



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

Finite system with third-type source boundary condition

Governing equation

One-dimensional solute-transport equation:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} - \lambda C \quad (48)$$

Boundary conditions:

$$VC_o = VC - D \frac{\partial C}{\partial x}, \quad x=0 \quad (49)$$

$$\frac{\partial C}{\partial x} = 0, \quad x=L \quad (50)$$

Initial condition:

$$C=0, \quad 0 < x < L \quad \text{at } t=0 \quad (51)$$

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 longitudinal dispersion coefficient (D), which is equivalent to D_x (eq. 7), is constant.

Analytical solution

The solution to equation 48 was first presented by Selim and Mansell (1976). The following equation is modified from a form presented in van Genuchten and Alves (1982, p. 66-67):

$$C(x,t) = C_o \left\{ \frac{\exp\left[\frac{(V-U)x}{2D}\right] + \frac{(U-V)}{(U+V)} \exp\left[\frac{(V+U)x}{2D} - \frac{UL}{D}\right]}{\left[\frac{(U+V)}{2V} - \frac{(U-V)^2}{2V(U+V)} \exp\left(-\frac{UL}{D}\right)\right]} \right.$$

$$\left. - 2 \frac{VL}{D} \exp\left[\frac{Vx}{2D} - \frac{V^2t}{4D} - \lambda t\right] \right\}$$

$$\cdot \sum_{i=1}^{\infty} \frac{\beta_i \left[\beta_i \cos\left(\frac{\beta_i x}{L}\right) + \left(\frac{VL}{2D}\right) \sin\left(\frac{\beta_i x}{L}\right) \right]}{\left[\beta_i^2 + \left(\frac{VL}{2D}\right)^2 + \frac{VL}{D} \right]}$$

$$\cdot \frac{\exp\left[-\frac{\beta_i^2 Dt}{L^2}\right]}{\left[\beta_i^2 + \left(\frac{VL}{2D}\right)^2 + \frac{VL}{D} \right]} \quad (52)$$

where $U = \sqrt{V^2 + 4\lambda D}$ and β_i are the roots of the equation

$$\beta \cot \beta - \frac{\beta^2 D}{VL} + \frac{VL}{4D} = 0. \quad (53)$$

For a solute that is not subject to first-order chemical transformation ($\lambda=0$), equation 52 can be simplified (Gershon and Nir, 1969, p. 837; van Genuchten and Alves, 1982, p. 13) as

$$C(x,t) = C_o \left\{ 1 - 2 \frac{VL}{D} \exp\left[\frac{Vx}{2D} - \frac{V^2t}{4D}\right] \right.$$

$$\cdot \sum_{i=1}^{\infty} \frac{\beta_i \left[\beta_i \cos\left(\frac{\beta_i x}{L}\right) + \left(\frac{VL}{2D}\right) \sin\left(\frac{\beta_i x}{L}\right) \right]}{\left[\beta_i^2 + \left(\frac{VL}{2D}\right)^2 + \frac{VL}{D} \right]}$$

$$\left. \cdot \frac{\exp\left[-\frac{\beta_i^2 Dt}{L^2}\right]}{\left[\beta_i^2 + \left(\frac{VL}{2D}\right)^2 + \frac{VL}{D} \right]} \right\}. \quad (54)$$

For large values of time (steady-state solution), equation 52 can be reduced (van Genuchten and Alves, 1982, p. 59) to

$$C(x) = C_o \left\{ \frac{\exp\left[\frac{(V-U)x}{2D}\right] + \frac{(U-V)}{(U+V)} \exp\left[\left(\frac{(V+U)x}{2D}\right) - \frac{UL}{D}\right]}{\left[\frac{(U+V)}{2V} - \frac{(U-V)^2}{2V(U+V)} \exp\left[-\frac{UL}{D}\right]\right]} \right\}. \quad (55)$$

Comments:

The roots of equation 53 can be found by standard root-search techniques. An iterative technique using Newton's second-order correction method was described in the preceding section.

Linear equilibrium adsorption and ion exchange can be simulated by first dividing the coefficients D and V by the retardation factor, R (eq. 15). (Note: U in eqs. 52 and 55 would be given by $U = \sqrt{V^* + 4\lambda D^*}$). Tempo-

ral variations in source concentration can be simulated through the principle of superposition (eq. 39).

Description of program FINITE

The analytical solution to the one-dimensional solute-transport equation for a finite system with a third-type (or first-type) source boundary condition at the inflow end is computed by the program FINITE, described in detail in the preceding section. 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 1.

The main program then calls subroutine ROOT3 to compute the positive roots of equation 53 when a third-type source boundary condition is specified, and executes a set of nested loops. The inner loop calls subroutine CNRML3 to calculate the concentration for a particular time value and distance; the outer loop cycles through all specified time values and prints a table of concentration in relation to distance for each time value. Graphs of concentration in relation to distance can also be plotted.

Subroutines ROOT3 and CNRML3

Subroutine ROOT3 calculates the roots of the equation $a \cdot \cot(a) - b \cdot a^2 + c = 0$. The procedure followed is similar to that for subroutine ROOT1 (described in the preceding section), with $\pi/2$ as an initial estimate for the first root.

Subroutine CNRML3 calculates the normalized concentration (C/C_0) for a particular time value and distance value, using equation 52 for a solute subject to first-order chemical transformation and equation 54 if the solute is conservative ($\lambda=0$). The number of terms taken in the infinite series summation is specified in the input data.

Sample problem 2

In sample problem 2, the solute introduced into the soil column is assumed to be conservative. Model variables are identical to those in sample problem 1a and are

Velocity (V)	=0.6 in/h
Longitudinal dispersion (D)	=0.6 in ² /h
System length (L)	=12 in
Solute concentration opposite inflow boundary (C_0)	=1.0 mg/L.

Concentrations are calculated for points 0.5 in apart at elapsed times of 2.5, 5, 10, 15, and 20 hours.

The input data set for sample problem 2 is shown in figure 6A; a computer plot of concentration profiles generated by the program FINITE is shown in figure 6B. Output for this sample problem is presented in

attachment 4. Sample problem 2 required 4.3 s of CPU time on a Prime model 9955 Mod II.

Comparison of figures 4B and 6B shows that the principal difference between the solutions for a first-type and a third-type source boundary condition is reflected in the solute concentrations near the inflow boundary at early times. As mentioned previously, these differences decrease with decreasing values for the quantity D/V .

Semi-infinite system with first-type source boundary condition

Governing equation

One-dimensional solute-transport equation:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} - \lambda C \quad (56)$$

Boundary conditions:

$$C = C_0, \quad x = 0 \quad (57)$$

$$C, \frac{\partial C}{\partial x} = 0, \quad x = \infty \quad (58)$$

Initial condition:

$$C = 0, \quad 0 < x < \infty \quad \text{at } t = 0 \quad (59)$$

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 longitudinal dispersion coefficient (D), which is equivalent to D_x (eq. 7), is constant.

Analytical solution

The following equation was modified from Bear (1972, p. 630) and van Genuchten and Alves (1982, p. 60):

$$C(x,t) = \frac{C_0}{2} \left\{ \exp \left[\frac{x}{2D}(V-U) \right] \cdot \operatorname{erfc} \left[\frac{x-Ut}{2\sqrt{Dt}} \right] + \exp \left[\frac{x}{2D}(V+U) \right] \cdot \operatorname{erfc} \left[\frac{x+Ut}{2\sqrt{Dt}} \right] \right\}, \quad (60)$$

where

$$U = \sqrt{V^2 + 4\lambda D}.$$

The analytical solution for a solute not subject to first-order chemical transformation ($\lambda=0$) was derived by Ogata and Banks (1961) as

A

Sample Problem 2 -- Solute transport in a finite-length soil column with a third-type boundary condition at $x=0$
 Model Parameters: $L=12$ in, $V=0.6$ in/h, $D=0.6$ in²/h
 $K1=0.0$ per h, $C0=1.0$ mg/L

3	25	05	50	1					
MG/L	IN/H	IN**2/H	PER HOUR	INCHES	HOURS				
1.0	0.6	0.6	0.6	0.0	12.0	1.2			
0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5		
4.0	4.5	5.0	5.5	6.0	6.5	7.0	7.5		
8.0	8.5	9.0	9.5	10.0	10.5	11.0	11.5		
12.0									
2.5	5.0	10.0	15.0	20.0					

B

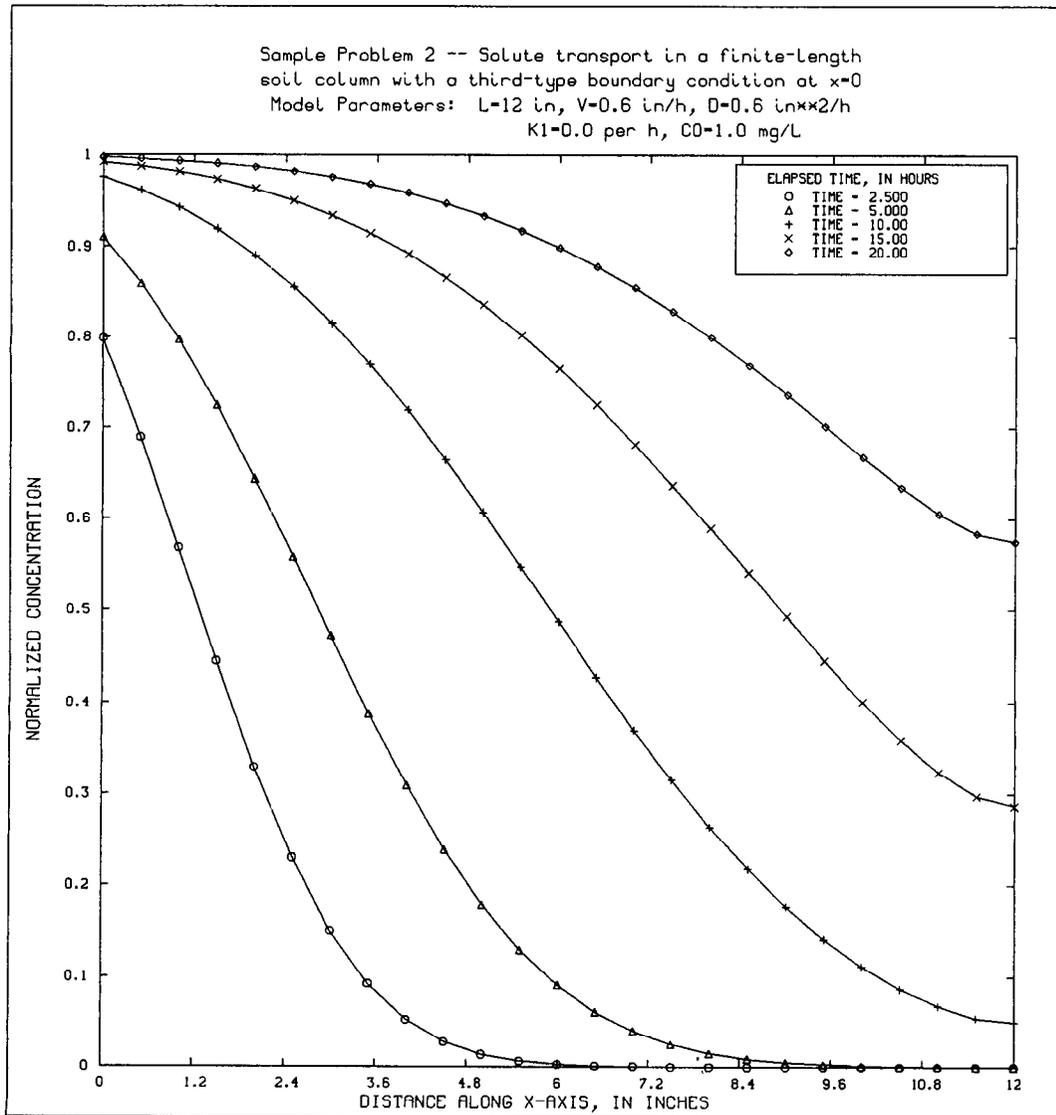


Figure 6.—(A) Sample input data set, and (B) concentration profiles generated by the program FINITE for a conservative solute in a finite-length system with third-type source boundary condition after 2.5, 5, 10, 15, and 20 hours (sample problem 2).

