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Techniques of Water-Resources Investigations
of the United States Geological Survey

Chapter B7

# ANALYTICAL SOLUTIONS FOR ONE-, TWO-, AND THREE-DIMENSIONAL SOLUTE TRANSPORT IN GROUND-WATER SYSTEMS WITH UNIFORM FLOW

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Book 3
APPLICATIONS OF HYDRAULICS

Table 7.—Measured solute concentrations in monitoring wells downgradient from the waste-disposal site in sample problem 8b

[Well locations shown in fig. 11]

| Well location (x and y coordinates), in feet | Measured solute concentration, in milligrams per liter | Calculated value of $\sigma$, in feet (from eq. 71) |
|---|---|---|
| 0, 200 | 2 | 70.9 |
| 0, 250 | 12 | 67.2 |
| 0, 300 | 65 | 64.2 |
| 0, 350 | 310 | 65.3 |
| 0, 400 | 725 | 62.3 |
| 0, 450 | 1,000 | -- |
| 0, 500 | 760 | 67.5 |
| 0, 550 | 290 | 63.6 |
| 0, 600 | 82 | 67.1 |
| 0, 650 | 9 | 65.2 |
| 0, 700 | 1 | 67.3 |

problems 8a and 8b required 24 s of CPU time on a Prime model 9955 Mod II.

# Three-Dimensional Solute Transport

Several analytical solutions are available for the three-dimensional form of the solute-transport equation (eq. 9), including those presented in Cleary and Ungs (1978), Huyakorn and others (1987), Codell and others (1982), Sagar (1982), and Hunt (1978). These solutions are particularly useful, as they can simulate transport of contaminants from sources in relatively thick aquifers when both vertical and horizontal spread of the solute is of interest. In addition to a solution modified from Cleary and Ungs (1978, p. 24–25), two solutions were derived by the author for this report. Detailed derivations of these solutions are presented in attachment 1.

In the first solution presented, the aquifer is assumed to be of infinite extent along all three coordinate axes. Fluid is injected into the aquifer through a point source at a constant rate and solute concentration ($C_o$). It is further assumed that the rate of injection is low and does not disturb the predominantly uniform flow field. In the remaining solutions presented in this section, the aquifer is assumed to be semi-infinite in length and to have a solute source located along the inflow boundary. The semi-infinite aquifer can be either finite in both width and height, extending from y=0 to y=W and from z=0 (the base

of the aquifer) to z=H, or infinite in width and height. A diagram of an idealized three-dimensional aquifer of semi-infinite length and finite width and height is presented in figure 18.

The solute source, referred to as a "patch" source (Cleary and Ungs, 1978), is of finite width and height and extends from $y=Y_1$ to $y=Y_2$ and from $z=Z_1$ to $z=Z_2$ at x=0 (fig. 18). The concentration within the patch is uniform and is equal to $C_o$, except along the boundary of the patch source, where it is equal to 0.5 $C_o$. Elsewhere along the inflow boundary, the concentration is 0. Combinations of patch sources could be used to simulate odd-shaped concentration distributions or multiple sources through the principle of superposition. First-order solute decay, adsorption, and ion exchange can also be simulated. A solution for a "gaussian source" of finite height along the boundary is given in Huyakorn and others (1987).

Three computer programs, POINT3, PATCHF, and PATCHI, were developed to calculate concentrations in these systems as a function of distance and elapsed time. They are described in this section.

## Aquifer of infinite extent with continuous point source

### Governing equation

The analytical solution for a continuous point source has been derived by first solving the solute-transport equation for an *instantaneous* point source and then integrating the solution over time. The three-dimensional solute-transport equation for an *instantaneous* point source is given by

$$\frac{\partial C}{\partial t} = D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} - \lambda C + \frac{Qdt}{n}C_o$$

$$\cdot \delta(x-X_c)\delta(y-Y_c)\delta(z-Z_c)\delta(t-t'). \tag{99}$$

*Boundary conditions:*

$$C, \frac{\partial C}{\partial x} = 0, \qquad x = \pm\infty \tag{100}$$

$$C, \frac{\partial C}{\partial y} = 0, \qquad y = \pm\infty \tag{101}$$

$$C, \frac{\partial C}{\partial z} = 0, \qquad z = \pm\infty, \tag{102}$$

where

    V = velocity in x-direction,
    Q = fluid injection rate,
    dt = infinitesimal time interval,
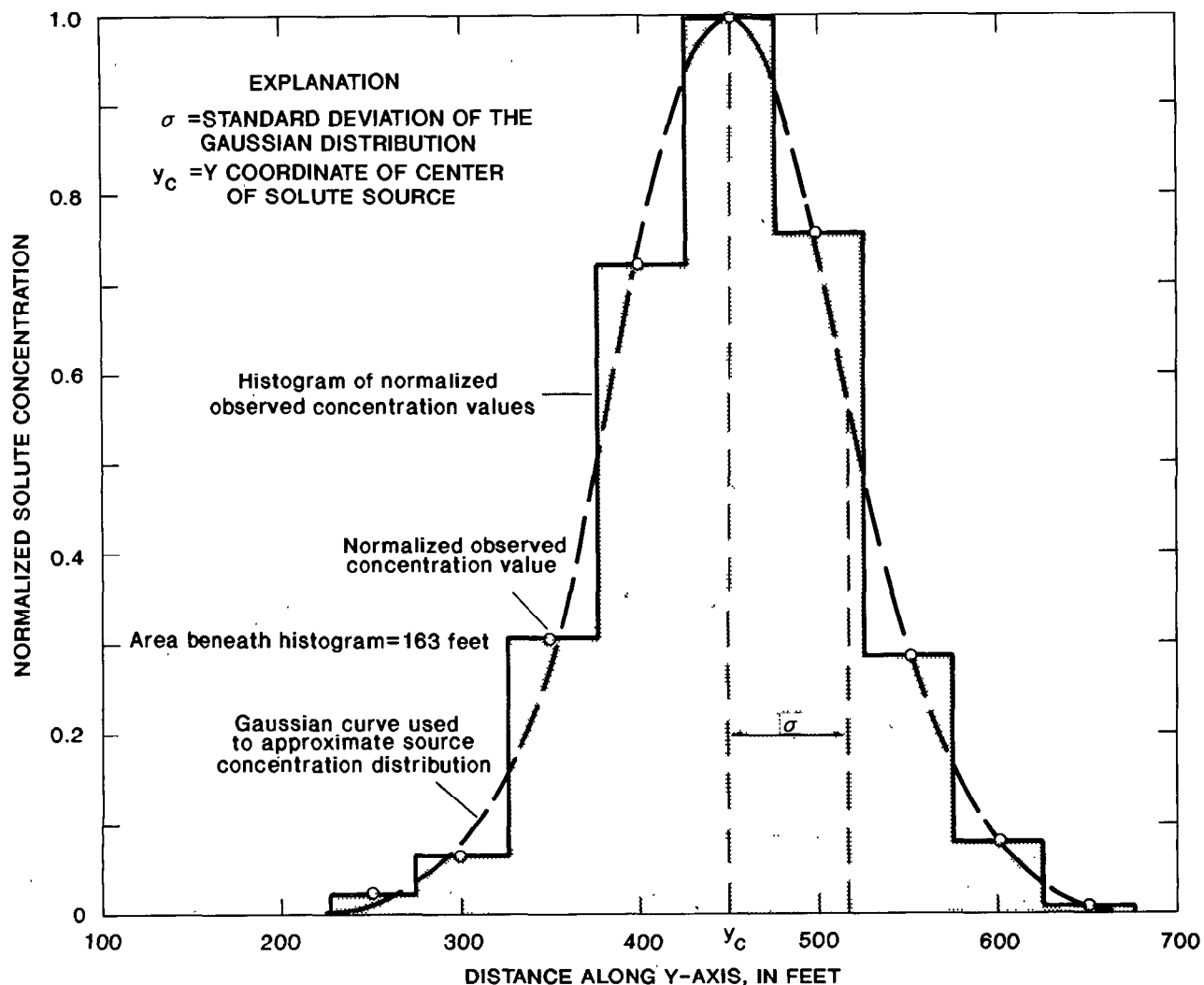    $\delta(\ )$ = dirac delta function,

Figure 15.—Normalized concentrations in relation to distance for the waste-disposal site in sample problem 8a and fitted gaussian distribution.

$X_c, Y_c, Z_c$ = coordinates of point source, and

t' = time at which instantaneous point source activates (assumed to be 0).

*Initial Condition:*

$C=0$,  $-\infty < x < \infty$,  $-\infty < y < \infty$,  $-\infty < z < \infty$  at $t'=0$  (103)

*Assumptions:*

1. Fluid is of constant density and viscosity.
2. Solute may be subject to first-order chemical transformation (for a conservative solute, $\lambda=0$).
3. Flow is in x-direction only, and velocity is constant. This presumes that the fluid injection rate is small

and that the spread of solute due to radially diverging flow paths is negligible.

4. The coefficients of longitudinal dispersion ($D_x$) and transverse dispersion ($D_y$, $D_z$), from equation 7, are constant.

