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Chapter B7

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

By Eliezer J. Wexler

Book 3
APPLICATIONS OF HYDRAULICS

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PREFACE

The series of manuals on techniques describes procedures for planning and executing specialized work in water-resources investigations. The material is grouped under major subject headings called books and further subdivided into sections and chapters; section B of book 3 is on ground-water techniques.

The unit of publication, the chapter, is limited to a narrow field of subject matter. This format permits flexibility in revision and publication as the need arises. Chapter 3B7 deals with analytical solutions to the solute-transport equation for a variety of boundary condition types and solute-source configurations in one-, two-, and three-dimensional systems with uniform ground-water flow.

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Copies of the computer codes and sample data sets described in this report are available on diskette from Book and Open-File Report Sales as USGS Open File Report 92–78. They are on a 5.25" (360K) double-density diskette formatted for the IBM PC. The computer programs were originally written for a Prime minicomputer but all programs should run using IBM-PC Fortrans with minor modifications as described in the report. The plot routines were written with DISSPLA software calls and can be used on the PC only with the PC version of the DISSPLA library. Alternatively, data can be easily extracted from the program output and plotted using PC graphics presentation programs.

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[1]This manual is a revision of "Measurement of Time of Travel and Dispersion in Streams by Dye Tracing," by E.F. Hubbard, F.A. Kilpatrick, L.A. Martens, and J.F. Wilson, Jr., Book 3, Chapter A9, published in 1982.

[2]Spanish translation also available.

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[1]This manual is a revision of TWRI 5–A3, "Methods of Analysis of Organic Substances in Water," by Donald F. Goerlitz and Eugene Brown, published in 1972.

[2]This manual supersedes TWRI 5–A4, "Methods for collection and analysis of aquatic biological and microbiological samples," edited by P.E. Greeson and others, published in 1977.

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METRIC CONVERSION FACTORS

For readers who wish to convert measurements from the inch-pound system of units to the metric system of units, the conversion factors are listed below:

Multiply inch-pound units	*By*	*To obtain metric units*
inch (in)	25.4	millimeter (mm)
inch per hour (in/h)	25.4	millimeter per hour (mm/h)
foot (ft)	0.3048	meter (m)
foot per day (ft/d)	0.3048	meter per day (m/d)
gallon (gal)	0.003785	cubic meter (m^3)
square inch per hour (in^2/h)	6.4516	square centimeter per hour (cm^2/h)
foot squared per day (ft^2/d)	0.09290	meter squared per day (m^2/d)
cubic foot (ft^3)	0.02832	cubic meter (m^3)
cubic foot per day (ft^3/d)	0.02832	cubic meter per day (m^3/d)
pound per cubic foot (lb/ft^3)	0.01602	gram per cubic centimeter (g/cm^3)

DEFINITION OF SYMBOLS

Symbol	*Dimension*	*Definitions*
C	M/L^3	Volumetric concentration
C_o	M/L^3	Specified concentration value along a boundary
CEC	$1/M$	Cation exchange capacity
$\underline{D}$	L^2/T	Coefficient of hydrodynamic dispersion for one-dimensional solute transport
$\underline{\underline{D}}$	L^2/T	Hydrodynamic dispersion tensor in an isotropic system
$\underline{\underline{D}}_d$	L^2/T	Molecular diffusion tensor
$\underline{\underline{D}}_m$	L^2/T	Mechanical dispersion tensor
D^*	L^2/T	Dispersion coefficient divided by the retardation factor, R
D_x, D_y, D_z	L^2/T	Magnitudes of the hydrodynamic dispersion tensor in a system having uniform flow
erf	—	Error function
erfc	—	Complimentary error function
exp	—	Exponential
h	L	Head
$\vec{J}$	M/L^2T	Solute flux due to dispersion or diffusion
k	L^3/M	Slope of the linear equilibrium adsorption isotherm
$\underline{\underline{k}}_d$	L^3/M	Distribution coefficient
$\underline{\underline{K}}$	L/T	Hydraulic conductivity tensor
K_s	—	Selectivity coefficient for ion exchange reactions
K_o	—	Modified Bessel function of second kind and zero order
n	—	Effective porosity
p	M/LT^2	Fluid pressure
P	—	Column Peclet number
R	—	Retardation factor for adsorbed solute
S	—	Mass concentration of adsorbed solute
t	T	Time
T	—	Number of displaced pore volumes
$T_{1/2}$	T	Half-life of radioactive solute
v	L/T	Magnitude of the average interstitial fluid velocity
v_x, v_y, v_z	L/T	Magnitudes of the average interstitial velocity components
V	L/T	Magnitude of uniform velocity
$\vec{V}$	L/T	Average interstitial fluid velocity
V^*	L/T	Average interstitial fluid velocity divided by the retardation factor, R
z	L	Elevation head
α_l	L	Longitudinal dispersivity
α_t	L	Transverse dispersivity
γ	M/L^2T^2	Specific weight of water
θ	—	Soil moisture content (equal to porosity for saturated soils)
λ	$1/T$	First-order chemical transformation rate
ρ	M/L^3	Density of water
ρ_b	M/L^3	Bulk density of aquifer material
Σ	—	Summation
∞	—	Infinity
$\vec{\nabla}$	—	Gradient operator
∂	—	Partial derivative

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

By Eliezer J. Wexler

Abstract

Analytical solutions to the advective-dispersive solute-transport equation are useful in predicting the fate of solutes in ground water. Analytical solutions compiled from available literature or derived by the author are presented for a variety of boundary condition types and solute-source configurations in one-, two-, and three-dimensional systems having uniform ground-water flow. A set of user-oriented computer programs was created to evaluate these solutions and to display the results in tabular and computer-graphics format. These programs incorporate many features that enhance their accuracy, ease of use, and versatility. Documentation for the programs describes their operation and required input data, and presents the results of sample problems. Derivations of selected solutions, source codes for the computer programs, and samples of program input and output also are included.

Introduction

Contamination of ground water by inorganic and organic chemicals has become an increasing concern in recent years. These chemicals enter the ground-water system by a wide variety of mechanisms, including accidental spills, land disposal of domestic and industrial waste, and application of agricultural fertilizers and pesticides. Once introduced into an aquifer, these solutes will be transported by flowing ground water and may degrade water quality at nearby wells and streams.

To improve management and protection of ground-water resources, it is important to first understand the physical, chemical, and biological processes that control the transport of solutes in ground water. Predictions of the fate of ground-water contaminants can then be made to assess the effect of these chemicals on local water resources and to evaluate the effectiveness of remedial actions.

Two physical processes that govern the movement of ground-water solutes are (1) advection, which describes the transport of solutes by the bulk motion of flowing ground water (Freeze and Cherry, 1979), and (2) hydrodynamic dispersion, which describes the spread of solutes along and transverse to the direction of flow resulting from both mechanical mixing and molecular diffusion (Bear, 1979, p. 230). Chemical reactions, including those mediated by microorganisms or caused by interaction with aquifer material or other solutes, may also affect the concentration of the solute.

These processes have been described quantitatively by a partial differential equation referred to as the "advective-dispersive solute-transport equation." Solution of the equation yields the solute concentration as a function of time and distance from the contaminant source. To apply the equation to a particular ground-water contamination problem, data must be provided on the ground-water velocity, coefficients of hydrodynamic dispersion, rates of chemical reactions, initial concentrations of solutes in the aquifer, configuration of the solute source, and boundary conditions along the physical boundaries of the ground-water flow system.

In ground-water systems having irregular geometry and nonuniform aquifer properties, numerical techniques are used to determine approximate solutions to the solute-transport equation. In aquifers having simple flow systems and relatively uniform hydrologic properties, analytical solutions, which represent exact mathematical solutions to the solute-transport equation, have been used to predict contaminant migration. These solutions are also used extensively in analysis of data from soil-column experiments and field tracer tests to determine aquifer properties, and have been used to verify the soundness of numerical models. In complex hydrogeologic systems, analytical solutions can still be useful to the hydrologist because they can provide estimates of

rates of solute spread and, thus, guide data collection and water-quality-monitoring efforts.

Although deriving an analytical solution for the solute-transport equation requires knowledge of higher mathematics, analytical solutions have already been derived and published for many combinations of solute-source configurations and boundary-condition types. After the solutions have been derived, they can be evaluated easily using electronic calculators or digital computers.

Purpose and scope

This report briefly describes the theoretical background of solute transport in a porous medium and then presents analytical solutions to the advective-dispersive solute-transport equation for a variety of aquifer and solute-source configurations and boundary conditions in systems having uniform (unidirectional) ground-water flow. Solutions for one-dimensional solute transport were compiled from various journals and reports, many of which are not readily available. Many of the solutions for two- and three-dimensional solute transport were modified from those presented in a report by Cleary and Ungs (1978), whereas others were derived by the author using integral transform techniques. (Detailed derivations of these solutions are provided in attachment 1.) All solutions are given in a simplified format, together with information on important assumptions in their derivation and limitations to their use.