$$C(x,t) = \frac{C_0}{2} \left\{ \operatorname{erfc} \left[\frac{x-Vt}{2\sqrt{Dt}} \right] + \exp \left[\frac{xV}{D} \right] \cdot \operatorname{erfc} \left[\frac{x+Vt}{2\sqrt{Dt}} \right] \right\}. \quad (61)$$

For large values of time (steady-state solution), equation 60 reduces (modified from Bear, 1972, p. 631) to

$$C(x) = C_0 \exp \left[\frac{x}{2D} (V-U) \right]. \quad (62)$$

Comments:

Equations 60 and 61 are presented in this form to utilize computer routines that accurately compute the product of an exponential term ($\exp [x]$) and the complementary error function (denoted as $\operatorname{erfc} [y]$).

Linear equilibrium adsorption and ion exchange can be simulated by first dividing the coefficients D and V by the retardation factor, R (eq. 15). (Note: U in eqs. 60 and 62 would be given by $U = \sqrt{V^* + 4\lambda D^*}$). Temporal variations in source concentration can be simulated through the principle of superposition (eq. 39).

Description of program SEMINF

The program SEMINF computes the analytical solution to the one-dimensional solute-transport equation for a semi-infinite system with a first-type or third-type source boundary condition at the inflow end. It consists of a main program and two subroutines—CNRML1 and CNRML3. The function of the main program and subroutine CNRML1 are outlined below; the program code listing is presented in attachment 2. Subroutine CNRML3, called when a third-type boundary condition is specified, is described in a subsequent section.

The program also calls the subroutine EXERFC and the output subroutines TITLE, OFILE, and PLOT1D, 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 2.

The program next executes a set of nested loops. The inner loop calls subroutine CNRML1 to calculate the concentration for a particular time value and distance. The outer loop cycles through all specified time values and prints a table of concentration in relation to distance for each time value. Graphs of concentration in relation to distance can also be plotted.

Subroutine CNRML1

Subroutine CNRML1 calculates the normalized concentration (C/C_0) for a particular time value and distance, using equation 60 for a solute subject to first-order chemical transformation and equation 61 if the solute is conservative ($\lambda=0$).

Sample problems 3a and 3b

Two sample problems are presented. In sample problem 3a, a conservative solute is introduced into a long soil column. The system is idealized as being semi-infinite in length, with model variables as

Velocity (V)	=0.6 in/h
Longitudinal dispersion (D)	=0.6 in ² /h
Solute concentration at inflow boundary (C_0)	=1.0 mg/L.

Concentrations are calculated for points 0.5 in apart at elapsed times of 2.5, 5, 10, 15, and 20 hours.

In sample problem 3b, solute is removed by both first-order solute decay and linear equilibrium adsorption. Additional model variables are

Solute half-life ($T_{1/2}$)	=7.6 days
Soil bulk density (ρ_b)	=0.047 lb(mass)/in ³
Porosity (n)	=0.45
Slope of adsorption isotherm (k)	=70 in ³ /lb (mass).

From these values, the following terms are obtained using equations 15 and 25:

Decay constant (λ)	=0.0038 per hour
Retardation factor (R)	=8.31
Scaled velocity (V^*)	=0.072 in/h
Scaled dispersion coefficient (D^*)	=0.072 in ² /h.

Concentrations are calculated for points 0.5 in apart at elapsed times of 20, 50, 100, and 150 hours.

Input data sets for sample problems 3a and 3b are shown in figures 7A and 8A; computer plots of concentration profiles generated by the program SEMINF are also shown. Output for sample problem 3a is presented in attachment 4. Sample problems 3a and 3b each required 3 s of CPU time on a Prime model 9955 Mod II.

Comparison of the concentration profiles at 20 hours in each plot (figs. 7B and 8B) shows the effect of both solute decay and adsorption on solute movement. Comparison of figures 7B and 4B shows the difference in concentration profiles that would result if the solution for a semi-infinite system were used to simulate transport in a finite system. The most significant difference is the lower solute concentrations and the

Table 2.—Input data format for the program SEMINF

Data set	Columns	Format	Variable name	Description
1	1 - 60	A60	TITLE	Data to be printed in a title box on 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	NBC	Boundary condition type (NBC = 1 for first-type boundary condition; NBC = 3 for third-type boundary condition).
	5 - 8	I4	NX	Number of x-coordinates at which solution will be evaluated.
	9 - 12	I4	NT	Number of time values at which solution will be evaluated.
	13 - 16	I4	IPLT	Plot control variable. Concentration profiles 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. ¹
	21 - 30	F10.0	DX	Longitudinal dispersion coefficient. ¹
	31 - 40	F10.0	DK	First-order solute decay coefficient. ¹
	41 - 50	F10.0	XSCLP	Scaling factor by which x-coordinate values are divided to convert them to plotter inches.
5	1 - 80	8F10.0	X(I)	X-coordinates at which solution will be evaluated (eight values per line).
6	1 - 80	8F10.0	T(I)	Time values at which solution will be evaluated (eight values per line).

¹All units must be consistent.

steeper gradients near $x=12.0$ in (fig. 7B). As mentioned previously, differences between the two solutions decrease with increased column Peclet number (P) and lower values for the number of displaced pore volumes (T).

Semi-infinite system with third-type source boundary condition

Governing equation

One-dimensional solute-transport equation:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} - \lambda C \quad (63)$$

Boundary conditions:

$$VC_0 = VC + D \frac{\partial C}{\partial x}, \quad x=0 \quad (64)$$

$$C, \frac{\partial C}{\partial x} = 0, \quad x = \infty \quad (65)$$

Initial condition:

$$C=0, \quad 0 < x < \infty \quad \text{at } t=0 \quad (66)$$

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 longitudinal dispersion coefficient (D), which is equivalent to D_x (eq. 7), is constant.

Analytical solution

The following equation is modified from Cleary and Ungs (1978, p. 10):

A

Sample Problem 3a -- Solute transport in a semi-infinite soil column with a first-type boundary condition at $x=0$
 Model Parameters: $V=0.6$ in/h, $D=0.6$ in²/h
 $K1=0.0$ per h, $C0=1.0$ mg/L

```

=====
      1 25 05 1
    MG/L  IN/H  IN**2/H  PER HOUR  INCHES  HOURS
      1.0   0.6   0.6     0.6     0.0     1.2
      0.0   0.5   1.0     1.0     1.5     2.0
      4.0   4.5   5.0     5.5     6.0     6.5
      8.0   8.5   9.0     9.5    10.0    10.5
      12.0  2.5   5.0    10.0    15.0    20.0
    
```

B

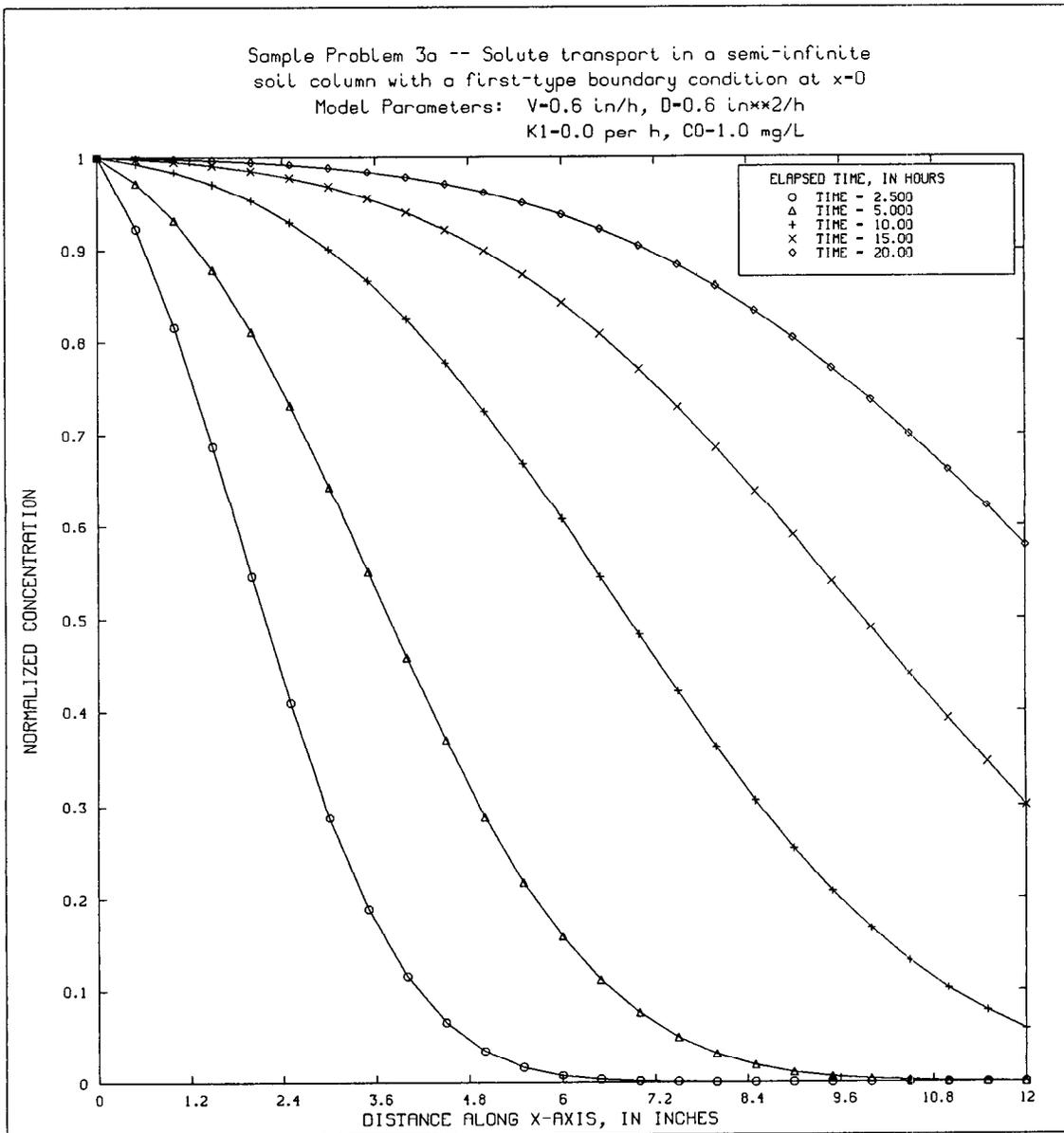


Figure 7.—(A) Sample input data set, and (B) concentration profiles generated by the program SEMINF for a conservative solute in a semi-infinite system with first-type source boundary condition after 2.5, 5, 10, 15, and 20 hours (sample problem 3a).