**Analytical solution**

Hunt (1978, p. 76) presented a solution for a point source with a conservative solute. A solution for the *instantaneous* point source with solute decay was derived by the author using exponential Fourier transforms (detailed derivation in attachment 1) and can be expressed as

*A*

```
Sample Problem 8a -- Solute transport in a semi-infinite
aquifer of infinite width with a continuous gaussian source
Model Data:  V=4.0 ft/d, DX-150.0 ft**2/d, DY-30.0 ft**2/d
             WS-130 ft, YC-450 ft, CO-1000.0 mg/L

  33  37   1 104   1
MG/L     FT/D       FT**2/D   PER DAY   FEET         DAYS
  1000.0     4.00     150.0      30.0       0.0
   450.0   130.0
     0.0     50.0     100.0     150.0     200.0     250.0     300.0     350.0
   400.0    450.0     500.0     550.0     600.0     650.0     700.0     750.0
   800.0    850.0     900.0     950.0    1000.0    1050.0    1100.0    1150.0
  1200.0   1250.0    1300.0    1350.0    1400.0    1450.0    1500.0    1550.0
  1600.0
     0.0     25.0      50.0      75.0     100.0     125.0     150.0     175.0
   200.0    225.0     250.0     275.0     300.0     325.0     350.0     375.0
   400.0    425.0     450.0     475.0     500.0     525.0     550.0     575.0
   600.0    625.0     650.0     675.0     700.0     725.0     750.0     775.0
   800.0    825.0     850.0     875.0     900.0
   300.0
   250.0    250.0       0.1
```
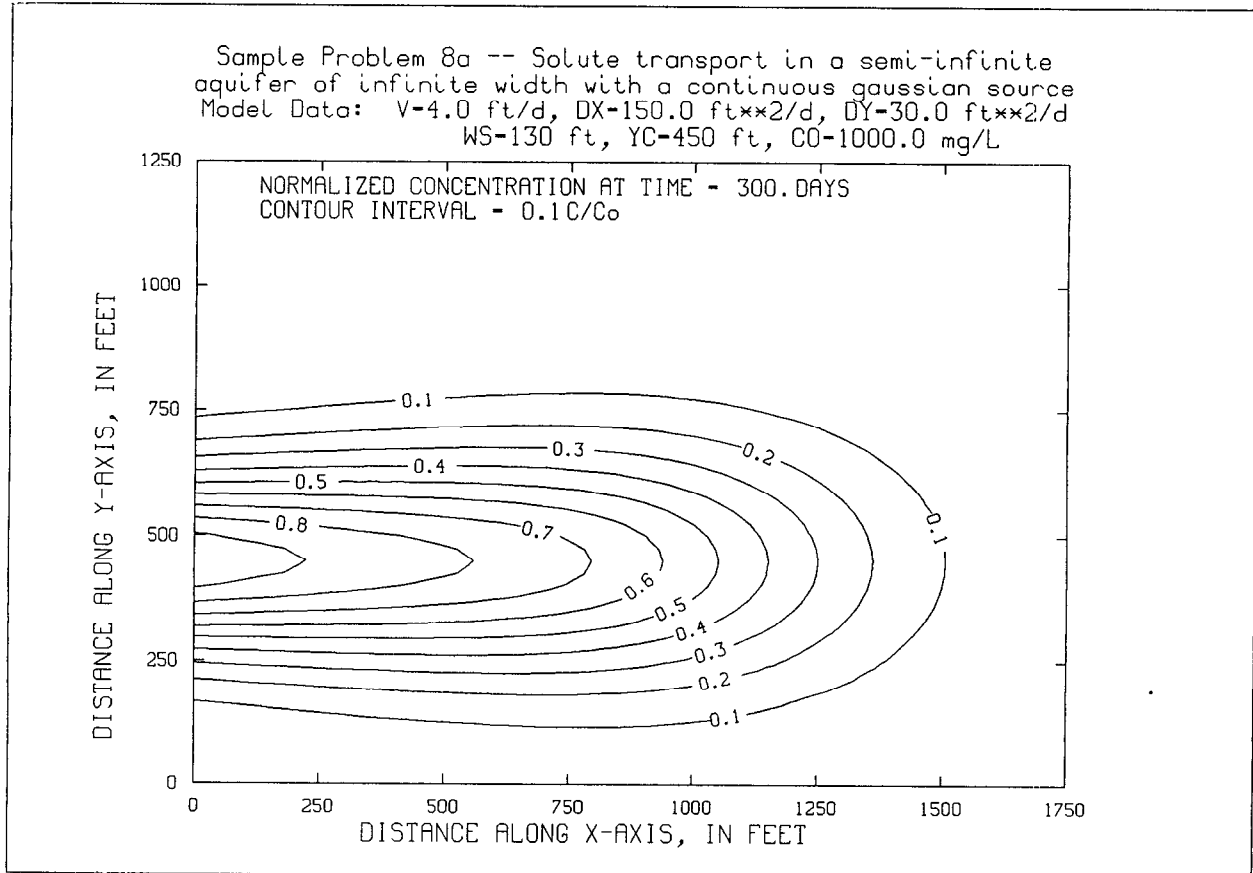
*B*



Figure 16.—(A) Sample input data set, and (B) normalized concentration contours generated by the program GAUSS for a conservative solute in an aquifer of infinite width having a gaussian concentration distribution ($\sigma$=150 feet) at the inflow boundary at 300 days (sample problem 8a).

*A*

```
Sample Problem 8b -- Solute transport in a semi-infinite
aquifer of infinite width with a continuous gaussian source
Model Data:   V=4.0 ft/d, DX=150.0 ft**2/d, DY=30.0 ft**2/d
              WS=65 ft, YC=450 ft, CO=1000.0 mg/L
────
  33   37   1 104    1
MG/L        FT/D       FT**2/D  PER DAY   FEET        DAYS
    1000.0     4.00     150.0     30.0       0.0
     450.0    65.0
       0.0    50.0     100.0     150.0     200.0     250.0    300.0    350.0
     400.0   450.0     500.0     550.0     600.0     650.0    700.0    750.0
     800.0   850.0     900.0     950.0    1000.0    1050.0   1100.0   1150.0
    1200.0  1250.0    1300.0    1350.0    1400.0    1450.0   1500.0   1550.0
    1600.0
       0.0    25.0      50.0      75.0     100.0     125.0    150.0    175.0
     200.0   225.0     250.0     275.0     300.0     325.0    350.0    375.0
     400.0   425.0     450.0     475.0     500.0     525.0    550.0    575.0
     600.0   625.0     650.0     675.0     700.0     725.0    750.0    775.0
     800.0   825.0     850.0     875.0     900.0
     300.0
     250.0   250.0       0.1
```
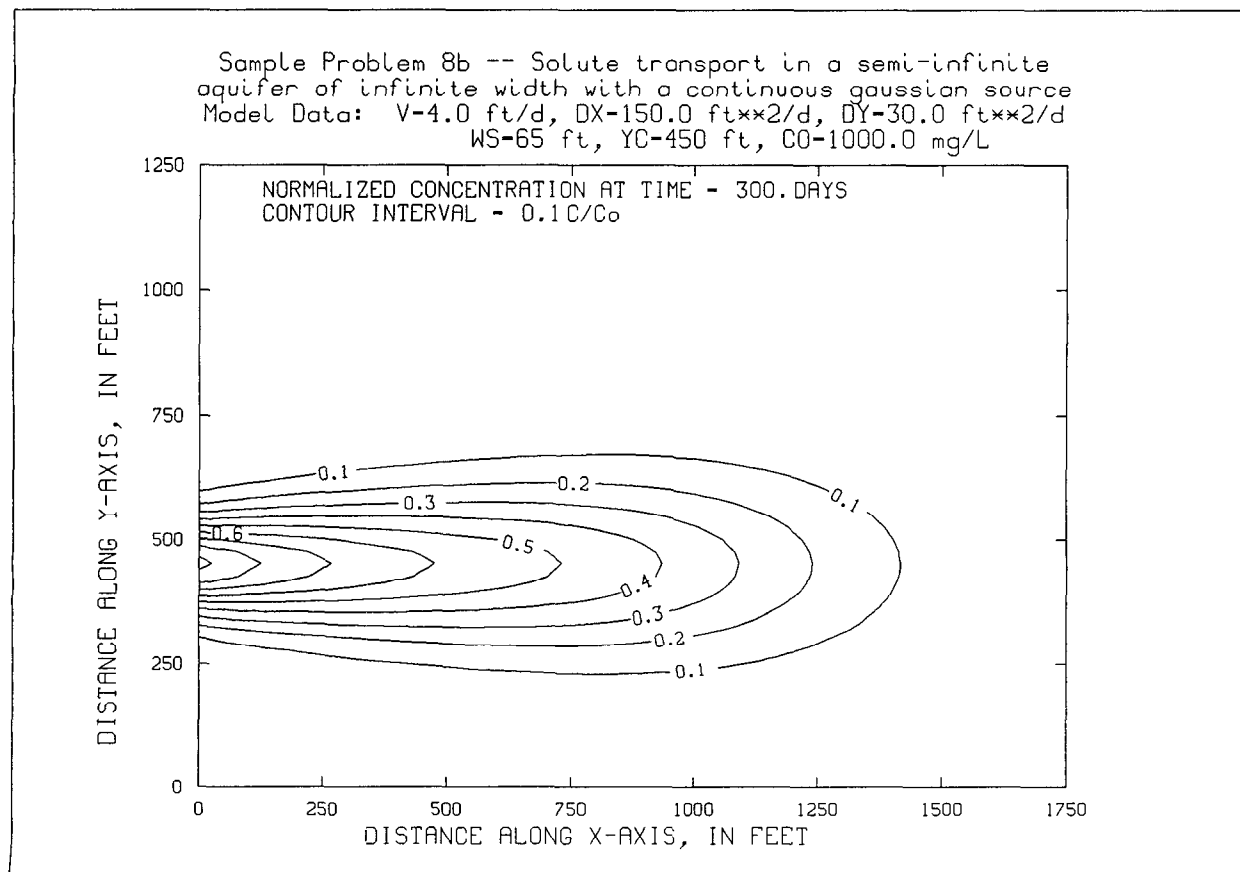
*B*



Figure 17.—(A) Sample input data set, and (B) normalized concentration contours generated by the program GAUSS for a conservative solute in an aquifer of infinite width having a gaussian concentration distribution ($\sigma$=65 feet) at the inflow boundary at 300 days (sample problem 8b).