Simple computer programs, written in FORTRAN-77, have been provided for evaluation of the analytical solutions presented. The programs were designed for ease of use and for enhanced accuracy. Documentation for these programs includes descriptions of program operation and the input data required. Source codes and samples of program output are provided at the end of the report. Subroutines that allow for graphical display of the program output, created using DISSPLA software, are also described. Computer-generated plots are presented within the report.

Previous studies

Analytical solutions for the one-dimensional form of the solute-transport equation have appeared in reports and journals concerning physical chemistry, soil science, and water resources. These solutions, generally determined through Laplace transform techniques, have been applied to studies of solute movement in laboratory columns, unsaturated soils, and natural-gradient tracer tests. Solutions to the one-dimensional solute-transport equation for most combinations of boundary and initial conditions are given in van Genuchten and Alves (1982); some of the more useful solutions appear in this report. Other sources that list several analytical solutions include Gershon and Nir (1969), Bear (1972), and Bear (1979).

Fewer analytical solutions have been published for the two- and three-dimensional forms of the solute-transport equation. Cleary and Ungs (1978) give several solutions derived using integral transform techniques, and Yeh (1981) presents a computer program that evaluates Green's function to model one-, two-, and three-dimensional transport.

Acknowledgments

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Theoretical Background

Most models that simulate migration of dissolved contaminants in ground water solve the advective-dispersive solute-transport equation. This partial differential equation is derived from the conservation-of-mass principle (continuity equation), whereby the net rate of change of solute mass within a volume of porous media is equal to the difference between the flux of solute into and out of the volume, adjusted for the loss or gain of solute mass due to chemical reactions (Freeze and Cherry, 1979). The flux of solute into the volume is controlled by two physical processes—advection and hydrodynamic dispersion. Hydrodynamic dispersion, in turn, represents the combined effects of two other physical processes—molecular diffusion and mechanical dispersion.

Advection

Advective transport describes the bulk movement of solute particles along the mean direction of fluid flow at a rate equal to the average interstitial fluid velocity. In a saturated medium, this velocity can be calculated from Darcy's law, such that

$$\vec{v} = -\frac{\overline{\overline{K}}}{n} \cdot \vec{\nabla} h, \qquad (1)$$

where

$\vec{v}$ = average interstitial fluid velocity [L/T],

$\overline{\overline{K}}$ = hydraulic conductivity tensor for medium [L/T],

n = effective porosity [dimensionless], and

$\vec{\nabla} h$ = gradient in head [dimensionless] (equal to dh/dx, the change in head per unit distance along the x-axis for uniform flow along the x-axis).

Head, h in equation 1, is equal to the sum of the elevation head, z, with respect to a datum level, and the pressure head, p/γ, where p is the fluid pressure (gage pressure) and γ is the specific weight of water (Bear, 1979, p. 62). Water flows from areas of higher head toward areas of lower head. Effective porosity, n, differs from total porosity (volume of pore space per unit volume of aquifer material) in that it does not include pores that are too small to transmit water or "dead-end" pores, those that are not interconnected with other pores.

In unsaturated porous media, the average interstitial fluid velocity can be approximated (Bear, 1979, p. 209) as

$$\vec{v} = -\frac{\overline{\overline{K}}(\theta)}{\theta} \cdot \vec{\nabla} h, \qquad (2)$$

where

$\vec{v}$ = average interstitial fluid velocity [L/T],

$\overline{\overline{K}}(\theta)$ = unsaturated hydraulic conductivity tensor for medium, which is a function of moisture content [L/T], and

θ = moisture content of soil [dimensionless].

This form of the equation assumes that the movement of air in the soil is negligible and that the density of water is constant.

Molecular diffusion

In addition to advective transport, solutes spread within the fluid in the porous medium by molecular diffusion. Diffusion results from the random collision of solute molecules and produces a flux of solute particles from areas of higher to lower solute concentration (Bear, 1979). The solute flux, $\vec{J}$, can be given by Fick's first law as

$$\vec{J} = \theta \overline{\overline{D}}_d \cdot \vec{\nabla} C, \qquad (3a)$$

where

$\overline{\overline{D}}_d$ = second-rank diagonal tensor of molecular diffusion [L^2/T],

$\vec{\nabla} C$ = concentration gradient [M/L^4], and

C = concentration of solute (mass of solute per unit volume of fluid) [M/L^3].

Bear and Bachmat (1967) state that the coefficients of molecular diffusion in an isotropic medium are dependent on the diffusion coefficient of the particular solute in water and the tortuosity of the medium. Rates of molecular diffusion are independent of ground-water velocity, and diffusion occurs even in the absence of fluid movement.

Mechanical dispersion

The average interstitial fluid velocity represents a mathematical approximation. True velocities at points in the aquifer will differ from this average value, in both magnitude and direction. Local variations in ground-water velocity may not greatly affect the bulk movement of ground water, but they do control the fate of solute particles.

Mechanical dispersion describes the mixing and spreading of solutes along and transverse to the direction of flow in response to local variations in interstitial fluid velocities. On a microscopic scale (the scale of individual pores), mechanical dispersion results from (1) the distribution of velocities within an individual pore due to friction effects along the surface of soil grains, (2) differences in size of pores, (3) differences in path length for individual solute particles, and (4) the effect of converging and diverging flow paths (Freeze and Cherry, 1979, p. 75). On a larger (macroscopic) scale, mechanical dispersion results from local variations in hydraulic conductivity, and thus fluid velocity, owing to the heterogeneity of aquifer material (Bear, 1979, p. 229).

Laboratory tests on soil columns have shown that the flux of solutes due to mechanical dispersion can also be described using Fick's first law, as

$$\vec{J} = -\theta \overline{\overline{D}}_m \cdot \vec{\nabla} C, \qquad (3b)$$

where $\overline{\overline{D}}_m$ is the second-rank symmetric tensor of mechanical dispersion [L^2/T].

Scheidegger (1961) stated that the coefficients of mechanical dispersion can be related to the average interstitial fluid velocity by means of the geometric dispersivity of the medium. For a saturated porous medium, geometric dispersivity depends on hydraulic conductivity, length of a characteristic flow path, and tortuosity (Bear, 1972, p. 614). In a medium that is isotropic with respect to dispersion, geometric dispersivity can be expressed in terms of just two coefficients—longitudinal dispersivity, α_l, and transverse dispersivity, α_t (Bear, 1979, p. 234).

The elements of the mechanical dispersion tensor can be expressed in terms of longitudinal and transverse dispersivities, the magnitude of the velocity

vector, v, and the magnitudes of its components, v_x, v_y, and v_z (Bear, 1979, p. 235) as

$$\begin{aligned}
D_{m_{xx}} &= [\alpha_l v_x^2 + \alpha_t (v_y^2 + v_z^2)]/v \\
D_{m_{yy}} &= [\alpha_l v_y^2 + \alpha_t (v_x^2 + v_z^2)]/v \\
D_{m_{xy}} &= D_{m_{yx}} = (\alpha_l - \alpha_t) v_x v_y / v \\
D_{m_{yz}} &= D_{m_{zy}} = (\alpha_l - \alpha_t) v_y v_z / v \\
D_{m_{xz}} &= D_{m_{zx}} = (\alpha_l - \alpha_t) v_x v_z / v \\
D_{m_{zz}} &= [\alpha_l v_z^2 + \alpha_t (v_x^2 + v_y^2)]/v. \qquad (4)
\end{aligned}$$

If a coordinate system is chosen, such that the direction of the average ground-water velocity is aligned with the x-direction ($v=v_x$ and $v_y=v_z=0$), the off-diagonal terms in the dispersion tensor (eq. 4) will equal zero, and the mechanical dispersion tensor can be simplified to

$$\begin{aligned}
D_{m_x} &= D_{m_{xx}} = \alpha_l v \\
D_{m_y} &= D_{m_{yy}} = \alpha_t v \\
D_{m_z} &= D_{m_{zz}} = \alpha_t v. \qquad (5)
\end{aligned}$$

Hydrodynamic dispersion

As stated earlier, hydrodynamic dispersion is the flux of solute due to the combined effect of molecular diffusion and mechanical dispersion. Solute flux, $\vec{J}$, is given by Fick's first law as

$$\vec{J} = -\theta \overline{\overline{D}} \cdot \vec{\nabla} C, \qquad (6)$$

where $\overline{\overline{D}}$ is the hydrodynamic dispersion tensor.

In a flow system having uniform flow aligned with the x-axis, the coefficients of the hydrodynamic dispersion tensor, D_x, D_y, and D_z, are given by

$$\begin{aligned}
D_x &= D_{m_x} + D_d = \alpha_l v + D_d \\
D_y &= D_{m_y} + D_d = \alpha_t v + D_d \\
D_z &= D_{m_z} + D_d = \alpha_t v + D_d. \qquad (7)
\end{aligned}$$

The effects of mechanical dispersion generally are much greater than those of molecular diffusion, and, except at low ground-water velocities, the contribution of molecular diffusion often is negligible.