A

Sample Problem 3b -- Solute transport in a semi-infinite soil column with a first-type boundary condition at $x=0$
 Model Parameters: $V=0.072$ in/h, $D=0.072$ in²/h
 $K_1=0.0038$ per h, $C_0=1.0$ mg/L
 Solute is subject to first-order decay and linear adsorption

MG/L	IN/H	IN**2/H	PER HOUR	INCHES	HOURS				
1	0.072	0.072	0.0038	1.2	1.2				
25	0.5	1.0	1.5	2.0	2.5	3.0	3.5		
04	4.0	5.0	5.5	6.0	6.5	7.0	7.5		
1	8.0	9.0	9.5	10.0	10.5	11.0	11.5		
	12.0								
	20.0	50.0	100.0	150.0					

B

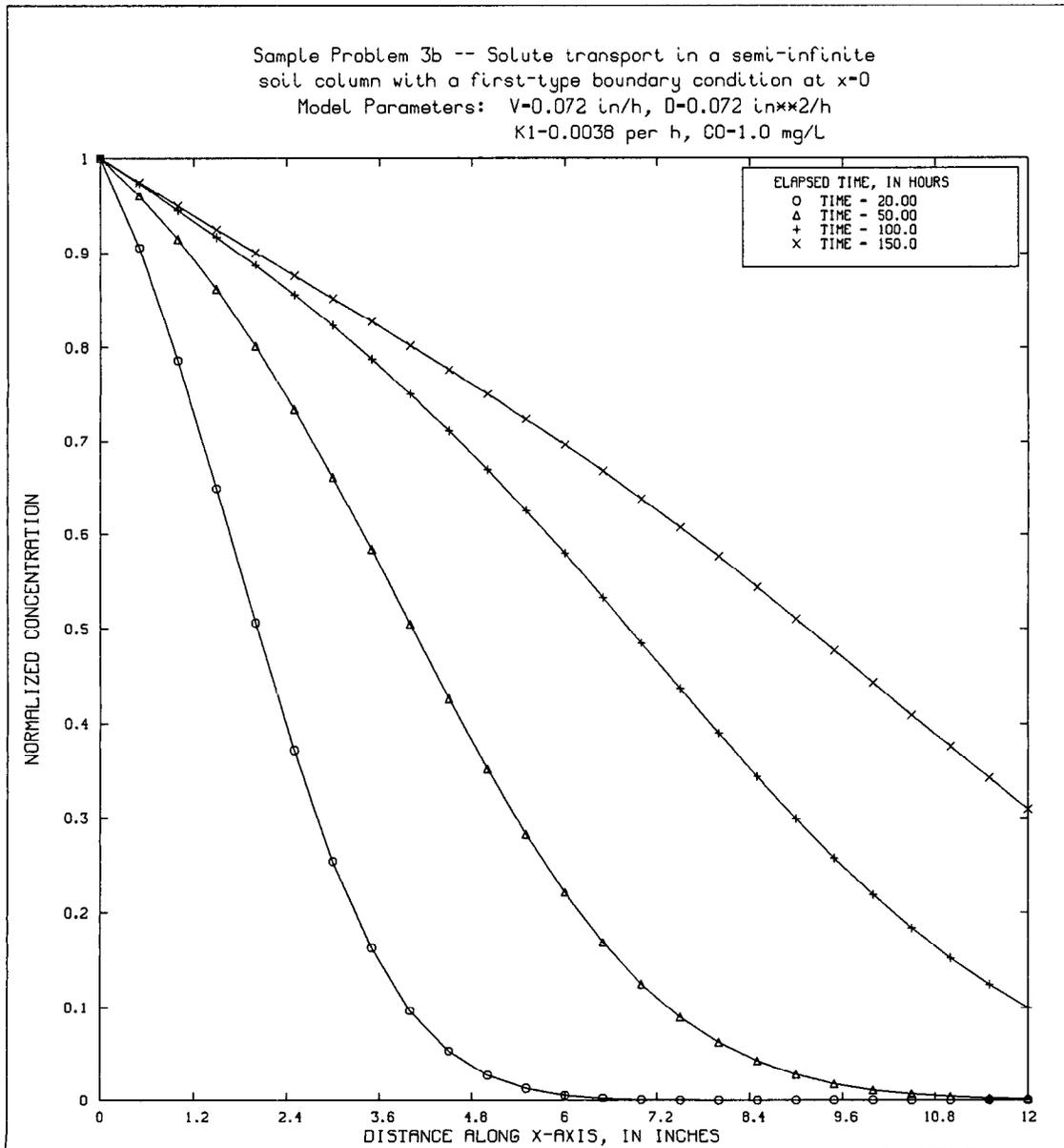


Figure 8.—(A) Sample input data set, and (B) concentration profiles generated by the program SEMINF for a solute subject to first-order decay and linear equilibrium adsorption in a semi-infinite system with first-type source boundary condition after 20, 50, 100, and 150 hours (sample problem 3b).

$$C(x,t) = \frac{C_o V^2}{4\lambda D} \left\{ 2 \exp\left[\frac{xV}{D} - \lambda t\right] \cdot \operatorname{erfc}\left[\frac{x+Vt}{2\sqrt{Dt}}\right] + \left(\frac{U}{V} - 1\right) \exp\left[\frac{x}{2D}(V-U)\right] \cdot \operatorname{erfc}\left[\frac{x-Ut}{2\sqrt{Dt}}\right] - \left(\frac{U}{V} + 1\right) \exp\left[\frac{x}{2D}(V+U)\right] \cdot \operatorname{erfc}\left[\frac{x+Ut}{2\sqrt{Dt}}\right] \right\}, \quad (67)$$

where

$$U = \sqrt{V^2 + 4\lambda D}.$$

For a conservative solute ($\lambda=0$), the solution to equation 63 is given by Lindstrom and others (1967) and van Genuchten and Alves (1982, p. 10) as

$$C(x,t) = C_o \left\{ \frac{1}{2} \operatorname{erfc}\left[\frac{x-Vt}{2\sqrt{Dt}}\right] + \sqrt{\frac{V^2 t}{\pi D}} \exp\left[-\frac{(x-Vt)^2}{4Dt}\right] - \frac{1}{2} \left[1 + \frac{Vx}{D} + \frac{V^2 t}{D} \right] \exp\left(\frac{Vx}{D}\right) \cdot \operatorname{erfc}\left[\frac{x+Vt}{2\sqrt{Dt}}\right] \right\}. \quad (68)$$

For large values of time (steady-state solution), equation 67 can be reduced (Gershon and Nir, 1969, p. 837) to

$$C(x) = C_o \frac{2V}{(V+U)} \cdot \exp\left[\frac{x}{2D}(V-U)\right]. \quad (69)$$

Comments:

Equations 67 and 68 are presented in this form to utilize computer routines that compute the product of an exponential term and the complementary error function. For extremely small values of λ , calculations of concentration values using equation 67 may be subject to round-off errors as both the denominator in the first term and the terms within the bracket approach zero.

Linear equilibrium adsorption can be simulated by dividing the coefficients D and V by the retardation factor, R (eq. 15). Temporal variations in source concentration can be simulated through the principle of superposition (eq. 39).

Description of program SEMINF

The analytical solution to the one-dimensional solute-transport equation for a semi-infinite system with a third-type (or first-type) source boundary condition is computed by the program SEMINF, described in detail in the preceding section. 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 2.

The program next executes a set of nested loops. The inner loop calls subroutine CNRML3 to calculate the concentration for a particular time value and distance. The outer loop cycles through all specified time values and prints a table of concentration in relation to distance for each time value. Graphs of concentration in relation to distance can also be plotted.

Subroutine CNRML3

Subroutine CNRML3 calculates the normalized concentration (C/C_o) for a particular time value and distance, using equation 67 for a solute subject to first-order chemical transformation and equation 68 if the solute is conservative ($\lambda=0$).

Sample problem 4

In sample problem 4, a conservative solute is introduced into a long soil column. The system is idealized as being semi-infinite in length, with model variables as

Velocity (V)	= 0.6 in/h
Longitudinal dispersion (D)	= 0.6 in ² /h
Solute concentration opposite inflow boundary (C_o)	= 1.0 mg/L.

Concentrations are calculated for points spaced 0.5 in apart at elapsed times of 2.5, 5, 10, 15, and 20 hours.

The input data set for sample problem 4 is shown in figure 9A; a computer plot of concentration profiles generated by the program SEMINF is shown in figure 9B. Because of the third-type boundary condition, solute concentration computed near $x=0$ at early times differs from C_o .

Program output for this sample problem is presented in attachment 4. Sample problem 4 required 3.6 s of CPU time on a Prime model 9955 Mod II.