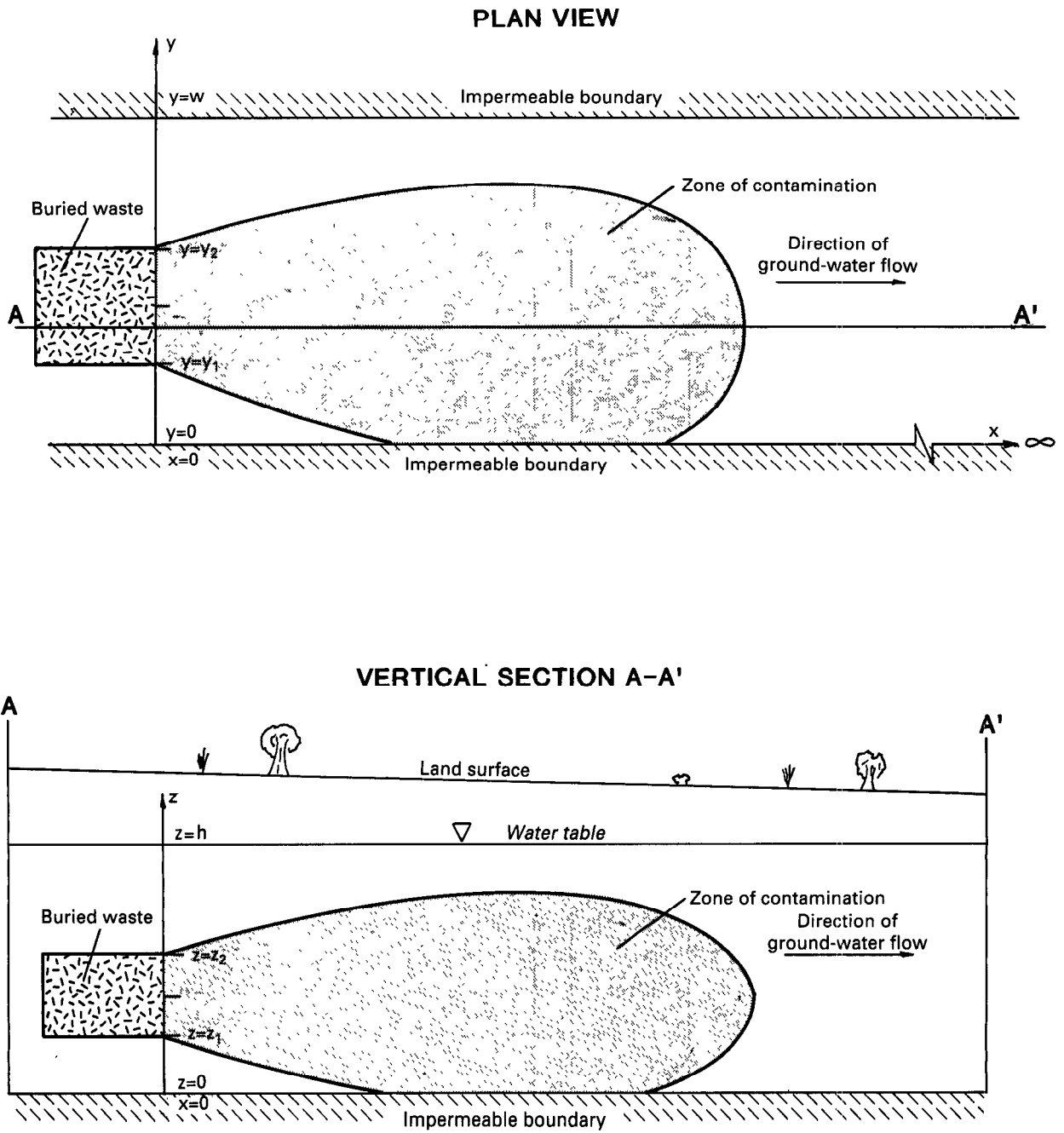## PLAN VIEW



## VERTICAL SECTION A-A'



Figure 18.—Plan view and vertical section of idealized three-dimensional transport in an aquifer of semi-infinite length and finite width and height.

$$C(x,y,z,t)=\frac{C_oQdt\;exp\left[\frac{V(x-X_c)}{2D_x}-\left(\frac{V^2}{4D_x}+\lambda\right)(t-t')\right]}{8n\pi^{3/2}\;(t-t')^{3/2}\;\sqrt{D_xD_yD_z}}$$

$$\cdot exp\left[-\frac{(x-X_c)^2}{4D_x(t-t')}-\frac{(y-Y_c)^2}{4D_y(t-t')}-\frac{(z-Z_c)^2}{4D_z(t-t')}\right].\quad(104)$$

Equation 104 can be integrated with respect to time to yield a closed-form solution for the continuous solute source as

$$C(x,y,z,t)=\frac{C_oQ\;exp\left[\frac{V(x-X_c)}{2D_x}\right]}{8n\pi\gamma\sqrt{D_yD_z}}\cdot\left\{exp\left[\frac{\gamma\beta}{2D_x}\right]erfc\left[\frac{(\gamma+\beta t)}{2\sqrt{D_x t}}\right]\right.$$

$$\left.+exp\left[\frac{-\gamma\beta}{2D_x}\right]erfc\left[\frac{(\gamma-\beta t)}{2\sqrt{D_x t}}\right]\right\},\quad(105)$$

where

$$\gamma=\left[(x-X_c)^2+\frac{D_x(y-Y_c)^2}{D_y}+\frac{D_x(z-Z_c)^2}{D_z}\right]^{1/2}$$

and

$$\beta=[V^2+4D_x\lambda]^{1/2}.$$

When $\lambda=0$, equation 105 reduces to a form similar to that presented in Hunt (1978, p. 77) for a continuous point source with a conservative solute.

*Comments*:

Equation 105 is valid only when $\gamma$ does not equal zero. Also, concentrations determined at locations close to the point source may exceed $C_o$ for certain combinations of values of Q, V, $D_x$, $D_y$, and $D_z$. In general, this can occur when Q is large relative to

$$\gamma\cdot\sqrt{D_yD_z}.$$

A solution that accounts for radial flow away from the point source would be more appropriate at large injection rates.

Linear equilibrium adsorption and ion exchange can be simulated by dividing the coefficients Q, V, $D_x$, $D_y$, and $D_z$ by the retardation factor, R (eq. 15). Temporal variations in solute concentration can be simulated through the principle of superposition.

### Description of program POINT3

The program POINT3 computes the analytical solution to the three-dimensional solute-transport equation for an aquifer of infinite extent with a continuous point source. It consists of a main program and the subroutine CNRML3. The functions of the main program and subroutine are outlined below; the program code listing is presented in attachment 2.

The program also calls the subroutine EXERFC and the output subroutines TITLE, OFILE, PLOT3, and CNTOUR, which are common to most programs described in this report. These subroutines are described in detail later.

#### Main program

The main program reads and prints all input data needed to specify model variables. The required input data and the format used in preparing a data file are shown in table 8.

The program next executes a set of four nested loops. The innermost loop calls subroutine CNRML3 to calculate the concentration at all specified y-coordinate values for a particular x-coordinate value, z-coordinate value, and time. The second loop cycles through all x-coordinate values. The third loop cycles through all z-coordinate values and prints a table of concentration in relation to x and y for each z value. The outer loop cycles through all specified time values. Model output can be plotted as a series of maps showing lines of equal solute concentration in a horizontal (x-y plane) cross section at each point along the z-axis.

#### Subroutine CNRML3

Subroutine CNRML3 calculates the normalized concentration ($C/C_o$) for a particular time value and distance using equation 105. A warning message is printed on the program output if the values of $(x-X_c)$, $(y-Y_c)$, and $(z-Z_c)$ all equal to zero are passed to the subroutine.

### Sample problem 9

In sample problem 9, a natural gradient tracer test was conducted by injecting a chloride solution into an aquifer. The solution was injected through three wells spaced 2 ft apart, laterally, each having a small screened interval centered about z=10 ft. A total of 22.5 gallons (3 ft$^3$) of solution was injected during a 24-hour period. Other model variables are

| | |
|---|---|
| Aquifer porosity (n) | =0.25 |
| Ground-water velocity ($V_x$) | =0.1 ft/d |
| Longitudinal dispersivity ($\alpha_l$) | =0.60 ft |
| Horizontal transverse dispersivity ($\alpha_{th}$) | =0.03 ft |
| Vertical transverse dispersivity ($\alpha_{tv}$) | =0.006 ft |
| Chloride concentration in injected solution | =1,000 mg/L |

Table 8.—Input data format for the program POINT3

| Data set | Columns | Format | Variable name | Description |
|---|---|---|---|---|
| 1 | 1 - 60 | A60 | TITLE | Data to be printed in a title box on the first page of program output. Last line in data set must have an "=" in column 1. First four lines are also used as title for plot. |
| 2 | 1 - 4 | I4 | NX | Number of x-coordinates at which solution will be evaluated. |
| | 5 - 8 | I4 | NY | Number of y-coordinates at which solution will be evaluated. |
| | 9 - 12 | I4 | NZ | Number of z-coordinates at which solution will be evaluated. |
| | 13 - 16 | I4 | NT | Number of time values at which solution will be evaluated. |
| | 17 - 20 | I4 | IPLT | Plot control variable. Contours of normalized concentration will be plotted if IPLT is greater than 0. |
| 3 | 1 - 10 | A10 | CUNITS | Character variable used as label for units of concentration in program output. |
| | 11 - 20 | A10 | VUNITS | Units of ground-water velocity. |
| | 21 - 30 | A10 | DUNITS | Units of dispersion coefficient. |
| | 31 - 40 | A10 | KUNITS | Units of solute-decay coefficient. |
| | 41 - 50 | A10 | LUNITS | Units of length. |
| | 51 - 60 | A10 | QUNITS | Units of solution injection rate. |
| | 61 - 70 | A10 | TUNITS | Units of time. |
| 4 | 1 - 10 | F10.0 | CO | Solute concentration in injected fluid. |
| | 11 - 20 | F10.0 | VX | Ground-water velocity in x-direction. |
| | 21 - 30 | F10.0 | DX | Longitudinal dispersion coefficient. |
| | 31 - 40 | F10.0 | DY | Transverse dispersion coefficient in y-direction. |
| | 41 - 50 | F10.0 | DZ | Transverse dispersion coefficient in z-direction. |
| | 51 - 60 | F10.0 | DK | First-order solute-decay coefficient. |
| 5 | 1 - 10 | F10.0 | XC | X-coordinate of continuous point source. |
| | 11 - 20 | F10.0 | YC | Y-coordinate of continuous point source. |
| | 21 - 30 | F10.0 | ZC | Z-coordinate of continuous point source. |
| | 31 - 40 | F10.0 | QM | Solution injection rate. |
| | 41 - 50 | F10.0 | POR | Aquifer porosity. |
| 6 | 1 - 80 | 8F10.0 | X(I) | X-coordinates at which solution will be evaluated (eight values per line). |
| 7 | 1 - 80 | 8F10.0 | Y(I) | Y-coordinates at which solution will be evaluated (eight values per line). |
| 8 | 1 - 80 | 8F10.0 | Z(I) | Z-coordinates at which solution will be evaluated (eight values per line). |
| 9 | 1 - 80 | 8F10.0 | T(I) | Time values at which solution will be evaluated (eight values per line). |
| [1]10 | 1 - 10 | F10.0 | XSCLP | Scaling factor by which x-coordinate values are divided to convert them to plotter inches. |
| | 11 - 20 | F10.0 | YSCLP | Scaling factor used to convert y-coordinates into plotter inches. |
| | 21 - 30 | F10.0 | DELTA | Contour increment for plot of normalized concentration (must be between 0.0 and 1.0). |

[1]Data line is needed only if IPLT (in data set 2) is greater than 0.