In laboratory experiments using homogeneous materials, values for longitudinal dispersivity, α_l, are typically between 0.004 and 0.4 inch (in), whereas in field studies, longitudinal dispersivities of as much as 328 feet (ft) have been determined (Freeze and Cherry, 1979). The larger field values can be attributed to increased mixing due to local variations in hydraulic conductivity (macrodispersion). A discussion of the apparent scale dependency of hydrodynamic dispersion is given in Anderson (1984). Transverse dispersivity is generally less than longitudinal dispersivity, by a factor of 5 to 20 (Freeze and Cherry, 1979, p. 400).

Advective-dispersive solute-transport equation

The advective-dispersive solute-transport equation describes the time rate of change of solute concentration for a single solute and can be written as

$$\frac{\partial \theta C}{\partial t} = -\vec{\nabla} \cdot [\theta \vec{v} C - \theta \overline{\overline{D}} \cdot \vec{\nabla} C] + \theta Q_s, \qquad (8)$$

where Q_s is used to represent a general source or sink term for production or loss of solute within the system.

Equation 8 (after Bear, 1979, p. 241) can be written in terms of volumetric rather than mass concentrations because the fluid density is assumed to be constant. This is usually valid for most ground-water flow systems in which solutes are present in relatively low concentrations.

The analytical solutions presented in this report are derived for idealized systems in which the ground-water velocity is assumed to be uniform, aligned with the x-axis, and of constant magnitude. The moisture content (equal to porosity for saturated material) and the coefficients of hydrodynamic dispersion (see eq. 7) are also assumed to be constant. Given these assumptions, the three-dimensional form of the solute-transport equation for a uniform flow system can be expressed as

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - V \frac{\partial C}{\partial x} + Q_s, \qquad (9)$$

where V represents the uniform velocity aligned with the x-axis.

In a thin aquifer in which the solute is uniformly mixed in the vertical (y-z) plane at the inflow boundary, the concentration gradient in the z-direction, $\partial C/\partial z$, equals zero. The two-dimensional solute-transport equation can be expressed as

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} + Q_s. \qquad (10)$$

Finally, if the solute concentration is uniform over the entire inflow boundary, such as in a soil column, the term $\partial C/\partial y$ would also equal zero, yielding the one-dimensional solute-transport equation that can be expressed as

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} + Q_s, \qquad (11)$$

where D represents the dispersion coefficient along the direction of flow.

Chemical transformation

In addition to physical mechanisms that govern the movement of solutes through the ground-water system, chemical transformations may alter the concentration of a contaminant species in solution. Possible chemical transformations include dissolution, precipitation, oxidation, reduction, biological degradation, radioactive decay, and adsorption and ion-exchange reactions between the solute and the solid matrix of the aquifer.

If the processes involved in chemical transformation can be described mathematically, they then can be incorporated in the source term, Q_s, in the solute-transport equation for each chemical species. The analytical solutions described herein have been derived for systems in which the chemical transformation terms are given by first-order (linear) relations. The relations and their incorporation in the solute-transport equation are described below.

Linear equilibrium adsorption

Many ionic inorganic solutes and nonpolar organic solutes can be removed from solution by adsorption onto the surface of soil particles. The solute may be attracted to soil surfaces by either electrical attraction, Van der Wals forces, or chemical bonding (chemisorption). A general expression for the change in solute concentration due to partitioning of solute particles on the solid matrix (in the absence of dispersive or advective fluxes) can be stated as

$$\theta\frac{\partial C}{\partial t}=-\rho_b\frac{\partial S}{\partial t}, \qquad (12)$$

where

ρ_b = bulk density of solid matrix measured as mass per unit volume of aquifer material [M/L^3], and

S = mass of solute adsorbed on solid matrix per unit mass of solid material [dimensionless].

The amount of solute remaining in solution depends on the amount of solute in the adsorbed phase. The functional relation is usually determined experimentally through a series of batch tests in which solutions of known initial concentration are mixed with differing amounts of adsorbate. After equilibrium is achieved, the final solute concentration of each solution is measured, and the mass of solute adsorbed is calculated. An equilibrium adsorption curve can then be fitted to these data. Equilibrium concentrations are dependent on temperature, and the adsorption curve at a particular temperature is termed an "equilibrium adsorption isotherm." A typical equilibrium adsorption isotherm is shown in figure 1.

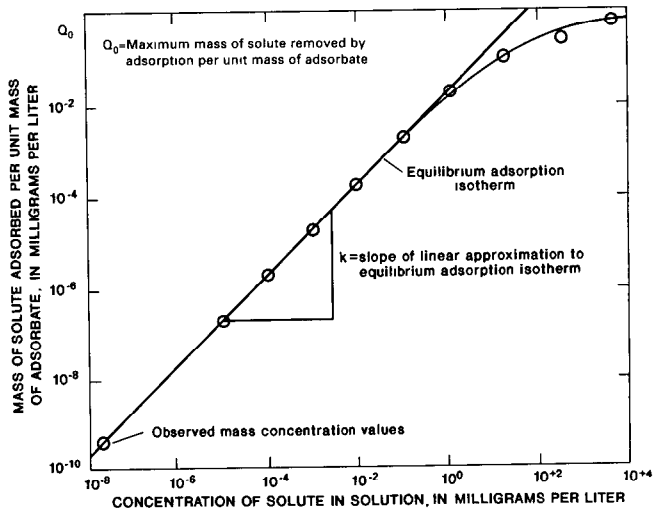

Figure 1.—Typical shape of equilibrium adsorption isotherm.

A linear approximation of the equilibrium adsorption isotherm is generally applicable in systems in which the solute concentration is low relative to the adsorptive capacity of the porous medium. The adsorption of various nonionic organic solutes at trace concentrations onto sediments and soils has also been shown to be linear (Cherry and others, 1984). Many nonlinear forms for the adsorption isotherm, some empirical and some that account for the physical mechanisms of adsorption, are suggested in the literature (see Helfferich, 1962). However, the transport equation that incorporates these other forms must be solved by numerical methods.

Because the amount adsorbed depends solely on the solute concentration, equation 12 can be expressed as

$$\theta\frac{\partial C}{\partial t}=-\rho_b\frac{\partial S}{\partial C}\frac{\partial C}{\partial t}, \qquad (13)$$

where $\partial S/\partial C$ is determined from the functional relation between C and S. For a linear equilibrium adsorption isotherm, $\partial S/\partial C$ is equal to the slope of the adsorption isotherm and often is termed k or the "partitioning coefficient." The source term can be incorporated in the general three-dimensional form of the solute-transport equation (eq. 9) to yield

$$R\frac{\partial C}{\partial t}=D_x\frac{\partial^2 C}{\partial x^2}+D_y\frac{\partial^2 C}{\partial y^2}+D_z\frac{\partial^2 C}{\partial z^2}-V\frac{\partial C}{\partial x}, \qquad (14)$$

where R is referred to as the "retardation factor," given by

$$R=1+\frac{k\rho_b}{\theta}. \qquad (15)$$

Dividing through by R yields

$$\frac{\partial C}{\partial t}=D_x^*\frac{\partial^2 C}{\partial x^2}+D_y^*\frac{\partial^2 C}{\partial y^2}+D_z^*\frac{\partial^2 C}{\partial z^2}-V^*\frac{\partial C}{\partial x}, \qquad (16)$$

where V^* and D_x^*, D_y^*, and D_z^* are the scaled (or retarded) velocity and dispersion coefficients, respectively. Equation 16 shows that transport of solutes subject to linear adsorption can be simulated in the same manner as a nonadsorbed solute using these scaled coefficients. Because the apparent velocity of the adsorbed solute is reduced, the solute will arrive at a given point later than a nonadsorbed solute.

The use of equilibrium isotherms assumes that equilibrium exists at all times between the porous medium and the solute in solution. This assumption is generally valid when the adsorption process is fast in relation to the ground-water velocity (Cherry and others, 1984). If adsorption proceeds slowly, kinetics of the reaction must be considered. Nonequilibrium adsorption relations can be incorporated in the transport equation, but numerical methods are needed for solution of the resulting equation.

The process of adsorption is also assumed to be reversible. If hysteresis effects during desorption are significant, other forms of the adsorption isotherms must be considered, and numerical methods would be required.

Ion exchange

Ion exchange is an adsorption process in which a cation in solution replaces another cation that is electrically bound to collodial material in the soil. Under certain conditions, ion exchange can be modeled in a manner similar to linear adsorption (R.W. Cleary, Princeton University, written commun., 1977). The exchange reaction for monovalent ions can be expressed as

$$A^+ + B^+R \rightleftarrows B^+ + A^+R, \qquad (17)$$

where A^+ is used to represent a cation in solution, R is the exchange medium, and B^+ represents the counter ion released from the exchanger. At equilibrium, a selectivity coefficient, K_s, can be defined, such that

$$K_s=\frac{[B^+][A^+R]}{[A^+][B^+R]}, \qquad (18)$$

where the bracketed terms represent the activities of each constituent.

Measured values of K_s can be used in simulating transport by making the following assumptions: (1) if all exchange sites are assumed to be occupied initially, then $[B^+R]$ represents the total cation exchange capacity (CEC) of the medium, which can be determined experimentally and then treated as a constant; (2) the counter ion, B^+, is usually present in solution at much greater concentrations than the solute A^+, and releases of additional amounts of the counter ion by exchange will not significantly alter its concentration; thus, $[B^+]$ can also be treated as a constant; and (3) the relation between the amount of solute on the exchange sites and the amount remaining in solution can be defined as

$$k_d=\frac{[A^+]}{[A^+R]}, \qquad (19)$$

where the distribution coefficient, k_d, is determined through laboratory batch tests.