Two-Dimensional Solute Transport

Several analytical solutions are available for the two-dimensional form of the solute-transport equation (eq. 10). These solutions can be used to simulate transport of contaminants from sources within relatively thin aquifers, provided the solute is generally well mixed throughout the thickness of the aquifer and vertical concentration gradients are negligible. Transport of contaminants within a vertical section along the centerline of a contaminant plume in a thick

A

Sample Problem 4 -- Solute transport in a semi-infinite soil column with a third-type boundary condition at $x=0$
 Model Parameters: $V=0.6$ in/h, $D=0.6$ in²/h
 $K1=0.0$ per h, $C0=1.0$ mg/L

3	25	05	1						
MG/L	IN/H	IN**2/H	PER HOUR	INCHES	HOURS				
1.0	0.6	0.6	0.6	0.0	1.2				
0.0	0.5	1.0	1.0	1.5	2.0	2.5	3.0	3.5	
4.0	4.5	5.0	5.5	6.0	6.5	7.0	7.5		
8.0	8.5	9.0	9.5	10.0	10.5	11.0	11.5		
12.0									
2.5	5.0	10.0	15.0	20.0					

B

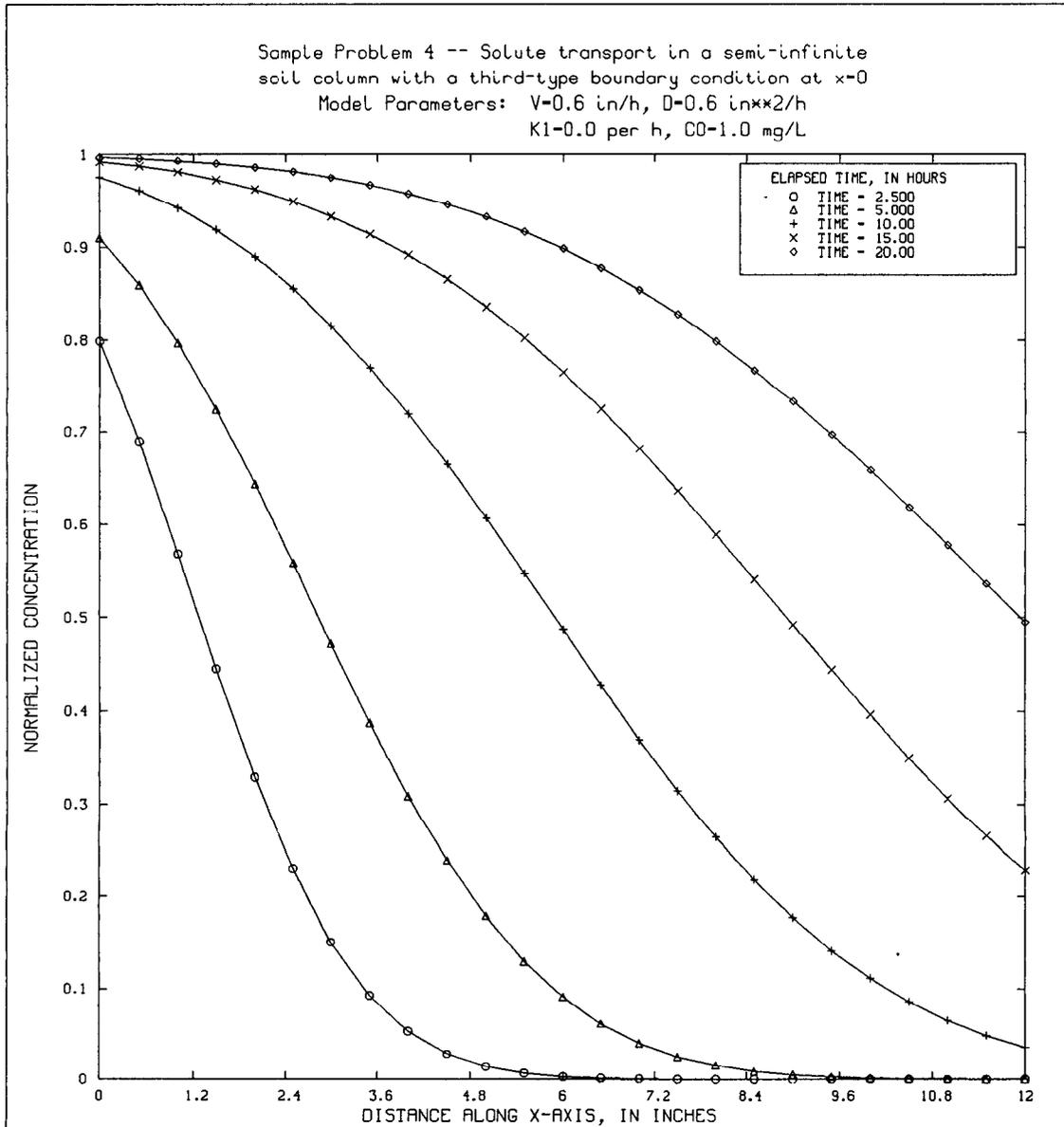


Figure 9. — (A) Sample input data set, and (B) concentration profiles generated by the program SEMINF for a conservative solute in a semi-infinite system with third-type source boundary condition after 2.5, 5, 10, 15, and 20 hours (sample problem 4).

aquifer can be simulated with these solutions if the solute source is wide enough that horizontal concentration gradients, which cause solute movement perpendicular to the centerline, are negligible.

In the first solution presented, the aquifer is assumed to be of infinite areal extent and to have a continuous point source in the x, y plane (equivalent to a line source extending the entire thickness of the aquifer). Fluid having a known solute concentration is injected into the aquifer at a constant rate. It is further assumed that the injection rate is small, and that the uniform flowfield around the well is not disturbed. Solutions in which radial flow away from an injection well is considered are discussed by Hseih (1986). A solution for an areal source where solute enters the aquifer at a known flux and concentration is given by Codell and others (1982).

For the remaining solutions presented in this section, aquifers are assumed to be of semi-infinite length and to have a solute source at the inflow boundary (at $x=0$). The width of the aquifer can be treated as being finite or infinite in extent. In an infinite-width system, impermeable boundaries at the edges of the aquifer are presumed to be far enough away as to have a negligible effect on solute distribution within the area of interest. Idealized diagrams of both types of systems are shown in figure 10.

One type of source configuration, referred to as a "strip" source (Cleary and Ungs, 1978), has a finite width extending from $y=Y_1$ to $y=Y_2$ at $x=0$ (fig. 10). The concentration within the strip is uniform and equal to C_0 . At the boundary of the strip source (at $y=Y_1$ or $y=Y_2$), the concentration is equal to $0.5 C_0$. Elsewhere along the inflow boundary, the concentration is zero. Combinations of strip sources could be used to simulate odd-shaped concentration distributions or multiple sources through use of the principle of superposition, as previously described.

A solute source can also have a "gaussian" concentration distribution (Cleary and Ungs, 1978, p. 80) given by

$$C = C_m \exp\left[-\frac{(y - Y_c)^2}{2\sigma^2}\right], \quad x=0, \quad (70)$$

where

C_m = maximum concentration at center of gaussian concentration distribution,

Y_c = y -coordinate of center of solute source ($X_c=0$), and

σ = standard deviation of the gaussian distribution.

A field situation in which a gaussian distribution can be found is shown in figure 11. The solute concentration at the waste-disposal pond is unknown, but a line of monitoring wells downgradient from the site and

normal to the direction of flow shows a concentration distribution that approximates a gaussian curve. (This is expected, as the concentration distribution along a cross section normal to the direction of flow taken at any point downgradient from an ideal point source would be gaussian.) The standard deviation of the distribution can be determined from the data as

$$\sigma = \frac{(y - Y_c)}{\sqrt{-2 \ln(C/C_m)}}, \quad (71)$$

where C is the concentration observed at a well a distance $(y - Y_c)$ away from the point of maximum concentration.

Solving equation 71 may lead to differing values of σ if the observed data are not perfectly gaussian. An alternative procedure (R.M. Cleary, Princeton University, written commun., 1978) is to (1) normalize the data by dividing the observed concentrations by C_m , (2) plot a histogram of the normalized concentration with respect to y , and (3) calculate the area under the curve. The standard deviation can be approximated by $\sigma = \text{area}/\sqrt{2\pi}$. A sample problem illustrating the use of both methods is presented later.

This section presents analytical solutions for an

- Aquifer of infinite areal extent with a continuous point source, when fluid is injected at a constant rate and concentration,
- Semi-infinite aquifer of finite width with a strip source,
- Semi-infinite aquifer of infinite width with a strip source, and
- Semi-infinite aquifer of infinite width with a gaussian source.

All solutions can account for first-order solute decay. Four computer programs (POINT2, STRIPF, STRIPI and GAUSS) were written to calculate concentrations in these systems as a function of distance and elapsed time.

Aquifer of infinite areal extent with continuous point source

Governing equation

The analytical solution for a continuous point source has been presented by several authors, including Bear (1972, 1979), Fried (1975, p. 132), and Wilson and Miller (1978). The solution is derived by first solving the solute-transport equation for an *instantaneous* point source and then integrating the solution over time. The two-dimensional solute-transport equation for an *instantaneous* point source is given by

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - V \frac{\partial C}{\partial x} - \lambda C + \frac{Q'}{n} \int_0^t C_0 \delta(x - X_c) \delta(y - Y_c) \delta(t - t') dt \quad (72)$$

Boundary conditions:

$$C, \frac{\partial C}{\partial x} = 0, \quad x = \pm \infty \quad (73)$$

$$C, \frac{\partial C}{\partial y} = 0, \quad y = \pm \infty, \quad (74)$$

where

$V = V_x$, velocity in x-direction,

Q' = fluid injection rate per unit thickness of aquifer,

n = aquifer porosity,

dt = infinitesimal time interval,

δ = dirac delta (impulse) function,

X_c, Y_c = x- and y-coordinates of point source, and

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

Initial condition:

$$C = 0, \quad -\infty < y < +\infty \text{ and } -\infty < x < +\infty \text{ at } t = 0 \quad (75)$$

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 (no radial flow).
4. The longitudinal and transverse dispersion coefficients (D_x and D_y) are constant.

Analytical solution

The following equation, modified from Bear (1979, p. 274), represents the analytical solution for an *instantaneous* point source integrated with respect to time, such that

$$C(x, y, t) = \frac{C_0 Q'}{4n\pi\sqrt{D_x D_y}} \exp\left[\frac{V(x - X_c)}{2D_x}\right] \int_0^t \frac{1}{\tau} \cdot \exp\left[-\left(\frac{V^2}{4D_x} + \lambda\right)\tau - \frac{(x - X_c)^2}{4D_x\tau} - \frac{(y - Y_c)^2}{4D_y\tau}\right] d\tau, \quad (76)$$

where τ is a dummy variable of integration for the time integral.

The steady-state solution is given (modified from Bear, 1979, p. 274) as

$$C(x, y) = \frac{Q' C_0 \exp\left[\frac{V(x - X_c)}{2D_x}\right]}{2n\pi\sqrt{D_x D_y} K_0 \left\{ \sqrt{\left(\frac{V^2}{4D_x} + \lambda\right) \left[\frac{(x - X_c)^2}{D_x} + \frac{(y - Y_c)^2}{D_y}\right]} \right\}}, \quad (77)$$

where K_0 is the modified Bessel function of second kind and zero order. Tables of values and polynomial approximations for $K_0(x)$ are given by Abramowitz and Stegun (1964, p. 37, p. 417-422).

Comments:

The integral in equation 76 cannot be simplified further and must, therefore, be evaluated numerically. A Gauss-Legendre numerical integration technique, used in the computer program written to evaluate the analytical solution (eq. 76), is described later.

The integral in equation 76 is difficult to evaluate correctly at x and y values near the point source. (Mathematically, when $(x - X_c)$ and $(y - Y_c)$ approach zero, the integral in eq. 76 becomes a form of the exponential integral, $E_1(t)$, which becomes infinite at $t = 0$; see Abramowitz and Stegun, 1964, p. 228.) Farther away from the point source, generally when $(x - X_c)^2$ is larger than V^2 , a meaningful solution can be obtained.

Linear equilibrium adsorption and ion exchange can be simulated by first dividing Q' and the coefficients D_x , D_y , and V by the retardation factor, R (eq. 15). Temporal variations in source concentration or multiple sources can be simulated through the principle of superposition.