Injection well coordinates $(X_c, Y_c, Z_c)$

Well 1   =(0, 98, 10)
Well 2   =(0, 100, 10)
Well 3   =(0, 102, 10).

From these values, the terms obtained are

Coefficient of longitudinal dispersion
  $(D_x)$   =0.06 ft$^2$/d
Coefficient of horizontal transverse
  dispersion $(D_y)$   =0.003 ft$^2$/d
Coefficient of vertical transverse
  dispersion $(D_z)$   = 0.0006 ft$^2$/d
Injection rate per well $(Q_m)$   =1.0 ft$^3$/d.

Chloride concentrations are computed in the z=10-ft plane at x=0 and at 2-ft intervals along the x-axis from x=20 ft to x=60 ft, and at 1-ft intervals along the y-axis from y=90 ft to y=110 ft, after an elapsed time of 400 days. The injection period was simulated using the principle of superposition by first calculating the concentrations resulting from a continuous point source after 400 days and then subtracting the concentrations resulting from a continuous point source after 399 days. The effect of the multiple injection wells was simulated by summing the calculated concentrations for each well.

Rather than running the program POINT3 six times and then summing all the concentration values manually, it was easier to *temporarily* modify the main program by adding nine lines within the innermost loop, as follows:

```
DO 50 IY=1,NY
YY=Y(IY)−YC
CALL  CNRML3(QM,POR,DK,T(IT),XX,YY,ZZ,
   DX,DY,DZ,VX,CN)
CXY(IX,IY)=CO*CN
   YY1=YY+2.0
   YY2=YY−2.0
   CALL  CNRML3(QM,POR,DK,T(IT),XX,YY1,
   ZZ,DX,DY,DZ,VX,CN1)
   CALL  CNRML3(QM,POR,DK,T(IT),XX,YY2,
   ZZ,DX,DY,DZ,VX,CN2)
   T1=T(IT)−1.0
   CALL  CNRML3(QM,POR,DK,T1,XX,YY,ZZ,
   DX,DY,DZ,VX,CN3)
   CALL  CNRML3(QM,POR,DX,T1,XX,YY1,ZZ,
   DX,DY,DZ,VX,CN4)
   CALL  CNRML3(QM,POR,DK,T1,XX,YY2,ZZ,
   DX,DY,DZ,VX,CN5)
   CXY(IX,IY) = CXY(IX,IY)+ CO*(CN1+ CN2
   −CN3−CN4−CN5)
50 CONTINUE
```

The input data set for sample problem 9 is shown in figure 19*A*; a computer-generated contour plot of normalized concentrations $(C/C_o)$ in the x-y plane at z=10 ft are shown in figure 19*B*. Sample problem 9 required 5 s of CPU time on a Prime model 9955 Mod II.

# Aquifer of finite width and height with finite-width and finite-height solute source

## Governing equation

*Three-dimensional solute-transport equation*:

$$\frac{\partial C}{\partial t}+D_x\frac{\partial^2 C}{\partial x^2}+D_y\frac{\partial^2 C}{\partial y^2}+D_z\frac{\partial^2 C}{\partial z^2}-V\frac{\partial C}{\partial x}-\lambda C \quad (106)$$

*Boundary conditions*:

$$C=C_o, \quad x=0 \text{ and } Y_1<y<Y_2 \quad (107a)$$
$$\text{and } Z_1<z<Z_2$$

$$C=0, \quad x=0 \text{ and } y<Y_1 \text{ or } y>Y_2 \quad (107b)$$
$$\text{and } z<Z_1 \text{ or } z>Z_2$$

$$C, \frac{\partial C}{\partial y}=0, \quad y=0 \quad (108)$$

$$C, \frac{\partial C}{\partial y}=0, \quad y=W \quad (109)$$

$$C, \frac{\partial C}{\partial z}=0, \quad z=0 \quad (110)$$

$$C, \frac{\partial C}{\partial z}=0, \quad z=H \quad (111)$$

$$C, \frac{\partial C}{\partial x}=0, \quad x=\infty \quad (112)$$

where
  V =velocity in x-direction,
  $Y_1$ =y-coordinate of lower limit of solute source,
  $Y_2$ =y-coordinate of upper limit of solute source,
  $Z_1$ =z-coordinate of lower limit of solute source,
  $Z_2$ =z-coordinate of upper limit of solute source at x=0,
  W =aquifer width, and
  H =aquifer height.

*Initial condition*:

C=0   0<x< $\infty$, 0<y<W, and 0<z< H   at t=0 (113)

*Assumptions*:

1. Fluid is of constant density and viscosity.

*A*

```
Sample Problem 9 -- Solute transport in an infinite aquifer
with multiple point sources of finite duration
Model Data:  V=0.1 ft/d, DX=0.06 ft**2/d, DY=0.003 ft**2/d
  DZ=0.0006 ft**2/d, QM=1.0 ft**3/d, CO=1000.0 mg/L, n=0.25
=====
  21  21   1  01   1
MG/L      FT/D       FT**2/D   PER DAY   FEET        FT**3/D    DAYS
   1000.0        0.1      0.06      0.003     0.0006
      0.0      100.0     10.0       1.00      0.25
     20.0       22.0     24.0      26.0      28.0      30.0      32.0      34.0
     36.0       38.0     40.0      42.0      44.0      46.0      48.0      50.0
     52.0       54.0     56.0      58.0      60.0
     90.0       91.0     92.0      93.0      94.0      95.0      96.0      97.0
     98.0       99.0    100.0     101.0     102.0     103.0     104.0     105.0
    106.0      107.0    108.0     109.0     110.0
     10.0
    400.0
      5.0        5.0      0.01
```
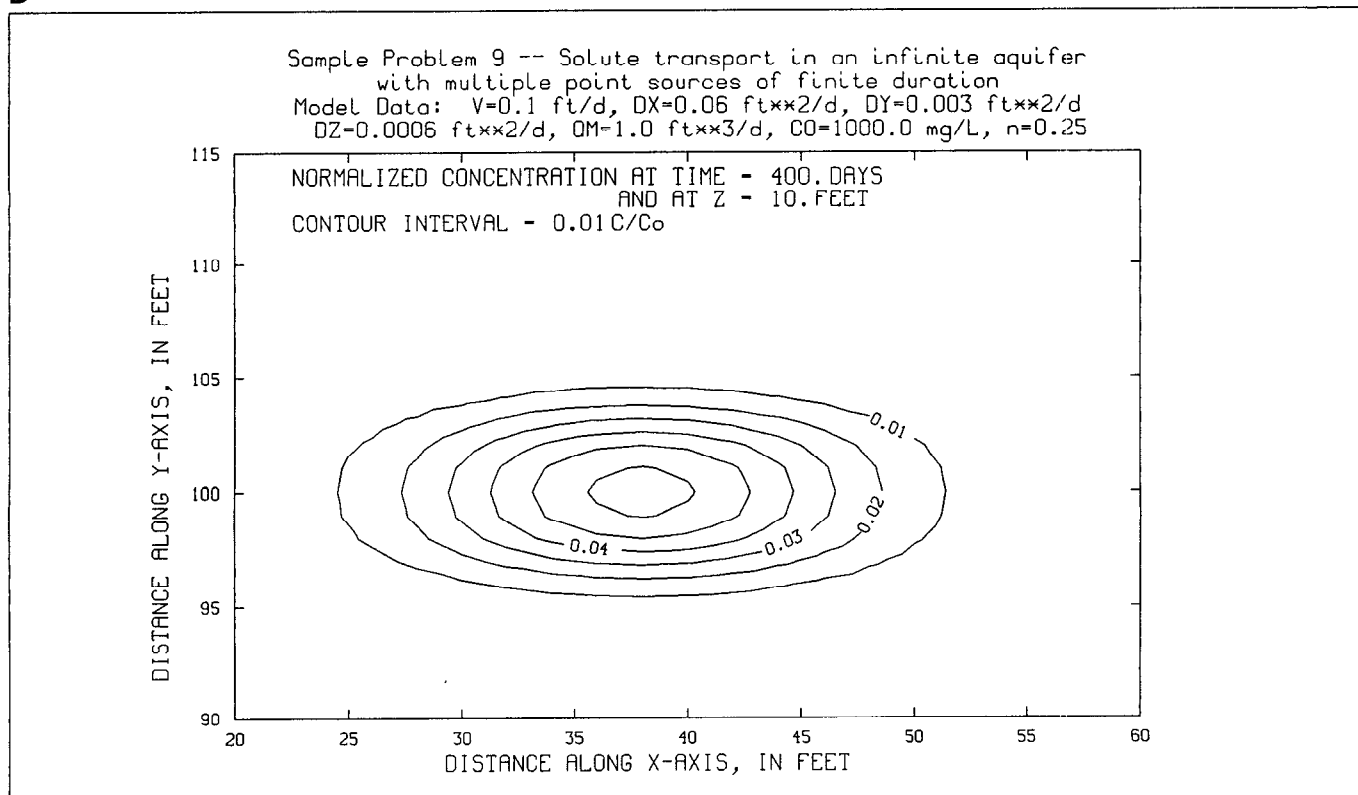
*B*



Figure 19.—(*A*) Sample input data set, and (*B*) normalized concentration contours generated by the program POINT3 for a natural gradient tracer test in an aquifer of infinite extent after 400 days in the $z=10$-foot plane (sample problem 9).