Given these assumptions, the general expression for the change in solute concentration due to cation exchange can be expressed as

$$\theta\frac{\partial C}{\partial t}=-\rho_b k_d\frac{\partial C}{\partial t}, \qquad (20)$$

where

$$k_d=\frac{K_s \cdot CEC}{[B^+]}. \qquad (21)$$

This term would replace k in equation 15. For monovalent-divalent cation exchange, where

$$A^{++}+2B^+R \rightleftarrows 2B^+ + A^{++}R, \qquad (22)$$

the distribution coefficient can be given by

$$k_d=\frac{K_s \cdot CEC^2}{[B^+]^2}. \qquad (23)$$

First-order chemical reactions

Simple chemical reaction terms can be formulated to account for the kinetics of reactions under nonequilibrium conditions. A first-order chemical process, such as radioactive decay or biological degradation, involves the irreversible unimolecular conversion of solute A to solute B (A→B). The rate of the reaction can be given by

$$\frac{d[A]}{dt}=-\lambda[A], \qquad (24)$$

where λ is the rate coefficient [1/T]. The rate coefficient can be expressed in terms of the half-life of the solute, $T_{1/2}$ (the time required for the concentration of the solute species to be reduced to half the initial concentration), as

$$\lambda=\ln(2)/T_{1/2}=0.693/T_{1/2}. \quad (25)$$

Equation 9 can be written to incorporate the first-order reaction as

$$\frac{\partial C}{\partial t}=D_x\frac{\partial^2 C}{\partial x^2}+D_y\frac{\partial^2 C}{\partial y^2}+D_z\frac{\partial^2 C}{\partial z^2}-V\frac{\partial C}{\partial x}-\lambda C. \quad (26)$$

If the solute is subject to linear adsorption and to first-order chemical transformation in both the solute and adsorbed phases, equation 9 can be expressed as

$$R\frac{\partial C}{\partial t}=D_x\frac{\partial^2 C}{\partial x^2}+D_y\frac{\partial^2 C}{\partial y^2}+D_z\frac{\partial^2 C}{\partial z^2}-V\frac{\partial C}{\partial x}-R\lambda C \quad (27)$$

where R is the retardation factor (eq. 15) or

$$\frac{\partial C}{\partial t}=D_x^*\frac{\partial^2 C}{\partial x^2}+D_y^*\frac{\partial^2 C}{\partial y^2}+D_z^*\frac{\partial^2 C}{\partial z^2}-V^*\frac{\partial C}{\partial x}-\lambda C, \quad (28)$$

where V^* and D^* represent the scaled velocity and dispersion coefficients. If the adsorbed phase is not subject to chemical transformation, λ in equation 28 should be replaced by λ^*, where

$$\lambda^*=\lambda/R. \quad (29)$$

Some multiple-ion reactions can be approximated as a first-order reaction if all ions, except the species being considered, are present at high concentrations (R.W. Cleary, Princeton University, written commun., 1977). For example, if the reaction involves the conversion of solutes A and B to form solute C(A+B →C), the rate of reaction would be given as

$$\frac{d[A]}{dt}=-\lambda_{AB}[A][B]. \quad (30)$$

If solute B is present at high concentration, its concentration will not change significantly due to conversion of A and [B] can be treated as a constant. Equation 26 or 28 can then be used with a modified λ term, where $\lambda=\lambda_{AB}[B]$. General bimolecular or multiple-ion reactions result in nonlinear chemical source terms. Reversible reactions and multistep reactions require simultaneous solution of the transport equation written for each species. Simulation of transport involving these chemical processes usually requires numerical methods.

Initial conditions

To solve the solute-transport equation, a complete set of boundary and initial conditions must be specified. Initial conditions are used to define the solute concentration in the aquifer at the time inflow of solute begins. For the analytical solutions presented in this report, the initial conditions are specified such that all initial concentrations are zero. If the solute is conservative, a constant initial background solute concentration can be added to the calculated concentrations. Analytical solutions for one-dimensional transport of nonconservative solute transport with nonzero initial concentrations are given in van Genuchten and Alves (1982).

Boundary conditions

Three types of boundary conditions are generally associated with the solute-transport equation. The first-type (or Dirichlet) boundary condition specifies the value of the concentration along a section of the flow-system boundary. The second-type (or Neumann) boundary condition specifies the gradient in solute concentration across a section of the boundary. The third-type (or Cauchy) boundary condition is applied where the flux of solute across the boundary is dependent on the difference between a specified concentration value on one side of the boundary and the solute concentration on the opposite side of the boundary. These three types of boundary conditions are used to describe conditions at the inflow and outflow ends of the flow system and also along the lateral boundaries of two- and three-dimensional systems.

Inflow boundary

The third-type boundary condition best describes solute concentrations at the inflow end in a uniform flow system (Bear, 1979, p. 268), where a well-mixed solute enters the system by advection across the boundary and is transported away from the boundary by advection and dispersion. The boundary conditions can be given as

$$VC-D_x\frac{\partial C}{\partial x}=VC_o, \qquad x=0, \quad (31)$$

where C_o is the known measured concentration in the influent water. The third-type boundary condition allows for solute concentration at the inflow boundary to be lower than C_o initially and then to increase as more solute enters the system. Over time, the concentration gradient across the boundary, $\partial C/\partial x$, decreases as the concentration at the inflow boundary approaches C_o.

Alternatively, a first-type boundary condition can be specified at the inflow end, such that

$$C=C_o, \qquad x=0. \quad (32)$$

Application of this simpler form of boundary condition presumes that the concentration gradient across the

boundary equals zero as soon as flow begins. However, this may lead to overestimation of the mass of solute in the system at early times.

Equation 31 indicates that the difference between concentrations predicted for a system having a first-type source boundary condition and a system having a third-type boundary condition should decrease as the quantity D/V decreases. Additional discussions of the effect and relative merits of the different types of inflow boundary conditions are presented in Gershon and Nir (1969), van Genuchten and Alves (1982), and Parker and van Genuchten (1984).

Outflow boundary

Often, the outflow boundary of the system being simulated is far enough away from the solute source that the boundary will not affect solute concentrations within the area of interest. Such a system can be treated as being "semi-infinite," and either a first-type or second-type boundary condition can be specified as

$$C, \quad \frac{\partial C}{\partial x}=0, \quad x=\infty. \tag{33}$$

When the system has a finite length, and solute concentrations near the outflow boundary are of interest, selection of an appropriate boundary condition becomes more difficult. In general, if the system discharges to a large, well-mixed reservoir and the additional solute will not significantly alter reservoir concentrations, then a third-type or first-type boundary condition (similar to the inflow boundary) can be used. If the reservoir is small or not well mixed, such as at the end of the soil column in figure 2*A*, concentrations in the reservoir would equal solute concentration at the discharge end of the system, and thus no concentration gradient would exist across the boundary. This can be specified by a second-type boundary condition as

$$\frac{\partial C}{\partial x}=0, \quad x=L, \tag{34}$$

where L represents the length of the finite system.

Van Genuchten and Alves (1982, p. 90–96) analyzed the difference between predicted concentrations obtained using analytical solutions for a semi-infinite system and a finite system having a second-type boundary condition in terms of two dimensionless numbers: (1) the column Peclet number (P) and (2) the number of displaced pore volumes (T), which are defined by

$$P=\frac{VL}{D} \tag{35}$$

and

$$T=\frac{Vt}{L}. \tag{36}$$

They found that the predicted concentration at points near the outflow boundary begins to differ significantly for T greater than 0.25 and that the differences increase as T approaches 1 (corresponding to movement of the solute front closer to the outflow boundary). The magnitude of the difference and distance inward from the outflow boundary at which the solutions diverge decreases as P values increase.

Lateral boundaries

In two- and three-dimensional systems, impermeable or no-flow boundaries may be present at the base, top, or sides of the aquifer. Because there is no advective flux across the boundary, and molecular diffusion across the boundary is assumed to be negligible, the general third-type boundary condition simplifies to a second-type boundary condition, expressed as

$$\frac{\partial C}{\partial y}=0, \quad y=0 \text{ and } y=W \tag{37a}$$

and

$$\frac{\partial C}{\partial z}=0, \quad z=0 \text{ and } z=H \tag{37b}$$

where W and H represent the width and height of the aquifer, respectively.