Description of program POINT2

The program POINT2 computes the analytical solution to the two-dimensional solute-transport equation for an aquifer of infinite areal extent with a continuous point source. It consists of a main program and the subroutine CNRML2. The functions of the main program and subroutine are outlined below; the program code listing is presented in attachment 2.

The program also calls subroutine GLQPTS and the output subroutines TITLE, OFILE, PLOT2D, 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

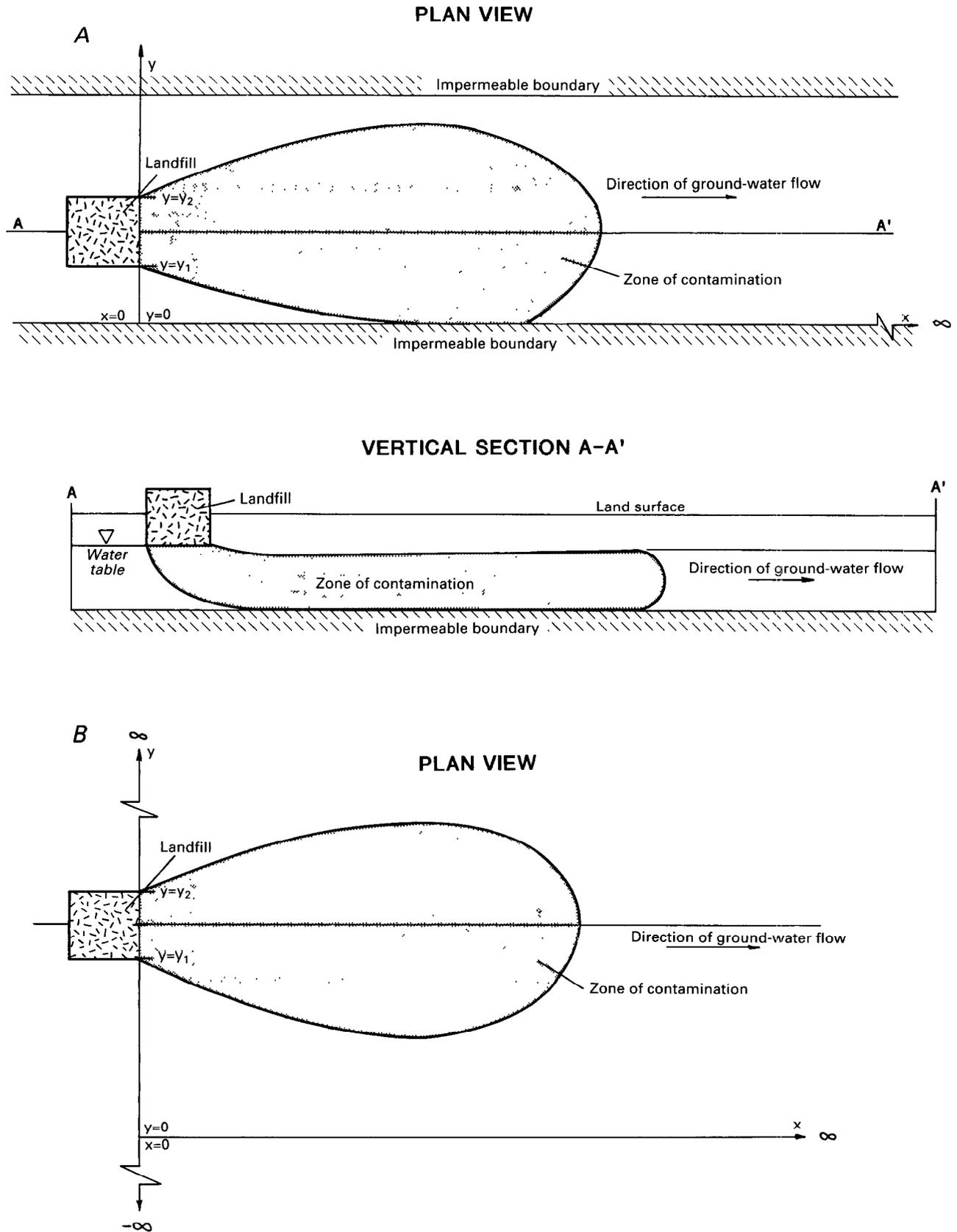


Figure 10.—(A) Plan view and vertical section of idealized two-dimensional solute transport in an aquifer of semi-infinite length and finite width, and (B) plan view of idealized two-dimensional solute transport in an aquifer of semi-infinite length and infinite width.

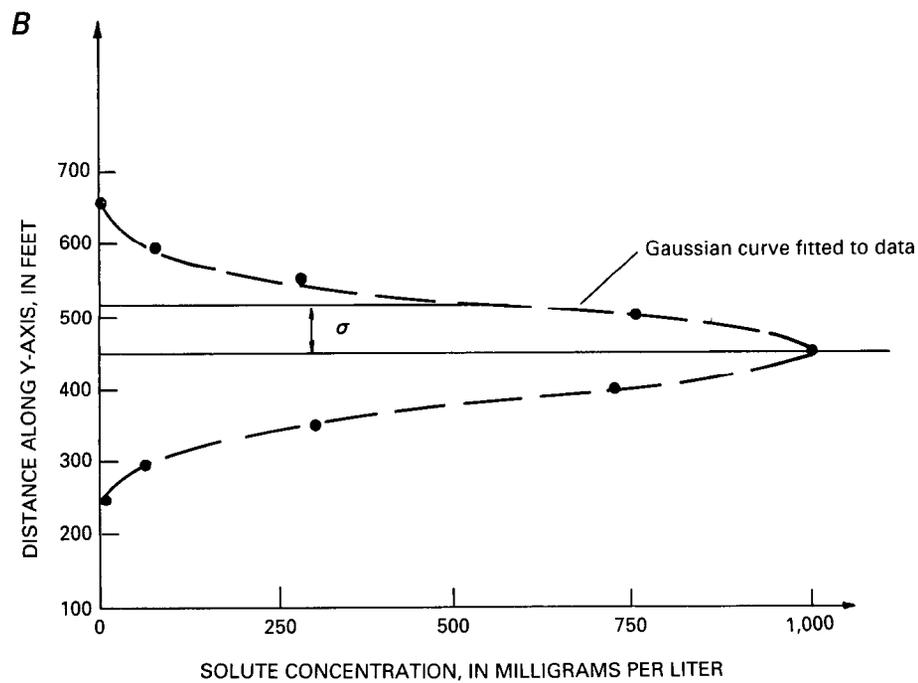
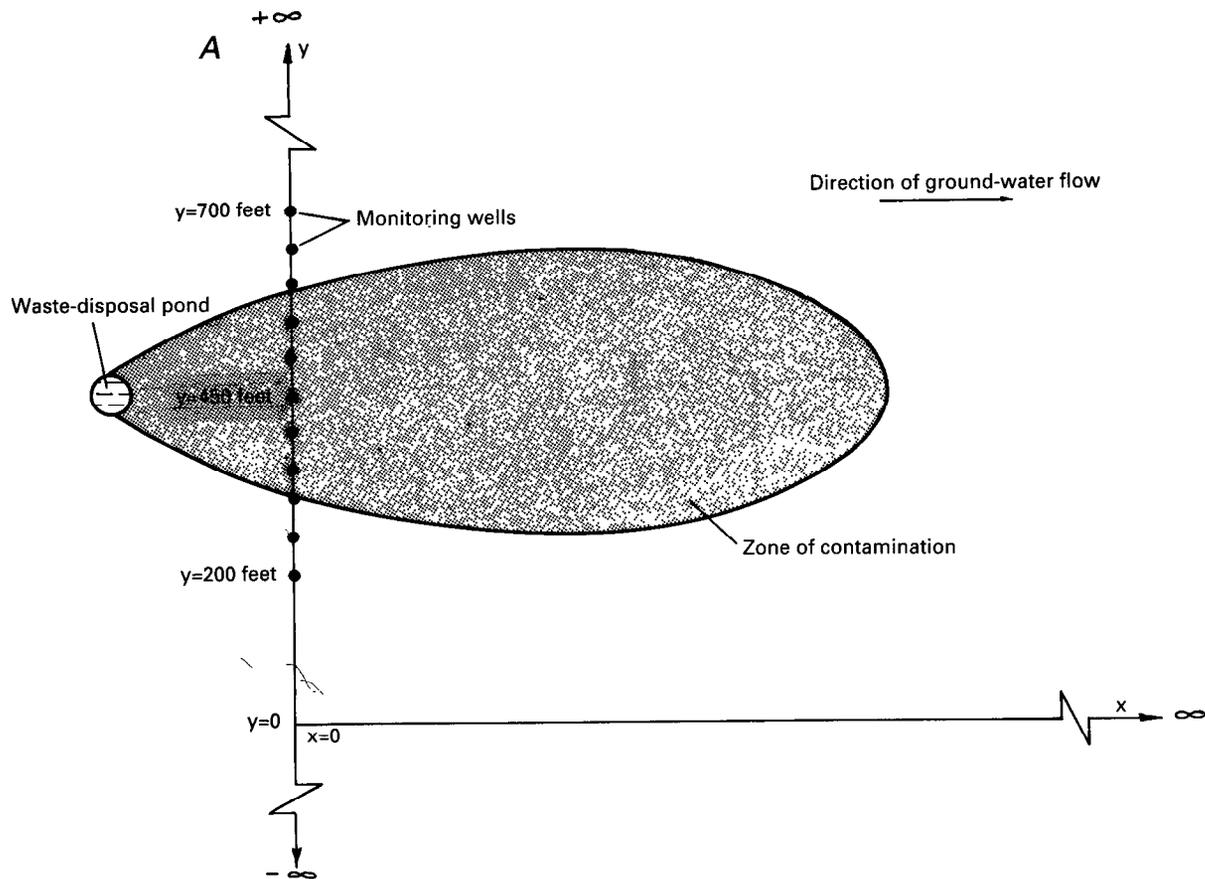


Figure 11.—(A) Plan view of a semi-infinite aquifer of infinite width showing location of waste-disposal pond and monitoring wells, and graph of (B) observed solute concentration values and gaussian curve used to approximate concentration distribution at $x=0$.

Table 3.—Input data format for the program POINT2

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	NT	Number of time values at which solution will be evaluated.
	13 - 16	I4	NMAX	Number of terms used in the numerical integration technique (must be equal to 4, 20, 60, 104, or 256).
	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	TUNITS	Units of time.
4	1 - 10	F10.0	C0	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.
	41 - 50	F10.0	DK	First-order solute-decay coefficient.
5	1 - 10	F10.0	XC	X-coordinate of point source.
	11 - 20	F10.0	YC	Y-coordinate of point source.
	21 - 30	F10.0	QM	Fluid injection rate per unit thickness of aquifer ¹ .
	31 - 40	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	T(I)	Time values at which solution will be evaluated (eight values per line).
² 9	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).

¹For the solution to be consistent, units of QM must be identical to those of the dispersion coefficients.