2. Solute may be subject to first-order chemical transformation (for a conservative solute, $\lambda=0$).
3. Flow is in x-direction only, and velocity is constant.
4. The coefficients of longitudinal dispersion ($D_x$) and transverse dispersion ($D_y$, $D_z$), from equation 7, are constant.

### Analytical solution

The solution to equation 106 was first derived by Cleary and Ungs (1978, p. 24–25). A modified form of the equation (derived in detail by the author in attachment 1) can be given as

$$C(x,y,z,t)=C_o\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}L_{mn}O_mP_n \cos (\zeta z) \cos (\eta y)$$

$$\cdot\left\{\exp\left[\frac{x(V-\beta)}{2D_x}\right]\cdot\text{erfc}\left[\frac{x-\beta t}{2\sqrt{D_xt}}\right]\right.$$

$$\left.+\exp\left[\frac{x(V+\beta)}{2D_x}\right]\cdot\text{erfc}\left[\frac{x+\beta t}{2\sqrt{D_xt}}\right]\right\}, \qquad (114)$$

where

$$L_{mn}=\begin{cases} \frac{1}{2} & m=0, \text{ and } n=0 \\ 1 & m=0, \text{ and } n>0 \\ 1 & m>0, \text{ and } n=0 \\ 2 & m>0, \text{ and } n>0 \end{cases}$$

$$O_m=\begin{cases} \dfrac{Z_2-Z_1}{H} & m=0 \\[2ex] \dfrac{[\sin (\zeta Z_2)-\sin (\zeta Z_1)]}{m\pi} & m>0 \end{cases}$$

$$P_n=\begin{cases} \dfrac{Y_2-Y_1}{W} & n=0 \\[2ex] \dfrac{[\sin (\eta Y_2)-\sin (\eta Y_1)]}{n\pi} & n>0 \end{cases}$$

$\zeta=m\pi/H$    $m=0,1,2,3...$

$\eta=n\pi/W$    $n=0,1,2,3...$

$\beta=\sqrt{V^2+4D_x(\eta^2D_y+\zeta^2D_z+\lambda)}.$

*Comments:*

The terms in the infinite series in equation 114 tend to oscillate, and the double series converges slowly for small values of x and time. Therefore, many terms may be needed to ensure convergence. A good initial estimate is 200 terms for each series.

The solution can yield results with either $D_y$, $D_z$, or $\lambda=0$. Linear equilibrium adsorption and ion exchange can be simulated by dividing the coefficients $D_x$, $D_y$, $D_z$, and V by the retardation factor, R (eq. 15). Temporal variations in solute concentration and odd-shaped source configurations can be simulated through the principle of superposition.

### Description of program PATCHF

The program PATCHF computes the analytical solution to the three-dimensional solute-transport equation for an aquifer of finite width and height with a finite-width and finite-height solute source at the inflow boundary. It consists of a main program and subroutine CNRMLF. The functions of the main program and subroutine are outlined below; the program code listing is presented in attachment 2.

The program also calls the subroutine EXERFC and output subroutines TITLE, OFILE, PLOT3D, and CNTOUR, which are common to most programs described in this report. These subroutines are described in detail later.

#### Main program

The main program reads and prints all input data needed to specify model variables. The required input data and the format used in preparing a data file are shown in table 9.

The program next executes a set of four nested loops. The innermost loop calls subroutine CNRMLF to calculate the concentration at all specified y-coordinate values for a particular x-coordinate value, z-coordinate value, and time. The second loop cycles through all x-coordinate values. The third loop cycles through all z-coordinate values and prints a table of concentration in relation to x and y for each z value. The outer loop cycles through all specified time values. Model output can be plotted as a series of maps showing lines of equal solute concentration in the horizontal (x-y) plane at each point along the z-axis.

#### Subroutine CNRMLF

Subroutine CNRMLF calculates the normalized concentration ($C/C_o$) for a particular time value and distance using equation 114. The maximum number of terms in the infinite series summation is specified by the user. Because terms in the series tend to oscillate, a subtotal of the last 10 terms is kept, and when the subtotal is less than a convergence criterion set at $1\times10^{-12}$, the series summation is halted. If the series does not converge after the specified maximum number of terms are taken, a warning message is printed on the program output.

Table 9.—Input data format for the program PATCHF

| Data set | Columns | Format | Variable name | Description |
|---|---|---|---|---|
| 1 | 1 - 60 | A60 | TITLE | Data to be printed in a title box on the first page of program output. Last line in data set must have an "=" in column 1. First four lines are also used as title for plot. |
| 2 | 1 - 4 | I4 | NX | Number of x-coordinates at which solution will be evaluated. |
|   | 5 - 8 | I4 | NY | Number of y-coordinates at which solution will be evaluated. |
|   | 9 - 12 | I4 | NZ | Number of z-coordinates at which solution will be evaluated. |
|   | 13 - 16 | I4 | NT | Number of time values at which solution will be evaluated. |
|   | 17 - 20 | I4 | NMAX | Maximum number of terms to be used in inner loop of the infinite series summation. |
|   | 21 - 24 | I4 | MMAX | Maximum number of terms to be used in outer loop of the infinite series summation. |
|   | 25 - 28 | I4 | IPLT | Plot control variable. Contours of normalized concentration will be plotted if IPLT is greater than 0. |
| 3 | 1 - 10 | A10 | CUNITS | Character variable used as label for units of concentration in program output. |
|   | 11 - 20 | A10 | VUNITS | Units of ground-water velocity. |
|   | 21 - 30 | A10 | DUNITS | Units of dispersion coefficient. |
|   | 31 - 40 | A10 | KUNITS | Units of solute-decay coefficient. |
|   | 41 - 50 | A10 | LUNITS | Units of length. |
|   | 51 - 60 | A10 | TUNITS | Units of time. |
| 4 | 1 - 10 | F10.0 | CO | Solute concentration at inflow boundary. |
|   | 11 - 20 | F10.0 | VX | Ground-water velocity in x-direction. |
|   | 21 - 30 | F10.0 | DX | Longitudinal dispersion coefficient. |
|   | 31 - 40 | F10.0 | DY | Transverse dispersion coefficient in y-direction. |
|   | 41 - 50 | F10.0 | DZ | Transverse dispersion coefficient in z-direction. |
|   | 51 - 60 | F10.0 | DK | First-order solute-decay coefficient. |
| 5 | 1 - 10 | F10.0 | W | Aquifer width (aquifer extends from y = 0 to y = W). |
|   | 11 - 20 | F10.0 | H | Aquifer thickness (aquifer extends from z = 0 to z = H). |
|   | 21 - 30 | F10.0 | Y1 | Y-coordinate of lower limit of patch solute source. |
|   | 31 - 40 | F10.0 | Y2 | Y-coordinate of upper limit of patch solute source. |
|   | 41 - 50 | F10.0 | Z1 | Z-coordinate of lower limit of patch solute source. |
|   | 51 - 60 | F10.0 | Z2 | Z-coordinate of upper limit of patch solute source. |
| 6 | 1 - 80 | 8F10.0 | X(I) | X-coordinates at which solution will be evaluated (eight values per line). |
| 7 | 1 - 80 | 8F10.0 | Y(I) | Y-coordinates at which solution will be evaluated (eight values per line). |
| 8 | 1 - 80 | 8F10.0 | Z(I) | Z-coordinates at which solution will be evaluated (eight values per line). |
| 9 | 1 - 80 | 8F10.0 | T(I) | Time values at which solution will be evaluated (eight values per line). |
| [1]10 | 1 - 10 | F10.0 | XSCLP | Scaling factor by which x-coordinate values are divided to convert them to plotter inches. |
|   | 11 - 20 | F10.0 | YSCLP | Scaling factor used to convert y-coordinates into plotter inches. |
|   | 21 - 30 | F10.0 | DELTA | Contour increment for plot of normalized concentration (must be between 0.0 and 1.0). |

[1]Data line is needed only if IPLT (in data set 2) is greater than 0.

## Sample problem 10

In sample problem 10, migration of chloride ion from a landfill, created by filling in a gravel pit excavated in a valley-fill aquifer, is simulated. Model variables are

| | |
|---|---|
| Aquifer width (W) | =3,000 ft |
| Aquifer height (H) | =100 ft |
| Y-coordinate of lower limit of source ($Y_1$) | =400 ft |
| Y-coordinate of upper limit of source ($Y_2$) | =2,000 ft |
| Z-coordinate of lower limit of source ($Z_1$) | =50 ft |
| Z-coordinate of upper limit of source ($Z_2$) | =100 ft |
| Source concentration ($C_o$) | =1,000 mg/L |
| Ground-water velocity (V) | =1 ft/d |
| Dispersion in x-direction ($D_x$) | =200 ft$^2$/d |
| Dispersion in y-direction ($D_y$) | =60 ft$^2$/d |
| Dispersion in z-direction ($D_z$) | =10 ft$^2$/d. |

Concentrations are calculated at 150-ft intervals along the x-axis for 3,900 ft, and at 100-ft intervals along the y-axis for 3,000 ft. Chloride concentration distributions after 3,000 days for z-coordinates of 50 and 75 ft (z=0 is at the base of the aquifer) are simulated.

The input data set for sample problem 10 is shown in figure 20A; computer-generated contour plots of normalized concentration ($C/C_o$) in x-y planes defined by the two z-coordinates are shown in figure 20B. The plot of concentrations along the centerline of the plume (at z=75 ft) can be compared with figure 13B to show the effect of vertical dispersion on both the shape of the chloride plume and simulated concentrations. This demonstrates the type of errors that can be introduced by using a two-dimensional solution when a three-dimensional solution is required.

Program output for sample problem 10 is presented in attachment 4. The sample problem required 7 min and 50 s of CPU time on a Prime model 9955 Mod II.