In many cases, lateral boundaries of the system may be far enough away from the area of interest that the system can be treated as being infinite along the y- and z-axes. Boundary conditions can then be specified as

$$C, \frac{\partial C}{\partial y}=0, \quad y=\pm\infty \tag{38a}$$

and

$$C, \frac{\partial C}{\partial z}=0, \quad z=\pm\infty. \tag{38b}$$

Superposition

Because the solute-transport equation is a linear partial-differential equation, the principle of superposition can be used to calculate concentrations in the system if solute concentrations at the inflow boundary vary over time. The general form of the solution can be expressed as

$$C=C_o \cdot A(x,y,z,t)+(C_1-C_o) \cdot A(x,y,z[t-t_1]), \tag{39}$$

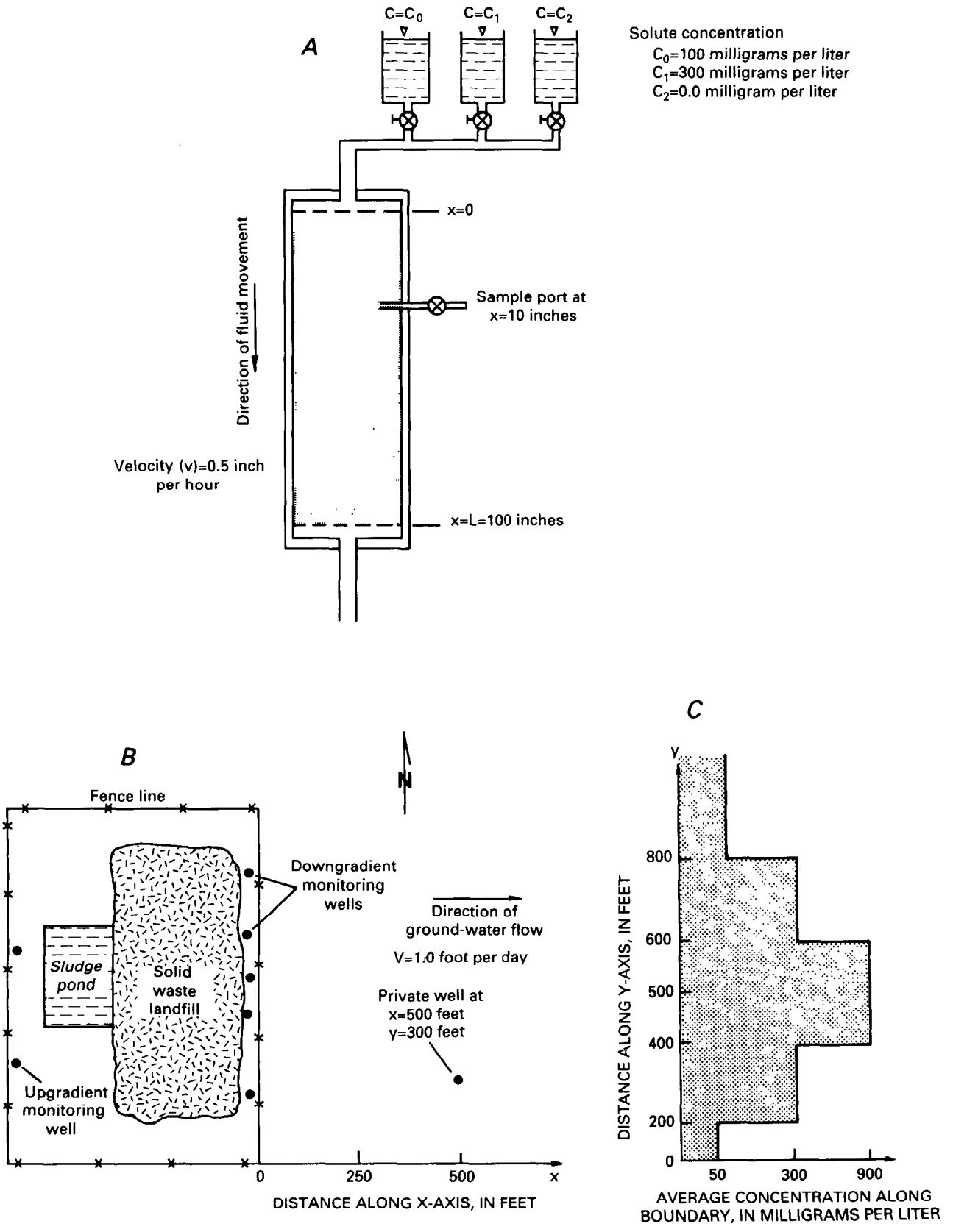

Figure 2.—Examples of situations in which the principle of superposition can be applied: A, soil column with time-varying input concentration (cases A and B in text), *B*, waste-disposal site with spatially varying input concentrations (case C in text), and *C*, plot of average concentration measured along waste-disposal site boundary.

where

C_o = initial solute concentration at boundary,

$A(x,y,z,t)$ = general form of analytical solution where concentration is a function of space and time,

C_1 = solute concentration at boundary after $t=t_1$, and

t_1 = time at which solute concentration changes at boundary.

The principle of superposition should be familiar to most hydrologists who have used analytical solutions (such as the Theis equation) in analyzing aquifer tests. Several examples are provided to illustrate its application to solute-transport simulation.

Case A:

A solution is passed through a 100-in-long soil column (fig. 2*A*) for a period of 10 hours, with V=0.5 inch per hour (in/h), D=0.05 square inch per hour (in^2/h), and C_o=100 milligrams per liter (mg/L). At the end of the 10-hour period, the concentration of the influent is increased to C_1=300 mg/L. Of interest is the concentration at x=10 in at the end of a total elapsed time of 20 hours.

The analytical solution for transport of a conservative solute in a semi-infinite column (assuming that boundary effects at x=L are negligible) with a first-type inflow boundary condition was given by Ogata and Banks (1961) as

$$A(x,t)=\frac{1}{2}\left\{\mathrm{erfc}\left[\frac{x-Vt}{2\sqrt{Dt}}\right]+\exp\left[\frac{Vx}{D}\right]\cdot\mathrm{erfc}\left[\frac{x+Vt}{2\sqrt{Dt}}\right]\right\},$$

where erfc is the complementary error function. (The solution is described in more detail later.) For the values given, equation 39 becomes

$$\begin{aligned}C(10\text{ in, }20\text{ hours})&=100\text{ mg/L}\cdot A(10\text{ in, }20\text{ hours})+(300\text{ mg/L}-100\text{ mg/L})\cdot A(10\text{ in, }[20\text{ hours}-10\text{ hours}])\\&=100\text{ mg/L}\cdot(0.984)+200\text{ mg/L}\cdot(0.088)\\&=116.0\text{ mg/L}.\end{aligned}$$

Case B:

This case is similar to case A, except that at the end of 10 hours, solute-free water (C_2=0.0 mg/L) is passed through the soil column, thus creating a solute pulse of finite duration. The concentration of solute at x=10 in and t=20 hours can be given from equation 39 as

$$\begin{aligned}C(10\text{ in, }20\text{ hours})&=100\text{ mg/L}\cdot A(10\text{ in, }20\text{ hours})+(0-100\text{ mg/L})\cdot A(10\text{ in, }[20-10\text{ hours}])\\&=100\text{ mg/L}\cdot(0.984)-100\text{ mg/L}\cdot(0.088)\\&=89.6\text{ mg/L}.\end{aligned}$$

The principle of superposition can also be used to simulate more complex solute configurations at the boundary of two- and three-dimensional systems, as shown in case C. Also, if solute sources are at two locations, the calculated concentration from the first source at a particular point of interest can simply be added to the calculated concentration from the second source at that point.

Case C:

A waste-disposal site, shown in plan view in figure 2*B*, has a solid-waste landfill and a smaller area for sludge disposal. Measured concentrations in fully screened wells along the eastern boundary downgradient from the landfill had chloride concentrations averaging 300 mg/L. Wells downgradient from both the sludge pond and the landfill had concentrations averaging 900 mg/L. Background chloride concentrations are 50 mg/L. Given V=1 foot per day (ft/d), D_x =20 feet squared per day (ft^2/d), and D_y=4 ft^2/d, calculate the concentration at a private well located at x=500 ft and y=300 ft at the end of 1 year.