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

data and the format used in preparing a data file are shown in table 3. The routine then calls the subroutine GLQPTS, which reads the data file GLQ.PTS containing values of the positive roots and weighting functions used in the Gauss-Legendre numerical integration technique.

The program next executes a set of three nested loops. The inner loop calls subroutine CNRML2 to calculate the concentration at all specified y-coordinate values for a particular x-coordinate value and time. The middle loop cycles through all x-coordinate values. The outer loop cycles through all

specified time values and prints a table of concentrations in relation to distance for each time value. Model output can also be plotted as a series of maps showing lines of equal solute concentration.

Subroutine CNRML2

Subroutine CNRML2 calculates the normalized concentration (C/C_0) for a particular time value and distance. The integral in equation 76 is evaluated through a Gauss-Legendre numerical integration technique. The Gauss integration formula used is given by Abramowitz and Stegun (1964) as

$$\int_{-1}^1 f(x)dx = \sum_{i=1}^n w_i \cdot f(z_i), \quad (78)$$

where

n = order of Legendre polynomial,

w_i = weighting functions,

$f(z_i)$ = value of integrand calculated with variable of integration equal to z_i , and

z_i = roots of n^{th} order polynomial.

The normalized roots of the Legendre polynomial and the corresponding weighting functions are passed by subroutine GLQPTS and scaled in the subroutine to account for the non-normalized limits of integration (from 0 to t 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 (from data in Cleary and Ungs, 1978) 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. Additional discussions of the numerical integration technique are presented in a later section describing subroutine GLQPTS.

Sample problem 5

In sample problem 5, an abandoned borehole that penetrates a brackish artesian formation is discharging into an overlying freshwater aquifer. Model variables are

Aquifer thickness	= 100 ft
Discharge rate	= 1,250 ft ³ /d
Ground-water velocity (V)	= 2 ft/d
Longitudinal dispersivity (α_1)	= 30 ft
Transverse dispersivity (α_t)	= 6 ft
Source concentration (C_0)	= 1,000 mg/L
Point-source location (X_0, Y_0)	= 0, 500 ft
Aquifer porosity (n)	= 0.25.

From these values, the terms obtained are

Discharge rate per unit thickness of aquifer (Q')	= 12.5 ft ² /d
Coefficient of longitudinal dispersion (D_x)	= 60 ft ² /d
Coefficient of transverse dispersion (D_y)	= 12 ft ² /d.

Concentrations are calculated at 10-ft intervals along the x-axis from $x = -60$ ft to $x = 200$ ft, and at 5-ft intervals along the y-axis from $y = 450$ ft to $y = 550$ ft. Chloride concentration distribution after 25 days and 100 days is simulated.

The input data set for sample problem 5 is shown in figure 12A. A computer-generated contour plot of normalized concentrations (C/C_0) at both time values is shown in figure 12B. Program output for this sample problem is presented in attachment 4. Sample problem 5 required 9 s of CPU time on a Prime model 9955 Mod II.

Aquifer of finite width with finite-width solute source

Governing equation

Two-dimensional solute-transport equation:

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - V \frac{\partial C}{\partial x} - \lambda C \quad (79)$$

Boundary conditions:

$$C = C_0, \quad x = 0 \text{ and } Y_1 < y < Y_2 \quad (80a)$$

$$C = 0, \quad x = 0 \text{ and } y < Y_1 \text{ or } y > Y_2 \quad (80b)$$

$$C, \frac{\partial C}{\partial y} = 0, \quad y = 0 \quad (81)$$

$$C, \frac{\partial C}{\partial y} = 0, \quad y = W \quad (82)$$

$$C, \frac{\partial C}{\partial x} = 0, \quad x = \infty \quad (83)$$

where

V = velocity in x-direction,

Y_1 = y-coordinate of lower limit of solute source at $x = 0$,

Y_2 = y-coordinate of upper limit of solute source at $x = 0$, and

W = aquifer width.

A

Sample Problem 5 -- Solute transport in an aquifer of infinite areal extent with a continuous point source
 Model Data: V=2.0 ft/d, DX=60.0 ft**2/d, DY=12.0 ft**2/d
 QM=12.5 ft**2/d, CO=1000.0 mg/L n=0.25

MG/L	26	21	02	104	3	FT**2/D	PER DAY	FEET	DAYS
1000.0	2.0	500.0	12.5	60.0	12.0	0.0	500.0	12.5	0.25
-60.0	-50.0	-40.0	50.0	60.0	-20.0	110.0	120.0	130.0	140.0
30.0	40.0	50.0	60.0	70.0	80.0	190.0	200.0	460.0	475.0
490.0	495.0	500.0	505.0	510.0	515.0	530.0	535.0	540.0	545.0
25.0	100.0	30.0	0.1						

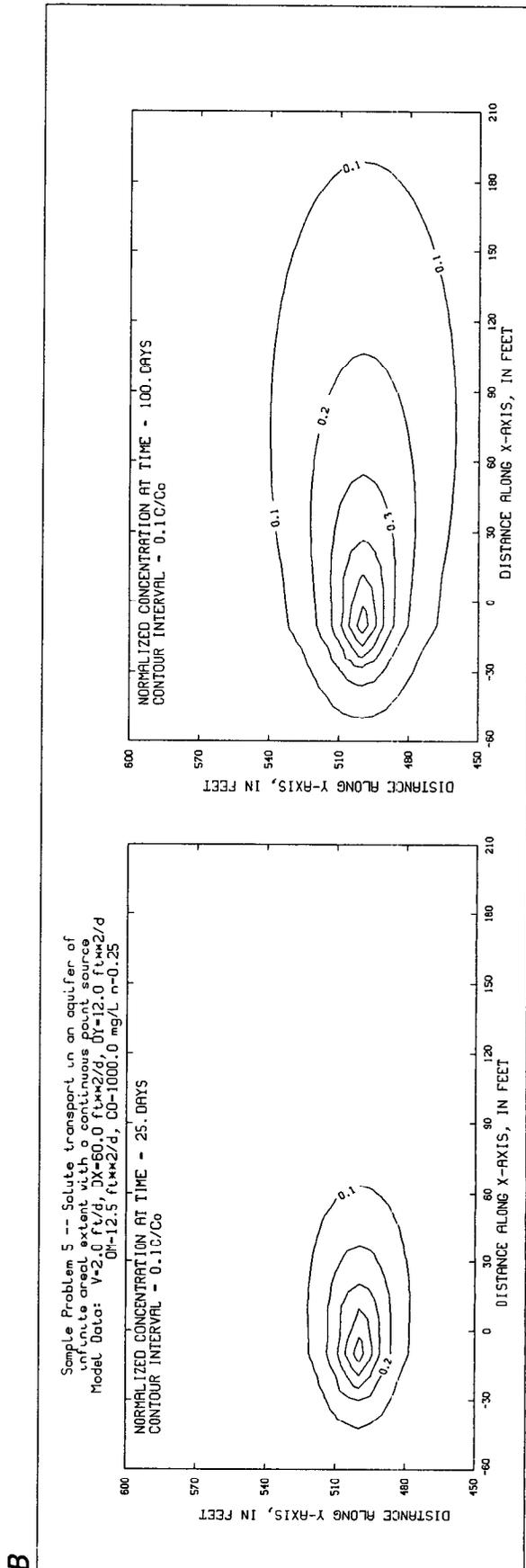


Figure 12. -- (A) Sample input data set, and (B) computer plot of normalized concentration contours generated by the program POINT2 for a conservative solute injected continuously into an aquifer of infinite areal extent after 25 and 100 days (sample problem 5).

Initial condition:

$$C=0, \quad 0 < x < \infty \text{ and } 0 < y < W \text{ at } t=0 \quad (84)$$

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 longitudinal and transverse dispersion coefficients (D_x , D_y) are constant.

Analytical solution

The following equation is modified from Hewson (1976):

$$C(x,y,t) = C_0 \sum_{n=0}^{\infty} L_n P_n \cos(\eta y) \cdot \left\{ \exp\left[\frac{x(V-\beta)}{2D_x}\right] \operatorname{erfc}\left[\frac{x-\beta t}{2\sqrt{D_x t}}\right] + \exp\left[\frac{x(V+\beta)}{2D_x}\right] \operatorname{erfc}\left[\frac{x+\beta t}{2\sqrt{D_x t}}\right] \right\} \quad (85)$$

where

$$L_n = \begin{cases} 1/2, & n=0 \\ 1, & n>0 \end{cases}$$

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

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

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

Comments:

Terms in the infinite series in equation 85 tend to oscillate, and the series converges slowly for small values of x ; thus, a large number of terms may be needed to ensure convergence. A good initial estimate is 100 terms. For larger values of x , the series converges more quickly.

The solution can yield results with either D_y or $\lambda=0$. Linear equilibrium adsorption and ion exchange can be simulated by first dividing the coefficients D_x , D_y , 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 STRIPF

The program STRIPF computes the analytical solution to the two-dimensional solute-transport equation for an aquifer of finite width with a finite-width or "strip" 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 the output subroutines TITLE, OFILE, PLOT2D, 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 4.

The program next executes a set of three nested loops. The inner loop calls subroutine CNRMLF to calculate the concentration at all specified y-coordinate values for a particular x-coordinate value and time. The middle loop cycles through all x-coordinate values. The outer loop cycles through all specified time values and prints a table of concentration in relation to distance for each time. Model output can also be plotted as a map showing lines of equal solute concentration.

Subroutine CNRMLF

Subroutine CNRMLF calculates the normalized concentration (C/C_0) for a particular time value and distance using equation 85. 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 1×10^{-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.

Sample problem 6

In sample problem 6, migration of chloride ion in landfill leachate through a narrow, relatively thin, valley-fill aquifer is simulated. Model variables are

Aquifer width (W)	=3,000 ft
Lower limit of solute source (Y_1)	=400 ft
Upper limit of solute source (Y_2)	=2,000 ft
Ground-water velocity (V_x)	=1 ft/d
Longitudinal dispersivity (α_1)	=200 ft
Transverse dispersivity (α_t)	=60 ft

Table 4.—Input data format for the program STRIPF

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	NT	Number of time values at which solution will be evaluated.
	13 - 16	I4	NMAX	Maximum number of terms used in the infinite series summation.
	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	TUNITS	Units of time.
4	1 - 10	F10.0	C0	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.
	41 - 50	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	Y1	Y-coordinate of lower limit of finite-width solute source.
	21 - 30	F10.0	Y2	Y-coordinate of upper limit of finite-width 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	T(I)	Time values at which solution will be evaluated (eight values per line).
¹ 9	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).

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

Source concentration (C_0) = 1,000 mg/L.

From these values, the terms obtained are

Dispersion in x-direction (D_x) = 200 ft²/d
 Dispersion in y-direction (D_y) = 60 ft²/d.

Concentrations are calculated at 150-ft intervals along the x-axis for 4,500 ft, and at 100-ft intervals along the y-axis for 3,000 ft. Chloride concentration distribution after 1,500 and 3,000 days is simulated.