# Aquifer of infinite width and height with finite-width and finite-height solute source

## Governing equation

*Three-dimensional solute-transport equation:*

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - V \frac{\partial C}{\partial x} - \lambda C \quad (115)$$

*Boundary conditions:*

$$C = C_o, \quad \begin{aligned} &x=0 \text{ and } Y_1 < y < Y_2 \\ &\text{and } Z_1 < z < Z_2 \end{aligned} \quad (116a)$$

$$C = 0, \quad \begin{aligned} &x=0 \text{ and } y < Y_1 \text{ or } y > Y_2 \\ &\text{and } z < Z_1 \text{ or } z > Z_2 \end{aligned} \quad (116b)$$

$$C, \frac{\partial C}{\partial y} = 0, \quad y = \pm \infty \quad (117)$$

$$C, \frac{\partial C}{\partial z} = 0, \quad z = \pm \infty \quad (118)$$

$$C, \frac{\partial C}{\partial x} = 0, \quad x = \infty \quad (119)$$

where
V = velocity in x-direction,
$Y_1$ = y-coordinate of lower limit of solute source,
$Y_2$ = y-coordinate of upper limit of solute source,
$Z_1$ = z-coordinate of lower limit of solute source, and
$Z_2$ = z-coordinate of upper limit of solute source at x=0.

*Initial condition:*

$$C=0, \quad 0 < x < \infty, \quad -\infty < y < +\infty, \text{ and } -\infty < z < +\infty \text{ at } t=0 \quad (120)$$

*Assumptions:*

1. Fluid is of constant density and viscosity.
2. Solute may be subject to first-order chemical transformation (for a conservative solute, $\lambda = 0$).
3. Flow is in x-direction only, and velocity is constant.
4. The coefficients of longitudinal dispersion ($D_x$) and transverse dispersion ($D_y$, $D_z$), from equation 7, are constant.

## Analytical solution

Sagar (1982, p. 49) presents a solution to the analogous problem of vertical leaching of a conservative solute from a patch source in the x-y plane. The following analytical solution was derived by the author using Fourier transforms (detailed derivation presented in attachment 1) for a patch source in the y-z plane with solute subject to decay:

Figure 20.—(A) Sample input data set, and (B) normalized concentration contours generated by the program PATCHF for a conservative solute in an aquifer of finite height and width after 3,000 days at heights of 75 and 50 feet above base of the aquifer (sample problem 10).

$$C(x,y,z,t)=\frac{C_o \text{ x } \exp\left[\frac{Vx}{2D_x}\right]}{8\sqrt{\pi D_x}}$$

$$\cdot \int_0^t \tau^{-\frac{3}{2}} \exp\left[-\left(\frac{V^2}{4D_x}+\lambda\right)\tau-\frac{x^2}{4D_x\tau}\right]$$

$$\cdot \left\{ \text{erfc}\left[\frac{(Y_1-y)}{2\sqrt{D_y\tau}}\right] - \text{erfc}\left[\frac{(Y_2-y)}{2\sqrt{D_y\tau}}\right]\right\}$$

$$\cdot \left\{ \text{erfc}\left[\frac{(Z_1-z)}{2\sqrt{D_z\tau}}\right] - \text{erfc}\left[\frac{(Z_2-z)}{2\sqrt{D_z\tau}}\right]\right\} d\tau. \quad (121a)$$

where $\tau$ is a dummy variable of integration for the time integral.

To improve the accuracy of the numerical integration, a variable substitution can be made where $\tau=Z^4$, yielding

$$C(x,y,z,t)=\frac{C_o \text{ x } \exp\left[\frac{Vx}{2D_x}\right]}{2\sqrt{\pi D_x}}$$

$$\cdot \int_0^{\tau^{1/4}} \frac{1}{Z^3}\exp\left[-\left(\frac{V^2}{4D_x}+\lambda\right)Z^4-\frac{x^2}{4D_xZ^4}\right]$$

$$\cdot \left\{ \text{erfc}\left[\frac{(Y_1-y)}{2Z^2\sqrt{D_y}}\right] - \text{erfc}\left[\frac{(Y_2-y)}{2Z^2\sqrt{D_y}}\right]\right\}$$

$$\cdot \left\{ \text{erfc}\left[\frac{(Z_1-z)}{2Z^2\sqrt{D_z}}\right] - \text{erfc}\left[\frac{(Z_2-z)}{2Z^2\sqrt{D_z}}\right]\right\} dZ. \quad (121b)$$

*Comments*:

The integral in equation 121b cannot be simplified further and must be evaluated numerically. A Gauss-Legendre numerical integration technique was used in the computer program written to evaluate the analytical solution and is described later. Round-off errors may still occur when evaluating the solution for very small values of x at late times.

Linear equilibrium adsorption and ion exchange can be simulated by dividing the coefficients $D_x$, $D_y$, $D_z$, and V by the retardation factor, R (eq. 15). Temporal variations in solute concentration and odd-shaped source configurations can be simulated through the principle of superposition. A solution where the patch source is located in the x-y plane at z=0 and velocity is in the x-direction can be found in Sagar (1982, p. 51).

## Description of program PATCHI

The program PATCHI computes the analytical solution to the three-dimensional solute-transport equation for an aquifer of infinite width and height with a finite-width and finite-height solute source at the inflow boundary. It consists of a main program and the subroutine CNRMLI. The functions of the main program and the subroutine are outlined below; the program code listing is presented in attachment 2.

The program also calls subroutines EXERFC and GLQPTS and the output subroutines TITLE, OFILE, and PLOT3D, which are common to most programs described in this report. These subroutines are described in detail later.

### Main program

The main program reads and prints all input data needed to specify model variables. The required input data and the format used in preparing a data file are shown in table 10.

The program next executes a set of four nested loops. The innermost loop calls subroutine CNRMLI to calculate the concentration at all specified y-coordinate values for a particular x-coordinate value, z-coordinate value, and time. The second loop cycles through all x-coordinate values. The third loop cycles through all z-coordinate values and prints a table of concentration in relation to x and y for each z value. The outer loop cycles through all specified time values. Model output can also be plotted as a series of maps showing lines of equal solute concentration in the horizontal (x-y) plane at each point along the z-axis.

### Subroutine CNRMLI

Subroutine CNRMLI calculates the normalized concentration ($C/C_o$) for a particular time value and distance. The integral in equation 121b is evaluated through a Gauss-Legendre numerical integration technique. The normalized roots of the Legendre polynomial and the corresponding weighting coefficients are passed by subroutine GLQPTS and scaled in the subroutine to account for the non-normalized limits of integration (from 0 to $t^{1/4}$ rather than from $-1$ to $+1$).

The number of terms summed in the numerical integration (equivalent to the order of the polynomial) is specified by the user. Roots of the Legendre polynomial of order 4, 20, 60, 104, and 256 are provided in data file GLQ.PTS. In general, the more terms used in the integration, the more accurate the approximation; however, this must be weighed against the corresponding increase in computational effort and time.

Table 10.—Input data format for the program PATCHI

| Data set | Columns | Format | Variable name | Description |
|---|---|---|---|---|
| 1 | 1 - 60 | A60 | TITLE | Data to be printed in a title box on the first page of program output. Last line in data set must have an "=" in column 1. First four lines are also used as titles for plot. |
| 2 | 1 - 4 | I4 | NX | Number of x-coordinates at which solution will be evaluated. |
|  | 5 - 8 | I4 | NY | Number of y-coordinates at which solution will be evaluated. |
|  | 9 - 12 | I4 | NZ | Number of z-coordinates at which solution will be evaluated. |
|  | 13 - 16 | I4 | NT | Number of time values at which solution will be evaluated. |
|  | 17 - 20 | I4 | NMAX | Number of terms to be used in numerical integration technique (must be equal to 4, 20, 60, 104, or 256). |
|  | 21 - 24 | I4 | IPLT | Plot control variable. Contours of normalized concentration will be plotted if IPLT is greater than 0. |
| 3 | 1 - 10 | A10 | CUNITS | Character variable used as label for units of concentration in program output. |
|  | 11 - 20 | A10 | VUNITS | Units of ground-water velocity. |
|  | 21 - 30 | A10 | DUNITS | Units of dispersion coefficient. |
|  | 31 - 40 | A10 | KUNITS | Units of solute-decay coefficient. |
|  | 41 - 50 | A10 | LUNITS | Units of length. |
|  | 51 - 60 | A10 | TUNITS | Units of time. |
| 4 | 1 - 10 | F10.0 | CO | Solute concentration at inflow boundary. |
|  | 11 - 20 | F10.0 | VX | Ground-water velocity in x-direction. |
|  | 21 - 30 | F10.0 | DX | Longitudinal dispersion coefficient. |
|  | 31 - 40 | F10.0 | DY | Transverse dispersion coefficient in y-direction. |
|  | 41 - 50 | F10.0 | DZ | Transverse dispersion coefficient in z-direction. |
|  | 51 - 60 | F10.0 | DK | First-order solute-decay coefficient. |
| 5 | 1 - 10 | F10.0 | Y1 | Y-coordinate of lower limit of finite width and height solute source. |
|  | 11 - 20 | F10.0 | Y2 | Y-coordinate of upper limit of finite width and height solute source. |
|  | 21 - 30 | F10.0 | Z1 | Z-coordinate of lower limit of finite width and height solute source. |
|  | 31 - 40 | F10.0 | Z2 | Z-coordinate of upper limit of finite width and height solute source. |
| 6 | 1 - 80 | 8F10.0 | X(I) | X-coordinates at which solution will be evaluated (eight values per line). |
| 7 | 1 - 80 | 8F10.0 | Y(I) | Y-coordinates at which solution will be evaluated (eight values per line). |
| 8 | 1 - 80 | 8F10.0 | Z(I) | Z-coordinates at which solution will be evaluated (eight values per line). |
| 9 | 1 - 80 | 8F10.0 | T(I) | Time values at which solution will be evaluated (eight values per line). |
| [1]10 | 1 - 10 | F10.0 | XSCLP | Scaling factor by which to divide x-coordinate values are divided to convert them to plotter inches. |
|  | 11 - 20 | F10.0 | YSCLP | Scaling factor used to convert y-coordinates into plotter inches. |
|  | 21 - 30 | F10.0 | DELTA | Contour increment for plot of normalized concentration (must be between 0.0 and 1.0). |

[1]Data line is needed only if IPLT (in data set 2) is greater than 0.

Additional discussions of the numerical integration technique are presented in a later section describing subroutine GLQPTS.