The analytical solution for transport of a conservative solute in an infinitely wide aquifer having a finite-width or "strip" source along the inflow boundary is modified from Cleary and Ungs (1978, p. 17):

$$A(x,y,Y_1,Y_2,t)=\frac{x}{4\sqrt{\pi D_x}}\exp\left(\frac{Vx}{2D_x}\right)\int_o^t \tau^{-\frac{3}{2}}\exp\left[\frac{-x^2}{4D_x\tau}-\frac{V^2\tau}{4D_x}\right]\cdot\left\{\mathrm{erfc}\left[\frac{Y_1-y}{2\sqrt{D_y\tau}}\right]-\mathrm{erfc}\left[\frac{Y_2-y}{2\sqrt{D_y\tau}}\right]\right\}d\tau,$$

where Y_1 and Y_2 are coordinates of the endpoints of the source on the y-axis and τ is a dummy variable of integration. The solute source can be represented by two strip sources, the first extending from Y_1=200 to Y_2=800 ft, with an effective concentration, C_1, of 250 mg/L (difference between measured and background concentration) and the second extending from Y_1= 400 to Y_2=600 ft, with a concentration, C_2, of 600 mg/L (measured concentration minus first-source effective concentration and background concentration). The concentration at the private well can be calculated as

$$C(500\text{ ft, }300\text{ ft})=C_{background}+C_1\cdot A(500\text{ ft, }300\text{ ft, }200\text{ ft, }800\text{ ft, }365\text{ days})+C_2\cdot A(500\text{ ft, }300\text{ ft, }400\text{ ft, }600\text{ ft, }365\text{ days})$$

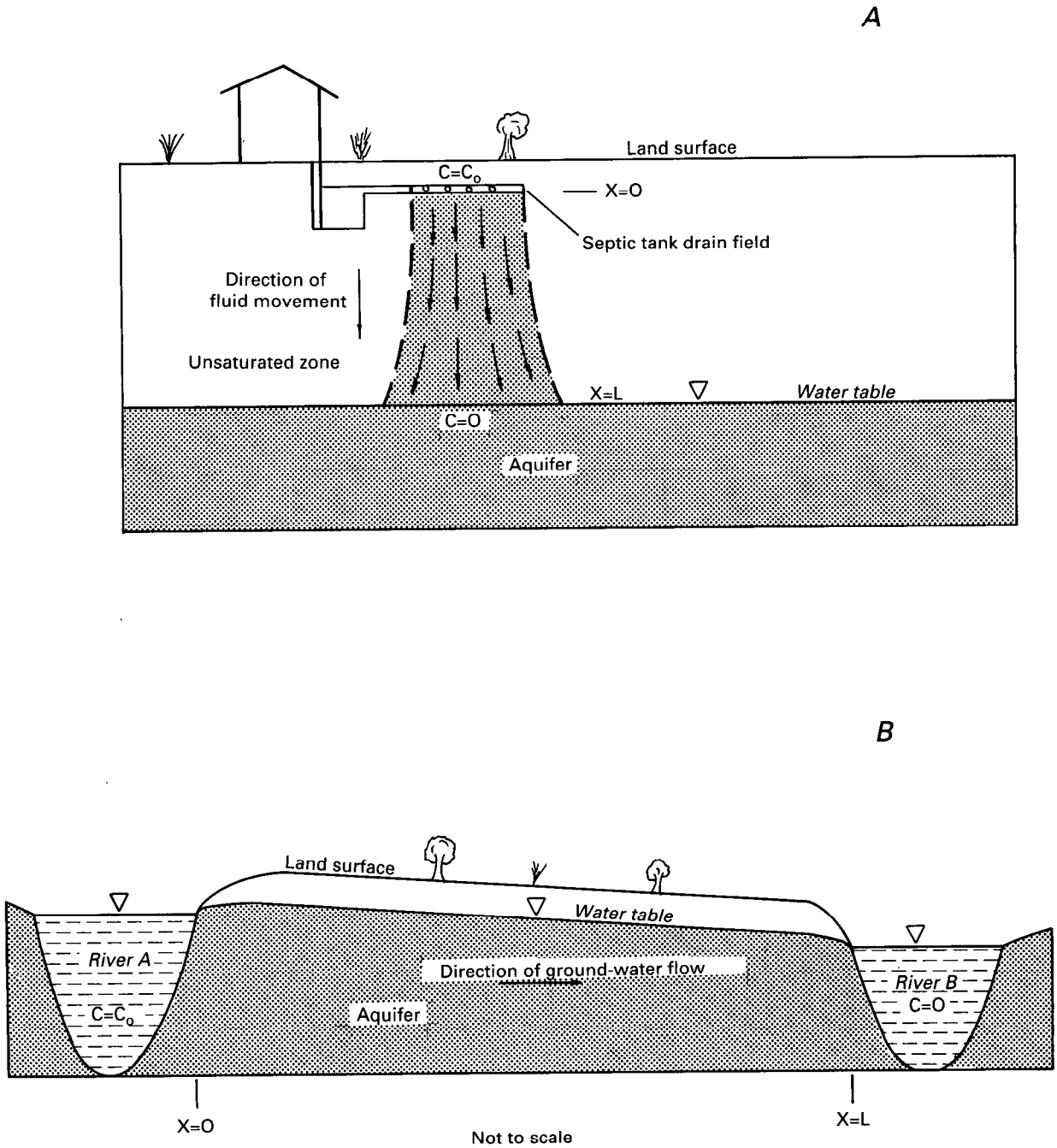

Figure 3.—Two examples (*A* and *B*) of contaminant movement in field settings that can be simulated as one-dimensional solute-transport systems.

$$=50 \text{ mg/L}+250 \text{ mg/L}\cdot(0.1612)+600 \text{ mg/L}\cdot(0.1354)$$
$$=171.5 \text{ mg/L}.$$

One-Dimensional Solute Transport

Many analytical solutions for the one-dimensional form of the solute-transport equation (eq. 11) were developed for study of dispersion phenomena in soil or adsorption columns. Some field situations can also be idealized as one-dimensional transport systems; two examples are shown in figure 3. Figure 3*A* represents steady vertical flow through the unsaturated zone beneath a septic tank drain field. Transport at the center of the field is simulated, and the horizontal spread of solutes along the edges of the field is ignored. Figure 3*B* represents a case of steady hori-

zontal ground-water flow from river A, which has been contaminated, to river B.

One-dimensional systems can be finite, semi-infinite, or infinite in extent. In the finite or semi-infinite systems, water containing a known concentration of a contaminant species enters the system at the origin (at x=0). Water and solute exit at the opposite end of the system (at x=L), which could represent the water table, a stream, or the end of a soil column (fig. 3).

In the finite-length system, the outflow boundary is close enough that it will have an effect on the magnitude of concentrations within the area of interest. If the outflow boundary is far enough away as to have negligible effect on solute concentrations in the area of interest (equivalent to $T<0.25$, where T is the number of displaced pore volumes), solutions for a semi-infinite system can be used and are generally easier to evaluate.

An example of transport in an infinite system might be the injection of a solute into the center of a long soil column. In this case, the spread of solute, both upgradient and downgradient from the source, is of interest. Solutions for an infinite system can be found in van Genuchten and Alves (1982) and Bear (1972, 1979).

For the four analytical solutions presented in this section, either a first- or third-type boundary condition is specified at the inflow end of a finite or semi-infinite system. Specifically, the solutions are for a

- Finite system with a first-type boundary condition at the inflow end,
- Finite system with a third-type boundary condition at the inflow end,
- Semi-infinite system with a first-type boundary condition at the inflow end, and
- Semi-infinite system with a third-type boundary condition at the inflow end.

Solutions for the finite systems assume a second-type boundary condition at the outflow end.

Two computer programs, FINITE and SEMINF, were developed to calculate concentrations in these four systems as a function of distance and elapsed time. These programs are also described in this section. The format used in presenting each of the solutions may seem repetitive, but it provides for easy reference.

Finite system with first-type source boundary condition

Governing equation

One-dimensional solute-transport equation:

$$\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial x^2}-V\frac{\partial C}{\partial x}-\lambda C \tag{40}$$

Boundary conditions:

$$C=C_o, \qquad x=0 \tag{41}$$

$$\frac{\partial C}{\partial x}=0, \qquad x=L \tag{42}$$

Initial condition:

$$C=0, \qquad 0<x<L \qquad \text{at } t=0 \tag{43}$$

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 van Genuchten and Alves (1982, p. 63–65):

$$C(x,t)=C_o\left\{\frac{\exp\left[\frac{(V-U)x}{2D}\right]+\frac{(U-V)}{(U+V)}\exp\left[\left(\frac{V+U}{2D}\right)x-\frac{UL}{D}\right]}{\left[1+\frac{(U-V)}{(U+V)}\exp\left[\frac{-UL}{D}\right]\right]}\right.$$

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

$$\left.\cdot\sum_{i=1}^{\infty}\frac{\beta_i\sin\left(\frac{\beta_i x}{L}\right)\left[\beta_i^2+\left(\frac{VL}{2D}\right)^2\right]\exp\left[-\frac{\beta_i^2Dt}{L^2}\right]}{\left[\beta_i^2+\left(\frac{VL}{2D}\right)^2+\frac{VL}{2D}\right]\left[\beta_i^2+\left(\frac{VL}{2D}\right)^2+\frac{\lambda L^2}{D}\right]}\right\}, \tag{44}$$

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

$$\beta\cot\beta+\frac{VL}{2D}=0. \tag{45}$$

Comments:

Values of the first six roots of equation 45, $a\cdot\cot(a)+c=0$, are tabulated in Carslaw and Jaeger (1959, p. 492) for various values of the constant c. Additional roots of equation 45 can be found through standard root-search techniques.

The maximum number of terms that should be computed in the infinite series summation depends on

how fast the series converges. Convergence is usually a problem at early times (or at $T << 1$) near the origin ($x=o$), especially when the column Peclet number (P in eq. 35) is relatively large. The program described below determines that the series has converged if the absolute value of the last term in the series is less than 1×10^{-12}. A good initial estimate for the maximum number of terms is 100, but more should be used if the program indicates that the series did not converge. A minimum of 25 roots is used by the program.

