Equation 2 as  $\Delta x$ ,  $\Delta y$ ,  $\Delta z$ , and  $\Delta t$  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  $\theta$  is the effective porosity or fractional void volume. The concentration gradient in the liquid phase is the driving force for mass transport 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

$$\begin{aligned} \frac{\partial C_T}{\partial x} + \frac{\partial(V_x C)}{\partial x} + \frac{\partial(V_y C)}{\partial y} + \frac{\partial(V_z C)}{\partial z} \\ = \frac{\partial}{\partial x} D_x \frac{\partial(\theta C)}{\partial x} + \frac{\partial}{\partial y} D_y \frac{\partial(\theta C)}{\partial y} + \frac{\partial}{\partial z} D_z \frac{\partial(\theta C)}{\partial z} + r_T \end{aligned} \quad (6)$$

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

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

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

$$\begin{aligned} \frac{\text{mass of tracer}}{\text{bulk volume}} &= \frac{\text{mass of tracer}}{\text{volume of solution}} \frac{\text{volume of solution}}{\text{bulk volume}} \\ &+ \frac{\text{mass of tracer}}{\text{mass of solids}} \frac{\text{mass of solids}}{\text{bulk volume}} \end{aligned} \quad (8)$$

Equation 8 can be written in terms of aquifer properties as

$$C_T = \theta C + \rho_B C_s \quad (9)$$

where  $\rho_B$  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

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

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

$$\frac{\partial C_s}{\partial t} = \frac{dC_s}{dC} \frac{\partial C}{\partial t} \quad (11)$$

For a linear adsorption isotherm,

$$C_s = K_d C \quad (12)$$

or

$$\frac{dC_s}{dC} = K_d \quad (13)$$

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:

$$\frac{\partial C_T}{\partial t} = \theta \frac{\partial C}{\partial t} + \rho_B K_d \frac{\partial C}{\partial t} \quad (14)$$

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

$$R_d \equiv 1 + \frac{K_d \rho_B}{\theta} \quad (15)$$

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

$$\frac{\partial C_T}{\partial t} = \theta R_d \frac{\partial C}{\partial t} \quad (14)$$

or

$$\frac{\partial C_T}{\partial t} = \theta \frac{\partial C}{\partial (t/R_d)} \quad (15)$$

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

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

and

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

where  $\lambda_f$  and  $\lambda_s$  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

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

Including the linear adsorption isotherm developed above

$$C_s = K_d C$$

and

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

or

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

where  $\lambda_T$  is an apparent overall first-order rate constant defined as

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

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  $t = t_{1/2}$

$$\int_{C_0}^{C_0/2} \frac{dC}{C} = - \lambda \int_0^{t_{1/2}} dt$$

or

$$\ln C \bigg|_{C_0}^{C_0/2} = - \lambda t_{1/2}$$

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 occurring, and

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

Equation 21 can then be written as

$$\lambda_T = R_d \lambda$$

and Equation 19 becomes

$$r_T = - \theta R_d \lambda C \quad (22)$$

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

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

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

$$V^* \equiv \frac{V}{\theta} \quad (24)$$

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

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

and

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

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

$$\left(\frac{\partial C}{\partial \tau}\right)_X = \left(\frac{\partial C}{\partial X}\right)_\tau \left(\frac{\partial X}{\partial \tau}\right)_X + \left(\frac{\partial C}{\partial t}\right)_X \left(\frac{\partial \tau}{\partial \tau}\right)_X \quad (27)$$

Also,

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



Substituting Equation 28 into Equation 27 yields

$$\left(\frac{\partial C}{\partial \tau}\right)_x = \left(\frac{\partial C}{\partial \tau}\right)_X - v \star \left(\frac{\partial C}{\partial x}\right)_\tau \quad (29)$$

For the second derivative term in x,

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

Substituting Equations 25, 29 and 30 into Equation 23 yields

$$\frac{\partial C}{\partial \tau} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - \lambda_T C \quad (31)$$

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 simplifying 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 mechanisms 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.