### Sample problem 11

In sample problem 11, a contaminant plume containing $^{90}$Sr (strontium-90) from a deep radioactive-waste storage facility migrates through a thick, confined aquifer. Model variables are

Source width ($W_s$)                              =1,200 ft
Source height ($H_s$)                             =  300 ft
Y-coordinate of lower limit of source ($Y_1$) =  900 ft
Y-coordinate of upper limit of source ($Y_2$) =2,100 ft
Z-coordinate of lower limit of source ($Z_1$) =1,350 ft
Z-coordinate of upper limit of source ($Z_2$) =1,650 ft
Ground-water velocity (V)                        =1 ft/d
Longitudinal dispersivity ($\alpha_l$)           =100 ft
Transverse dispersivity ($\alpha_t$)             = 20 ft
Source concentration ($C_o$)                     =100 mg/L
Half-life of $^{90}$Sr                           =28 years.

From these values, the terms obtained are

Coefficient of longitudinal
 dispersion ($D_x$)              =100 ft$^2$/d
Coefficients of transverse
 dispersion ($D_y$ and $D_z$)    = 20 ft$^2$/d
First-order solute-decay
 coefficient ($\lambda$)         =6.78$\times$10$^{-5}$ per day.

Concentrations are calculated at 150-ft intervals along the x-axis for 3,900 ft, and at 100-ft intervals along the y-axis for 2,600 ft. The $^{90}$Sr concentration distribution after 10 years (3,652.5 days) for z-coordinates of 1,650, 1,700, and 1,750 ft (z=0 at the base of the aquifer and z=1,650 at the top of the storage facility) is simulated.

The input data set for sample problem 11 is shown in figure 21*A*; computer-generated contour plots of the normalized concentration (C/C$_o$) in x-y planes defined by the three z-coordinates are shown in figure 21*B*. Program output for this sample problem is presented in attachment 4. Sample problem 11 required 3 min 20 s of CPU time on a Prime model 9955 Mod II.

# Description of Subroutines

The subroutines described in this section are common to most of the programs developed to evaluate the analytical solutions. Subroutines EXERFC and GLQPTS are used in evaluating terms in the analytical solutions, OFILE and TITLE are used in program input and output, and PLOT1D, PLOT2D, PLOT3D, and CNTOUR are used to graphically display program results. Subroutine listings are presented in attachment 3.

## Mathematical subroutines

### Subroutines EXERFC and GLQPTS

Subroutine EXERFC is called to evaluate the product of an exponential and complementary error function (exp[x]• erfc[y]), where the error function, erf(y), is defined as

$$\text{erf}(y) = \frac{2}{\sqrt{\pi}} \int_o^y \exp[-\epsilon^2] d\epsilon, \qquad (122)$$

and the complementary error function, erfc(y), is defined as

$$\text{erfc}(y) = 1.0 - \text{erf}(y). \qquad (123)$$

Often, the values of x and y are such that erfc(y) is very small (less than $1 \times 10^{-12}$ for y=5), whereas exp(x) is very large. To accurately calculate the product of the two functions, a high degree of accuracy is needed in the calculation of erfc(y). Subroutine EXERFC uses a rational Chebyshev approximation (Cody, 1969), accurate to between 10 and 13 significant figures, to calculate erf(y) or erfc(y). The two variables x and y are passed to the subroutine. To calculate only erfc(y), the routine EXERFC can be called with the value of x set to zero.

For absolute values of y less than 0.469, the rational Chebyshev approximation is given by

$$\text{erf}(y) = y \sum_{i=0}^{n} P1_i y^{2i} / \sum_{i=0}^{n} Q1_i y^{2i}, \qquad (124)$$

where P1 and Q1 are the coefficients of the rational approximation given by Cody (1969) for n=5. For negative values of y, the symmetry condition that erf(-y)=-erf(y) (Abramowitz and Stegun, 1964) is used. Erfc(y) is then given by equation 123.

For absolute values of y between 0.469 and 4.0, a rational approximation for erfc(y) is used, given by

$$\text{erfc}(y) = \exp[-y^2] \sum_{i=0}^{n} P2_i y^i / \sum_{i=0}^{n} Q2_i y^i, \qquad (125)$$

where P2 and Q2 are the coefficients given by Cody (1969) for n=8. For negative values of y, the identity that erfc(-y)=2-erfc(y) is used.

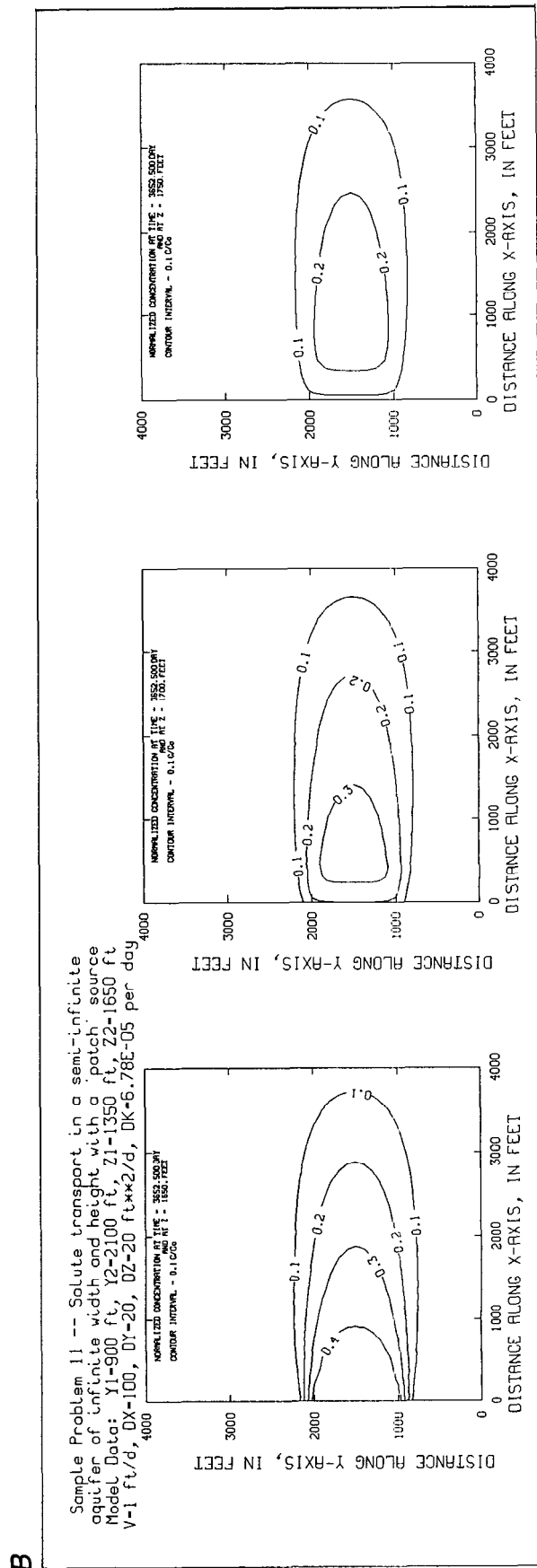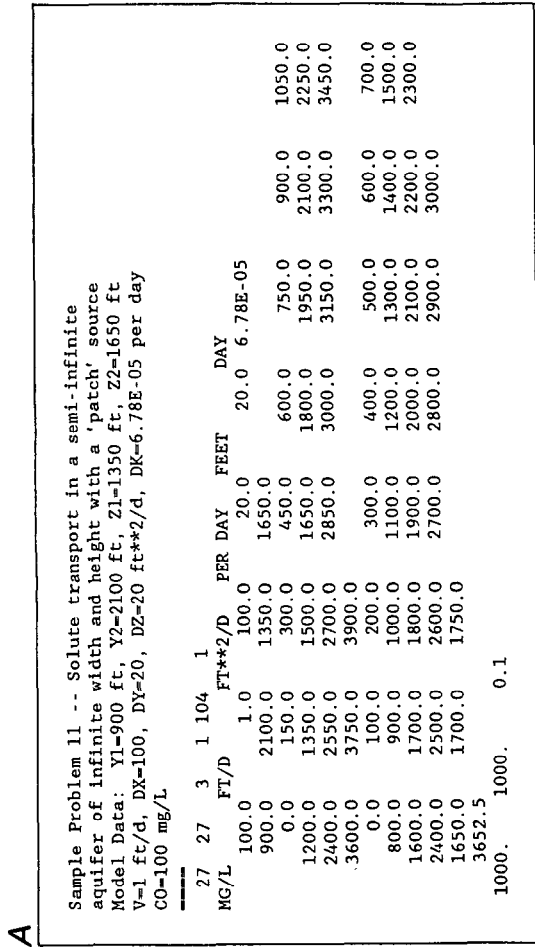For absolute values of y greater than 4.0, a second rational approximation for erfc(y) is used, given by

Figure 21.—(A) Sample input data set, and (B) normalized concentration contours generated by the program PATCHI for a solute subject to first-order chemical transformation in an aquifer of infinite height and width with a solute source of finite height and width after 3,652.5 days at heights of 1,650, 1,700, and 1,750 feet above base of the aquifer (sample problem 11).

$$\text{erfc}(y) = \frac{\exp[-y^2]}{y} \left\{ \frac{1}{\sqrt{\pi}} + \frac{1}{y^2} \sum_{i=0}^{n} P3_i y^{-2i} \Big/ \sum_{i=0}^{n} Q3_i y^{-2i} \right\}, \qquad (126)$$

where P3 and Q3 are coefficients given by Cody (1969) for n=5. When a product of exp(x) and erfc(y) is calculated, the arguments for the exponential in equations 125 and 126 are changed to $(x-y^2)$.

Subroutine GLQPTS is called to numerically evaluate the time integral found in several of the analytical solutions. The Gauss integration formula used is given by Abramowitz and Stegun (1964) as

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{n} w_i f(z_i), \qquad (127)$$

where

$z_i$ = roots of Legendre polynomial for a particular value of n, and

$w_i$ = corresponding weighting functions.

Positive roots of the Legendre polynomials for n=4, 20, 60, 104, and 256 and their weighting functions, as given in Cleary and Ungs (1978), have been tabulated and are read from a data file called GLQ.PTS. Subroutine GLQPTS calculates the negative roots and their weighting coefficients. These values are passed to the other subroutines through an array in common. A listing of file GLQ.PTS is presented in attachment 3.