The input data set for sample problem 6 is shown in figure 13A. A computer-generated contour plot of normalized concentration (C/C_0) at each time value is shown in figure 13B. The lack of symmetry about the centerline of the chloride plume is due to the effect of the closer lateral boundary (at $y=0$). Lines of equal concentration are perpendicular to the lateral boundary, indicating that concentration gradients in the y-direction equal zero and, thus, no solute flux occurs across the boundary. Program output for this sample

A

Sample Problem 6 -- Solute transport in a semi-infinite aquifer of finite width with a continuous 'strip' source
 Model Data: $V=1.0$ ft/d, $DX=200.0$ ft**2/d, $DY=60.0$ ft**2/d
 $W=3000$ ft, $Y1=400$ ft, $Y2=2000$ ft, $CO=1000.0$ mg/L

MG/L	31	27	02	300	1	FT/D	FT**2/D	PER DAY	FEET	DAYS
1000.0	1000.0	400.0	1.0	200.0	60.0	0.0				
3000.0	0.0	150.0	300.0	450.0	600.0	750.0	900.0	1050.0		
1200.0	1200.0	1350.0	1500.0	1650.0	1800.0	1950.0	2100.0	2250.0		
2400.0	2400.0	2550.0	2700.0	2850.0	3000.0	3150.0	3300.0	3450.0		
3600.0	3600.0	3750.0	3900.0	4050.0	4200.0	4350.0	4500.0			
0.0	0.0	100.0	200.0	300.0	400.0	500.0	600.0	700.0		
800.0	800.0	900.0	1000.0	1100.0	1200.0	1300.0	1400.0	1500.0		
1600.0	1600.0	1700.0	1800.0	1900.0	2000.0	2100.0	2200.0	2300.0		
2400.0	2400.0	2500.0	2600.0	2700.0	2800.0	2900.0	3000.0			
1500.0	750.0									

B

Sample Problem 6 -- Solute transport in a semi-infinite aquifer of finite width with a continuous 'strip' source
 Model Data: $V=1.0$ ft/d, $DX=200.0$ ft**2/d, $DY=60.0$ ft**2/d
 $W=3000$ ft, $Y1=400$ ft, $Y2=2000$ ft, $CO=1000.0$ mg/L

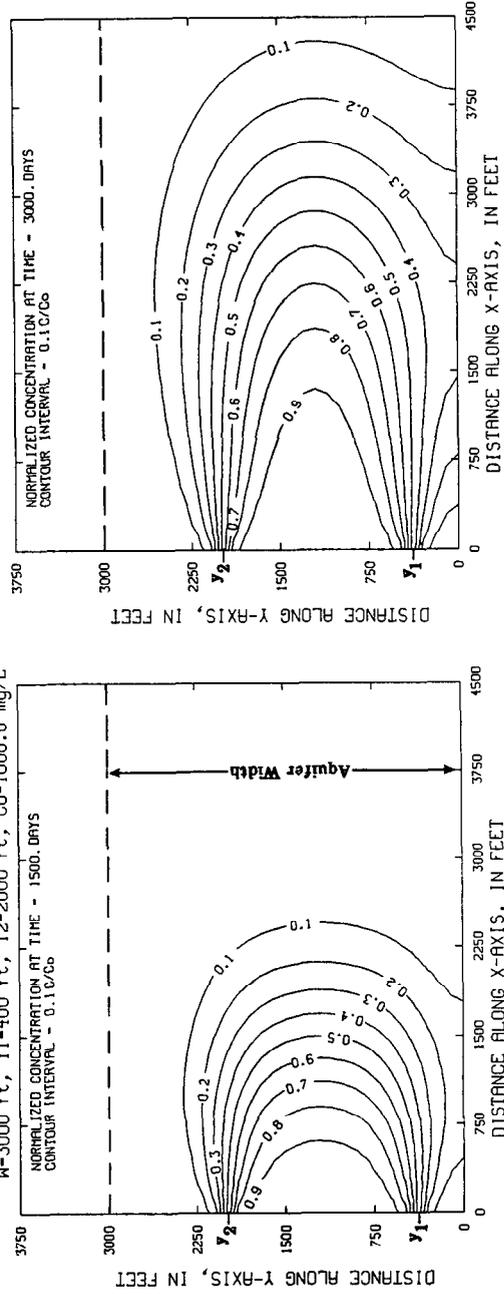


Figure 13. — (A) Sample input data set, and (B) computer plot of normalized concentration contours generated by the program STRIPF for a conservative solute in an aquifer of finite width with finite-width source after 1,500 and 3,000 days (sample problem 6).

problem is presented in attachment 4. Sample problem 6 required 52 s of CPU time on a Prime model 9955 Mod II.

Aquifer of infinite width with finite-width solute source

Governing equation

Two-dimensional solute-transport equation:

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - V \frac{\partial C}{\partial x} - \lambda C \quad (86)$$

Boundary conditions:

$$C = C_o, \quad x=0 \text{ and } Y_1 < y < Y_2 \quad (87a)$$

$$C = 0, \quad x=0 \text{ and } y < Y_1 \text{ or } y > Y_2 \quad (87b)$$

$$C, \frac{\partial C}{\partial y} = 0, \quad y = \pm\infty \quad (88)$$

$$C, \frac{\partial C}{\partial x} = 0, \quad x = \infty, \quad (89)$$

where

V = velocity in x -direction,

Y_1 = y -coordinate of lower limit of solute source at $x=0$, and

Y_2 = y -coordinate of upper limit of solute source at $x=0$.

Initial condition:

$$C = 0, \quad 0 < x < \infty \text{ and } -\infty < y < +\infty \quad \text{at } t=0 \quad (90)$$

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 longitudinal and transverse dispersion coefficients (D_x , D_y) are constant.

Analytical solution

The following equation is modified from Cleary and Ungs (1978, p. 17):

$$C(x,y,t) = \frac{C_o x}{4\sqrt{\pi D_x}} \exp\left(\frac{Vx}{2D_x}\right) \cdot \int_{\tau=0}^{\tau=t} \tau^{-\frac{3}{2}} \exp\left[-\left(\frac{V^2}{4D_x} + \lambda\right)\tau - \frac{x^2}{4D_x\tau}\right] d\tau$$

$$\cdot \left\{ \operatorname{erfc}\left[\frac{(Y_1-y)}{2\sqrt{D_y\tau}}\right] - \operatorname{erfc}\left[\frac{(Y_2-y)}{\sqrt{D_y\tau}}\right] \right\} d\tau, \quad (91a)$$

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

$$C(x,y,t) = \frac{C_o x}{\sqrt{\pi D_x}} \exp\left[\frac{Vx}{2D_x}\right] \cdot \int_0^{t^{1/4}} \frac{1}{Z^3} \exp\left[-\left(\frac{V^2}{4D_x} + \lambda\right)Z^4 - \frac{x^2}{4D_x Z^4}\right] \cdot \left\{ \operatorname{erfc}\left[\frac{(Y_1-y)}{2Z^2\sqrt{D_y}}\right] - \operatorname{erfc}\left[\frac{(Y_2-y)}{2Z^2\sqrt{D_y}}\right] \right\} dz \quad (91b)$$

Comments:

The integral in equation 91b 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 , 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 STRIPI

The program STRIPI computes the analytical solution to the two-dimensional solute-transport equation for an aquifer of infinite width with a finite-width or "strip" solute source at the inflow boundary. It consists of a main program and the subroutine CNRMLI. The functions of the main program and 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, PLOT2D, 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 5. The routine then calls the subroutine GLQPTS, which reads the data file GLQ.PTS containing values of the positive roots and weighting functions used in the Gauss-Legendre numerical integration technique.

Table 5.—Input data format for the program STRIPI

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	NT	Number of time values at which solution will be evaluated.
	13 - 16	I4	NMAX	Number of terms used in the numerical integration techniques (must be equal to 4, 20, 60, 104, or 256).
	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	TUNITS	Units of time.
4	1 - 10	F10.0	C0	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.
	41 - 50	F10.0	DK	First-order solute-decay coefficient.
5	1 - 10	F10.0	Y1	Y-coordinate of lower limit of finite-width solute source.
	11 - 20	F10.0	Y2	Y-coordinate of upper limit of finite-width 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	T(I)	Time values at which solution will be evaluated (eight values per line).
¹ 9	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).

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

The program next executes a set of three nested loops. The inner loop calls subroutine CNRMLI to calculate the concentration at all specified y-coordinate values for a particular x-coordinate value and time. The middle loop cycles through all x-coordinate values. The outer loop cycles through all specified time values and prints a table of concentration in relation to distance for each time. Model output can also be plotted as a map showing lines of equal solute concentration.

Subroutine CNRMLI

Subroutine CNRMLI calculates the normalized concentrations (C/C_0) for a particular time value and distance. The integral in equation 91 is evaluated through a Gauss-Legendre numerical integration technique. The normalized roots of the Legendre polynomial and the corresponding weighting functions 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. Additional discussions of the numerical integration technique are presented in a later section describing subroutine GLQPTS.

Sample problem 7

In sample problem 7, contaminant migration from a waste-disposal pond through the upper glacial aquifer of Long Island, N.Y., is simulated. Data are from a numerical modeling study by Pinder (1973). Model variables are

Lower limit of solute source (Y_1)	=635 ft
Upper limit of solute source (Y_2)	=865 ft
Ground-water velocity (V)	=1.42 ft/d
Longitudinal dispersivity (α_1)	=70 ft
Transverse dispersivity (α_t)	=14 ft
Source concentration (C_0)	=40 mg/L.

Lateral boundaries are far enough from the area of interest that the aquifer can be treated as being infinite in width. From these values, the terms obtained are

Dispersion in x-direction (D_x)	=100 ft ² /d
Dispersion in y-direction (D_y)	= 20 ft ² /d.

Concentrations are calculated at 100-ft intervals along the x-axis for 3,000 ft, and at 50-ft intervals on the y-axis for 1,500 ft. Concentration distributions after 5 years (1,826 days) are simulated.

The input data set for sample problem 7 is shown in figure 14A. A computer-generated contour plot of normalized concentration (C/C_0) is shown in figure 14B. Program output for this sample problem is presented in attachment 4. Sample problem 7 required 1 min (minute) 25 s of CPU time on a Prime model 9955 Mod II.

Aquifer of infinite width with solute source having gaussian concentration distribution

Governing equation

Two-dimensional solute-transport equation:

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - V \frac{\partial C}{\partial x} - \lambda C \quad (92)$$

Boundary conditions:

$$C = C_m \exp\left[\frac{-(y - Y_c)^2}{2\sigma^2}\right], \quad x = 0 \quad (93)$$

$$C, \frac{\partial C}{\partial y} = 0, \quad y = \pm\infty \quad (94)$$

$$C, \frac{\partial C}{\partial x} = 0, \quad x = \infty, \quad (95)$$

where

C_m = maximum concentration at center of gaussian solute source,

Y_c = y-coordinate of center of solute source at $x = 0$, and

σ = standard deviation of gaussian distribution.