For a solute that is not subject to first-order chemical transformation ($\lambda=0$), equation 44 can be replaced (Cleary and Adrian, 1973; Wexler and Cleary, 1979) by

$$C(x,t)=C_o\left\{1-2\exp\left[\frac{Vx}{2D}-\frac{V^2t}{4D}\right]\cdot\sum_{i=1}^{\infty}\frac{\beta_i\sin\left(\frac{\beta_i x}{L}\right)\exp\left(-\frac{\beta_i^2Dt}{L^2}\right)}{\beta_i^2+\left(\frac{VL}{2D}\right)^2+\frac{VL}{2D}}\right\}. \quad (46)$$

For large values of time (steady-state solution), equation 44 can be reduced (van Genuchten and Alves, 1982, p. 58) to

$$C(x)=C_o\exp\frac{\left[\frac{(V-U)x}{2D}\right]+\frac{(U-V)}{(U+V)}\exp\left[\frac{(V+U)x}{2D}-\frac{UL}{D}\right]}{\left[1+\frac{(U-V)}{(U+V)}\exp\left(\frac{-UL}{D}\right)\right]}. \quad (47)$$

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. 44 and 47 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 FINITE

The program FINITE computes the analytical solution to the one-dimensional solute-transport equation for a finite system with a first-type (eq. 44) or third-type (eq. 52) source boundary condition at the inflow end. It consists of a main program and four subroutines—ROOT1, ROOT3, CNRML1, and CNRML3. The function of the main program and subroutines ROOT1 and CNRML1 are outlined below; the program code listing is presented in attachment 2. Subroutines ROOT3 and CNRML3 are called when a third-type boundary condition is specified and are described in a subsequent section.

The program also calls the output subroutines TITLE, OFILE, and PLOT1D, which are common to most of the 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 1.

The program calls subroutine ROOT1 to compute the positive roots of equation 45 when a first-type source boundary condition is specified and then 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.

Subroutines ROOT1 and CNRML1

Subroutine ROOT1 calculates the roots of the equation

$$a\cdot\cot(a)+c=0$$

by an iterative procedure. The first root is known to lie between $\pi/2$ and π, and an initial estimate of $0.75\,\pi$ is made. Newton's second-order method (Salvadori and Baron, 1961, p. 6) is used to correct and update the estimate at each iteration. A maximum of 50 iterations and a convergence criterion of 1.0×10^{-10} are set in the subroutine. Each subsequent root of the equation is about π greater than the previous one. This value is used as an initial estimate in the search for the remaining roots.

Subroutine CNRML1 calculates the normalized concentration (C/C_o) for a particular time value and x-distance value, using equation 44 for a solute subject to first-order chemical transformation and equation 46 if the solute is conservative ($\lambda=0$). The number of terms taken in the infinite series summation is specified in the input data.

Sample problems 1a and 1b

Two sample problems are presented that use data similar to the data given in Lai and Jurinak (1972). In sample problem 1a, a conservative solute is introduced into a saturated soil column under steady flow. Model variables are

Velocity (V)	=0.6 in/h
Longitudinal dispersion (D)	=0.6 in^2/h
System length (L)	=12 in

Table 1.—Input data format for the program FINITE

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 a first-type boundary condition; NBC = 3 for a 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	NROOT	Number of terms used in infinite series summation.
	17 - 20	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	XL	Length of flow system.[1]
	51 - 60	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).

[1]All units must be consistent.

Solute concentration at inflow boundary (C_o) =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 1b, a solute is removed by linear equilibrium adsorption. Additional model variables are

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 and equations 15 and 16 (substituting n for θ), the terms obtained are

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.

The input data sets for sample problems 1a and 1b are shown in figures 4*A* and 5*A*; computer plots of concentration profiles generated by the program FINITE are shown in figures 4*B* and 5*B*. Comparison of the concentration profiles at 20 hours shows the retarding effect of adsorption on solute movement.

Program output for sample problem 1a is presented in attachment 4. Sample problems 1a and 1b each required 3.9 seconds (s) of central processing unit (CPU) time on a Prime model 9955 *Mod II*.

A

```
Sample Problem 1a -- Solute transport in a finite-length
soil column with a first-type boundary condition at x=0
Model Parameters:  L=12 in, V=0.6 in/h, D=0.6 in**2/h
                   K1=0.0 per h, C0=1.0 mg/L
====
   1  25  05  50   1
MG/L      IN/H      IN**2/H   PER HOUR  INCHES    HOURS
      1.0        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

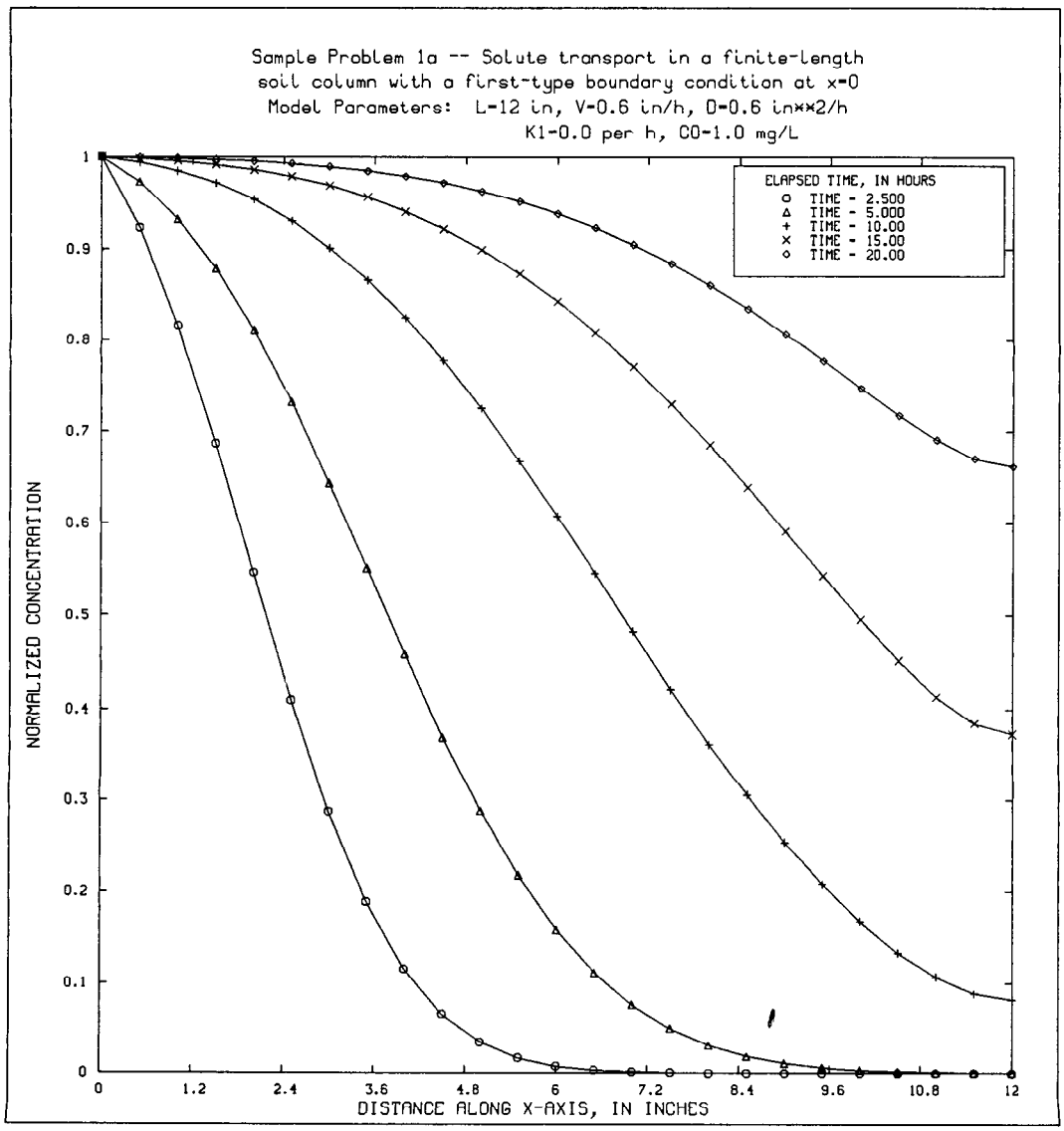

Figure 4.—(*A*) Sample input data set, and (*B*) concentration profiles generated by the program FINITE for a conservative solute in a finite-length system with first-type source boundary condition after 2.5, 5, 10, 15, and 20 hours (sample problem 1a).

A