As stated earlier, the accuracy of the numerical integration is increased if the user selects a larger value for n. However, computational effort is also increased. Checks can be made to determine whether a smaller value for n produces reasonable results by comparing the solution for a particular n with that obtained using the next higher value. Roots and weighting coefficients for additional values of n can be found in Abramowitz and Stegun (1964, p. 916–919).

.The subroutine is set up to read data file GLQ.PTS on logical unit 77 on the Prime system. For systems other than Prime, this routine should be modified to include the correct system-dependent file opening statements. Also, file-naming conventions for the particular system must be observed, and the data file renamed appropriately.

## Input/Output subroutines

### Subroutines OFILE and TITLE

Subroutine OFILE is used to open disk files for program input and output on the Prime computer system. It assigns logical unit 15 to the input data file and logical unit 16 to the file for program output. The user is queried at the terminal (logical unit 1) for the name of the appropriate disk files, and any file name up to 50 characters in length can be entered. For output to be sent directly to the terminal, the user should type an asterisk (*) in column 1 when asked for the output file name.

For systems other than the Prime, this routine should be modified to include the correct system-dependent file opening statements. Also, the logical units (1, 15, and 16) should be changed if they are not appropriate for the particular system.

Subroutine TITLE is called by all programs to print a title box on the first page of model output. Titles are supplied as the first lines of the input data set. Titles are automatically centered, and the routine closes the title box when it encounters an equal sign (=) in column 1 of a data line. The routine also prints the date and time the program execution began. The first four title lines are used as titles for plots.

Subroutine TITLE calls the Prime-supplied functions TIME\$A and DATE\$A found in the library VAPPLB. For non-Prime systems, these calls should be modified or, if similar functions are not available, deleted.

## Graphics subroutines

Four subroutines, PLOT1D, PLOT2D, PLOT3D, and CNTOUR, were developed to graphically display selected output from the programs described in this report. These subroutines contain calls for DISSPLA graphics software (Integrated Software Systems Corporation, 1981), and the DISSPLA library must be loaded when compiling the programs. Users who do not have access to DISSPLA software can easily modify the DISSPLA software calls to those appropriate to their own graphics software.

Subroutines PLOT1D, PLOT2D, and PLOT3D contain a call to COMPRS, which creates a META file that can be output, at a later time, to a wide variety of plotter devices through the DISSPLA postprocessor. This call can be replaced with a call to directly nominate a plotter device (such as a graphics terminal) so that plots can be drawn as the programs execute. The user should consult the DISSPLA users manual (Integrated Software Systems Corporation, 1981) for more information.

### Subroutines PLOT1D, PLOT2D, PLOT3D, and CNTOUR

Subroutine PLOT1D is called by the programs FINITE and SEMINF to create plots of the normalized concentration $C/C_0$ in relation to distance for each of the time values specified in the input data. An example of typical plotter output is shown in figure 4B. DISSPLA software calls are used to draw the axes and to plot the data points. The height of the plot is 12.5 in. The width is controlled by the difference

between the minimum and maximum x-coordinate value and by the scale factor XSCLP specified in data set 4 (tables 1, 2). If no plotter is available, the user can either specify a value of 0 for IPLT in data set 2 (tables 1, 2) or delete the call to PLOT1D in the main programs of FINITE and SEMINF.

Subroutine PLOT2D is called by the programs POINT2, STRIPF, STRIPI, and GAUSS to initialize a plot of lines of equal normalized concentration (C/C$_o$) in the x-y plane for each of the specified time values. A typical example is shown in figure 13B.

The size of each subplot depends on the difference between the maximum and minimum x- and y-coordinate values and the plot scaling factors XSCLP and YSCLP specified by the user in data set 9 (tables 3–5). The overall length of the plot is determined by the number of time values specified. The contour increment DELTA (a value between 0.0 and 1.0) is specified by the user in data set 9.

Subroutine PLOT2D defines the plot and subplot sizes, draws and labels the axes, and then calls subroutine CNTOUR, which draws and labels the contours. If no plotter is available, IPLT in data set 2 (tables 3–6) can be set to 0, or the call to PLOT2D in the main programs STRIPF, STRIPI, and GAUSS can be deleted.

Subroutine PLOT3D is called by the programs POINT3, PATCHF, and PATCHI to initialize a plot of lines of equal normalized concentration (C/C$_o$) in the x-y plane for each of the z-coordinates and time values specified in the input data. An example of plotter output from this subroutine is shown in figure 20B.

The size of each subplot depends on the difference between the maximum and minimum x- and y-coordinates and the plot scaling factors XSCLP and YSCLP specified by the user in data set 10 (tables 8–10). The overall length of the plot is determined by the number of z-values specified. Separate plots are drawn for each specified time value. The contour increment DELTA (a value between 0.0 and 1.0) can also be specified by the user, in data set 10.

Subroutine PLOT3D defines the plot and subplot sizes, draws and labels the axes, and then calls subroutine CNTOUR, which draws and labels the contours. If no plotter is available, IPLT in data set 2 (tables 8–10) can be set to zero, or the call to PLOT3D in the main programs of POINT3, PATCHF, and PATCHI can be deleted.

Subroutine CNTOUR is called to produce simplified plots of lines of equal normalized concentration (C/C$_o$) in the x-y plane for each of the time values or z-coordinates specified in the input data. Although there are many software packages that contour gridded data, such as concentration in relation to x and y, some of these require the grid to be equally spaced

and others, such as that contained in DISSPLA, can interpolate scattered data onto regular grids, but at the cost of considerable computational effort and time.

The subroutine first creates a rectangular grid based on the x- and y-coordinates supplied in the input data. Each rectangular block in the grid is then subdivided into two triangles defined by a diagonal drawn across the block. Next, contour segments are drawn by connecting points of equal concentration determined by linear interpolation along the axes of each triangular element.

The number of contours drawn is determined by the difference between the maximum and minimum normalized concentration values and the contour increment, DELTA. The subroutine uses a relatively complex algorithm to connect the contour segments defining a contour line and to determine whether a contour line has exited the grid or formed a closed loop. Contour lines are labeled after all NUM contour segments are drawn. NUM is set to 40 in the code, but this can be changed by the user. The routine requires three work arrays—XPC, YPC, and IFLAG—to store contouring data. IFLAG must be dimensioned to twice the number of rectangular blocks. XPC and YPC are dimensioned by 50 in the subroutine and in common block PDAT in the main programs. This number must be changed if the user increases the value of NUM to greater than 50.

## Running the programs

### Array dimensions

Dimensions of arrays used by the programs are set by a PARAMETER statement, as follows:

PARAMETER (MAXX=100, MAXY=50, MAXZ =30, MAXT=20, MAXXY=5000, MAXXY2=10000, MAXRT=1000)

where
    MAXX =maximum number of x-coordinates,
    MAXY =maximum number of y-coordinates,
    MAXZ =maximum number of z-coordinates,
    MAXT =maximum number of time values,
  MAXXY =product of MAXX and MAXY,
MAXXY2 =twice MAXXY, and
  MAXRT =maximum number of roots used in series summation in program FINITE.

The user can modify the PARAMETER statement to increase or decrease these limits.

### Compiling and loading

The following describes the procedure for compiling and running the programs on the Prime system. For convenience, the user should first create a single file

called SUBS.F77 that contains the following subroutines: EXERFC, GLQPTS, OFILE, TITLE, PLOT1D, PLOT2D, PLOT3D, AND CNTOUR. The user should then type

```
F77 PROGRAM.F77 -BIG -SILENT
F77 SUBS.F77 -BIG -SILENT
SEG -LOAD
LOAD PROGRAM
LOAD SUBS
LIBRARY DISSPLA
LIBRARY VAPPLB
LI
SAVE
QUIT
```

where PROGRAM indicates the name of the main program (for example, STRIPF or GAUSS). After the message "LOAD COMPLETE" is received at the terminal, the user can run the program by typing

SEG PROGRAM

The following message will appear

"TYPE IN INPUT FILE NAME"

The user can respond with the name of the file containing the data set (see description of subroutine OFILE). The following will then appear:

"TYPE IN OUTPUT FILE NAME"

The user can respond with the name of the output file name or an asterisk (*) to cause output to come to the terminal.

These programs can be run on other computer systems, although some device-dependent subroutine calls may have to be modified. These statements are identified in the previous section.

# Summary

The physical, chemical, and biological processes that govern transport of solutes in ground water can be described quantitatively by the advective-dispersive solute-transport equation. Analytical solutions, which are exact mathematical solutions for this partial differential equation, have been derived for many combinations of aquifer geometry, solute-source configurations, and boundary and initial conditions. These solutions can be used to mathematically model the movement of solutes in homogeneous aquifers having simple flow systems in which the chemical and biological processes can be described by linear relations.

This report presents analytical solutions for solute transport in one-, two-, and three-dimensional systems having uniform flow. The solutions were compiled from those published in various journals and reports or were derived by the author. The solutions for one-dimensional solute transport are for (1) a finite-length system with a first-type boundary condition at the inflow end, (2) a finite-length system with a third-type boundary condition at the inflow end, (3) a semi-infinite system with a first-type boundary condition at the inflow end, and (4) a semi-infinite system with a third-type boundary condition at the inflow end. Solutions for the finite-length system assume a second-type boundary condition at the outflow end.

Solutions for two-dimensional solute transport were presented for (1) an aquifer of infinite areal extent with a continuous point source at which fluid is injected at a constant rate and concentration, (2) a semi-infinite aquifer of finite width with a strip source along the inflow boundary, (3) a semi-infinite aquifer of infinite width with a strip source along the inflow boundary, and (4) a semi-infinite aquifer of infinite width with a solute source having a gaussian concentration distribution. Solutions for three-dimensional solute transport were presented for (1) an aquifer of infinite extent with a continuous point source, (2) a semi-infinite aquifer of finite height and width with a patch source along the inflow boundary, and (3) a semi-infinite aquifer of infinite width and height with a patch source along the inflow boundary. All the solutions presented can account for first-order solute decay due to chemical or biological processes and linear equilibrium adsorption.

A set of computer programs was written to evaluate these solutions and to produce tables and graphs of solute concentration as a function of time and distance from the solute source. Documentation of these programs includes instruction on their use, description of input data format, sample problems, and sample data sets. Source codes for the programs and output for the sample problems are presented in attachments to the report.

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