Initial condition:

$$C = 0, \quad 0 < x < \infty \text{ and } -\infty < y < +\infty \text{ at } t = 0 \quad (96)$$

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 ($V_y = 0$), and velocity is constant.
4. The longitudinal and transverse dispersion coefficients (D_x, D_y) are constant.

Analytical solution

The following equation is modified from Gureghian and others (1980, p. 905):

$$C(x, y, t) = \frac{C_m x \sigma}{\sqrt{8\pi D_x}} \exp\left[\frac{Vx}{2D_x}\right] \int_0^t \frac{\exp\left[-\beta\tau - \frac{x^2}{4D_x\tau} - \frac{(y - Y_c)^2}{4(D_y\tau + \sigma^2)}\right] d\tau}{\tau^{\frac{3}{2}} \sqrt{D_y\tau + \sigma^2}}, \quad (97)$$

where

$$\beta = \frac{V^2}{4D_x} + \lambda$$

and τ is a dummy variable of integration for the time integral.

To improve the accuracy of the numerical integration, a variable substitution (modified from Cleary and Unga, 1978, p. 20) can be made where $\tau = Z^4$, yielding

A

Sample Problem 7 -- Solute transport in a semi-infinite aquifer of infinite width with a continuous 'strip' source
 Model Data: $V=1.42$ ft/d, $DX=100.0$ ft**2/d, $DY=20.0$ ft**2/d
 $Y1=635$ ft, $Y2=865$ ft, $C0=40.0$ mg/L

MG/L	31	31	1	104	1	FT**2/D	PER DAY	FEET	DAYS
40.0			1.42			100.0	20.0	0.0	
635.0			865.0						
0.0			100.0			200.0	300.0	400.0	500.0
800.0			900.0			1000.0	1100.0	1200.0	1300.0
1600.0			1700.0			1800.0	1900.0	2000.0	2100.0
2400.0			2500.0			2600.0	2700.0	2800.0	2900.0
0.0			50.0			100.0	150.0	200.0	250.0
400.0			450.0			500.0	550.0	600.0	650.0
800.0			850.0			900.0	950.0	1000.0	1050.0
1200.0			1250.0			1300.0	1350.0	1400.0	1450.0
1826.0									
500.			500.			0.1			

B

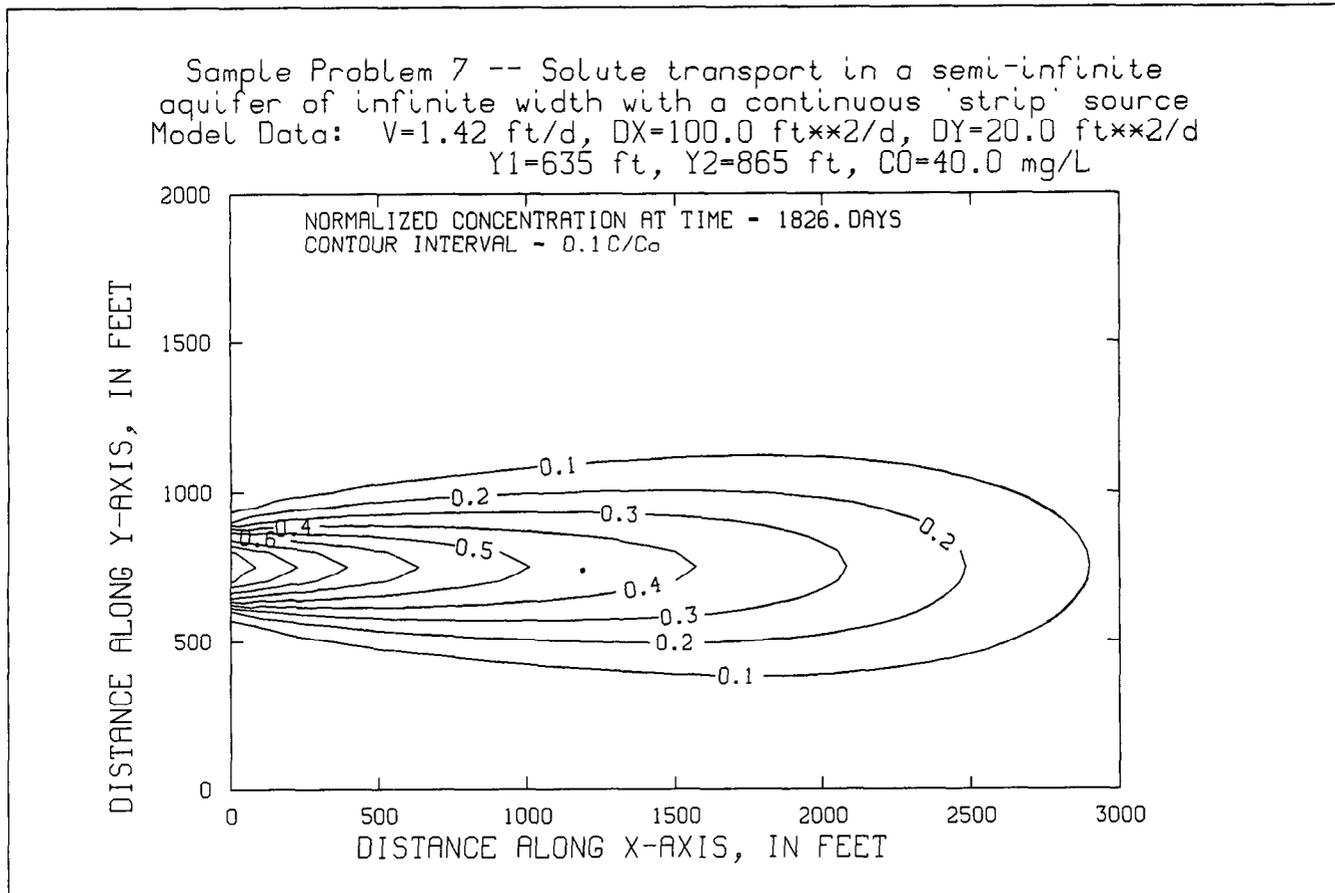


Figure 14.—(A) Sample input data set, and (B) computer plot of normalized concentration contours generated by the program STRIPI for a conservative solute in an aquifer of infinite width with finite-width solute source after 1,826 days (sample problem 7).

$$C(x,y,t) = \frac{2C_m x \sigma}{\sqrt{2\pi D_x}} \exp\left[\frac{Vx}{2D_x}\right] \int_0^{t^{1/4}} \frac{\exp\left[-\beta Z^4 - \frac{x^2}{4D_x Z^4} - \frac{(y-Y_c)^2}{4\gamma}\right] dZ}{Z^3 \sqrt{\gamma}}, \quad (98)$$

where

$$\gamma = \left[D_y Z^4 + \frac{\sigma^2}{2} \right].$$

Comments:

The integral in equation 98 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.

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

Description of program GAUSS

The program GAUSS computes the analytical solution to the two-dimensional solute-transport equation for an aquifer of infinite width with a solute source having a gaussian concentration distribution along the inflow boundary. It consists of a main program and the subroutine CNRMLG. 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 GLQPTS and the output subroutines TITLE, OFILE, and PLOT2D, 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 6. The routine then calls the subroutine GLQPTS, which reads the data file GLQ.PTS containing values of the positive roots and weighting functions used in the Gauss-Legendre numerical integration technique.

The program next executes a set of three nested loops. The inner loop calls subroutine CNRMLG to calculate the concentration at all specified y-coordinate values for a particular x-coordinate value and time. The middle loop cycles through all x-

coordinate values. The outer loop cycles through all specified time values and prints a table of concentration in relation to distance for each time value. Model output can also be plotted as a map showing lines of equal solute concentration.

Subroutine CNRMLG

Subroutine CNRMLG calculates the normalized concentration (C/C_m) for a particular time value and distance. The integral in equation 98 is evaluated through a Gauss-Legendre numerical integration technique. The normalized roots of the Legendre polynomial and the corresponding weighting functions 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. Additional discussions of the numerical integration technique are presented in a later section describing subroutine GLQPTS.

Sample problems 8a and 8b

Two sample problems are presented. Sample problem 8a is modified from an example presented in Gureghian and others (1980) for a conservative solute uniformly mixed in a thin aquifer of infinite width. Model variables are

Maximum concentration (C_m)	=1,000 mg/L
Standard deviation of gaussian distribution (σ)	=130 ft
Center of solute source (Y_c)	=450 ft
Ground-water velocity (V_x)	=4 ft/d
Coefficient of longitudinal dispersion (D_x)	=150 ft ² /d
Coefficient of transverse dispersion (D_y)	=30 ft ² /d.

Concentrations are calculated at 50-ft intervals along the x-axis for 1,700 ft, and at 25-ft intervals on the y-axis for 900 ft. The chloride concentration distribution after 300 days is simulated.

Sample problem 8b demonstrates two methods of calculating a value for σ . Aquifer dimensions, ground-water velocity, and dispersion coefficients are the same as in problem 8a. Concentrations measured in monitoring wells 500 ft downgradient from a waste-disposal site are presented in table 7; figure 15 presents a plot of the normalized concentration (C/C_m) in

Table 6.—Input data format for the program GAUSS

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	NT	Number of time values at which solution will be evaluated.
	13 - 16	I4	NMAX	Number of terms used in the numerical integration technique (must be equal to 4, 20, 60, 104, or 256).
	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	TUNITS	Units of time.
4	1 - 10	F10.0	CM	Maximum 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.
	41 - 50	F10.0	DK	First-order solute-decay coefficient.
5	1 - 10	F10.0	YC	Y-coordinate of center of gaussian-distributed solute source.
	11 - 20	F10.0	WS	Standard deviation of gaussian distribution describing 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	T(I)	Time values at which solution will be evaluated (eight values per line).
¹ 9	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).

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

relation to distance along the y-axis (normal to the direction of flow). An average value of σ , calculated from the observed concentrations (table 7) using equation 70, is 66.1 ft. The area under the curve in figure 15 can also be approximated and yields a σ value of 65.0 ft. A value of 65 ft was used in the input data for sample problem 8b.

Input data sets for sample problems 8a and 8b are shown in figures 16A and 17A. Computer-generated contour plots of normalized concentration (C/C_m) are shown in figures 16B and 17B. Comparison of figures 16B and 17B shows the effect of varying σ on the concentration distribution. Program output for sample problem 8a is presented in attachment 4. Sample

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 σ , 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_0). 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_0 , except along the boundary of the patch source, where it is equal to $0.5 C_0$. 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

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - V \frac{\partial C}{\partial x} - \lambda C + \frac{Q dt}{n} C_0 \cdot \delta(x - X_0) \delta(y - Y_0) \delta(z - Z_0) \delta(t - t'). \quad (99)$$

Boundary conditions:

$$C, \frac{\partial C}{\partial x} = 0, \quad x = \pm \infty \quad (100)$$

$$C, \frac{\partial C}{\partial y} = 0, \quad y = \pm \infty \quad (101)$$

$$C, \frac{\partial C}{\partial z} = 0, \quad z = \pm \infty, \quad (102)$$

where

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