```
Sample Problem 1b -- Solute transport in a finite-length
soil column with a first-type boundary condition at x=0
Model Parameters:  L=12 in, V=0.072 in/h, D=0.072 in**2/h
                   K1=0.0 per h, C0=1.0 mg/L
Solute is subject to linear adsorption
====
   1  25  04  50   1
MG/L      IN/H      IN**2/H   PER HOUR  INCHES    HOURS
      1.0     0.072     0.072       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
     20.0      50.0     100.0     150.0
```

B

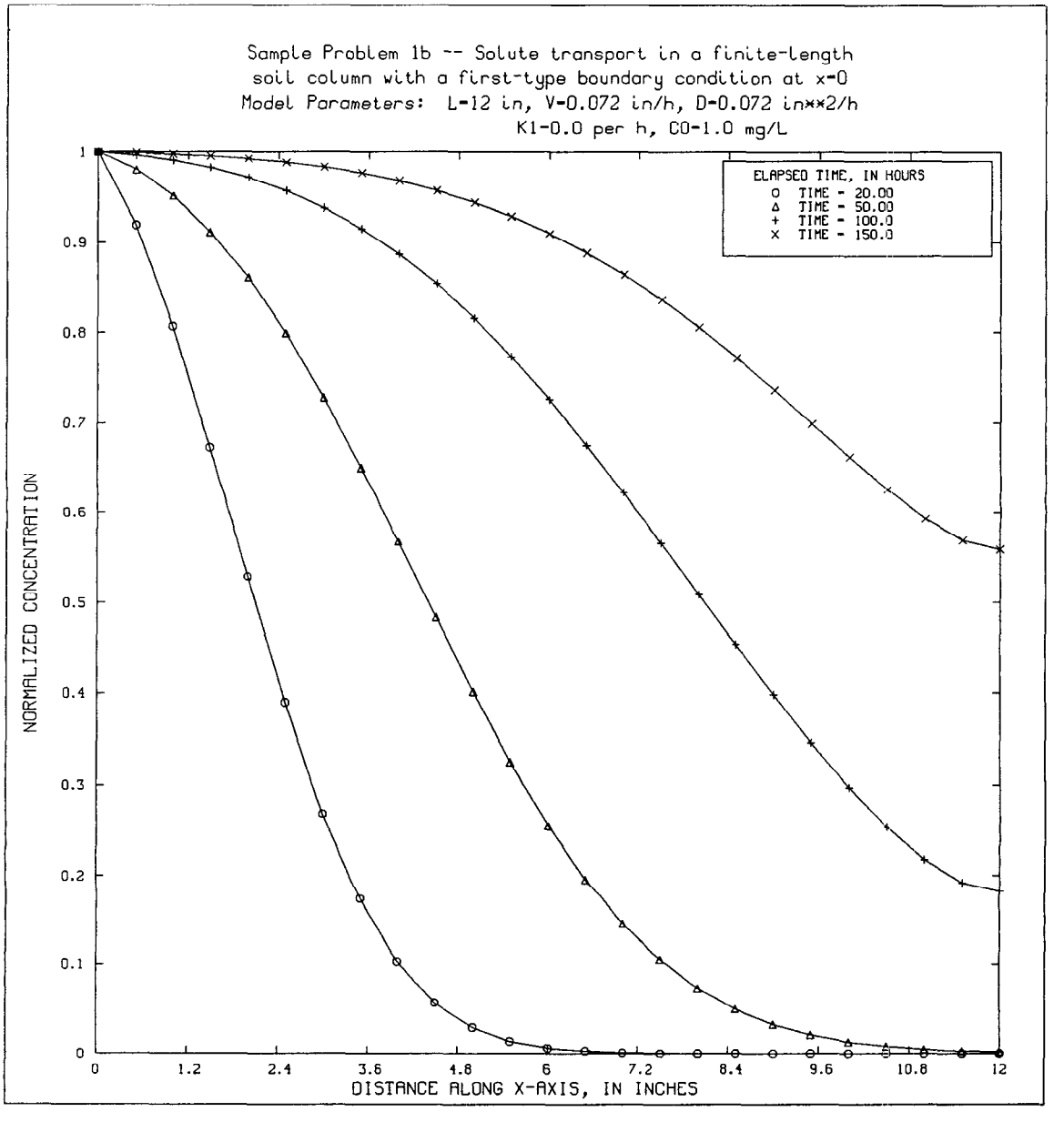

Figure 5.—(*A*) Sample input data set, and (*B*) concentration profiles generated by the program FINITE for a solute subject to linear adsorption in a finite-length system with first-type source boundary condition after 20, 50, 100, and 150 hours (sample problem 1b).

Finite system with third-type source boundary condition

Governing equation

One-dimensional solute-transport equation:

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

Boundary conditions:

$$VC_o=VC-D\frac{\partial C}{\partial x}, \qquad x=0 \tag{49}$$

$$\frac{\partial C}{\partial x}=0, \qquad x=L \tag{50}$$

Initial condition:

$$C=0, \qquad 0<x<L \qquad \text{at } t=0 \tag{51}$$

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):

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

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

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

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

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

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

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

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

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

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

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

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

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_o) 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_o)	=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 6*A*; a computer plot of concentration profiles generated by the program FINITE is shown in figure 6*B*. 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 4*B* and 6*B* 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:

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

Boundary conditions:

$$C = C_o, \qquad x = 0 \qquad (57)$$

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

Initial condition:

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

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):

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

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 in**2/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       0.0      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

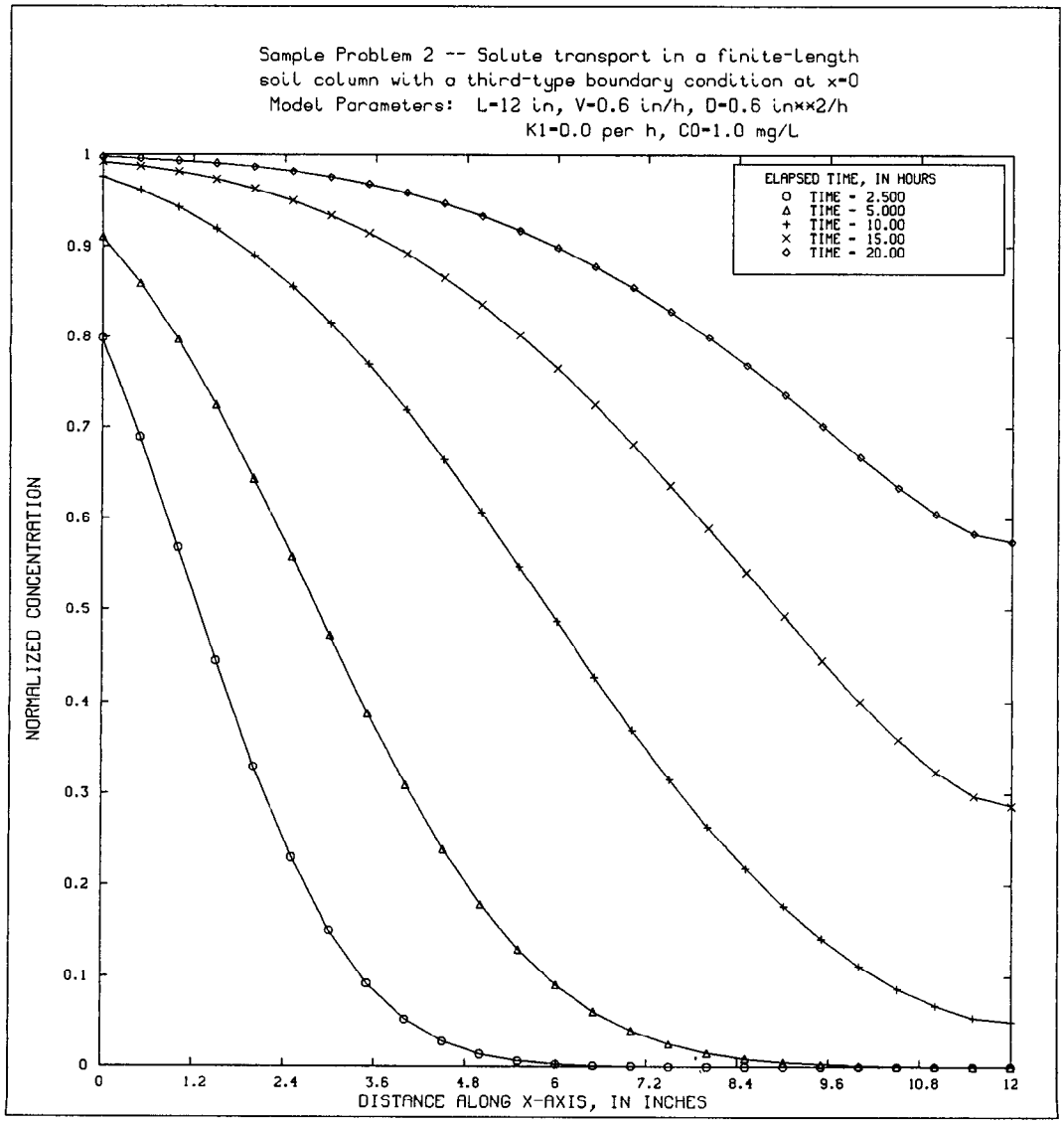

Figure 6.—(*A*) Sample input data set, and (*B*) concentration profiles generated by the program FINITE for a conservative solute in a finite-length system with third-type source boundary condition after 2.5, 5, 10, 15, and 20 hours (sample problem 2).

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

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

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

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 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_o) 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_o)	=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 7*A* and 8*A*; 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. 7*B* and 8*B*) shows the effect of both solute decay and adsorption on solute movement. Comparison of figures 7*B* and 4*B* 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).

[1]All units must be consistent.

steeper gradients near x=12.0 in (fig. 7*B*). 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:

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

Boundary conditions:

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

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

Initial condition:

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

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 in**2/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       0.0       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

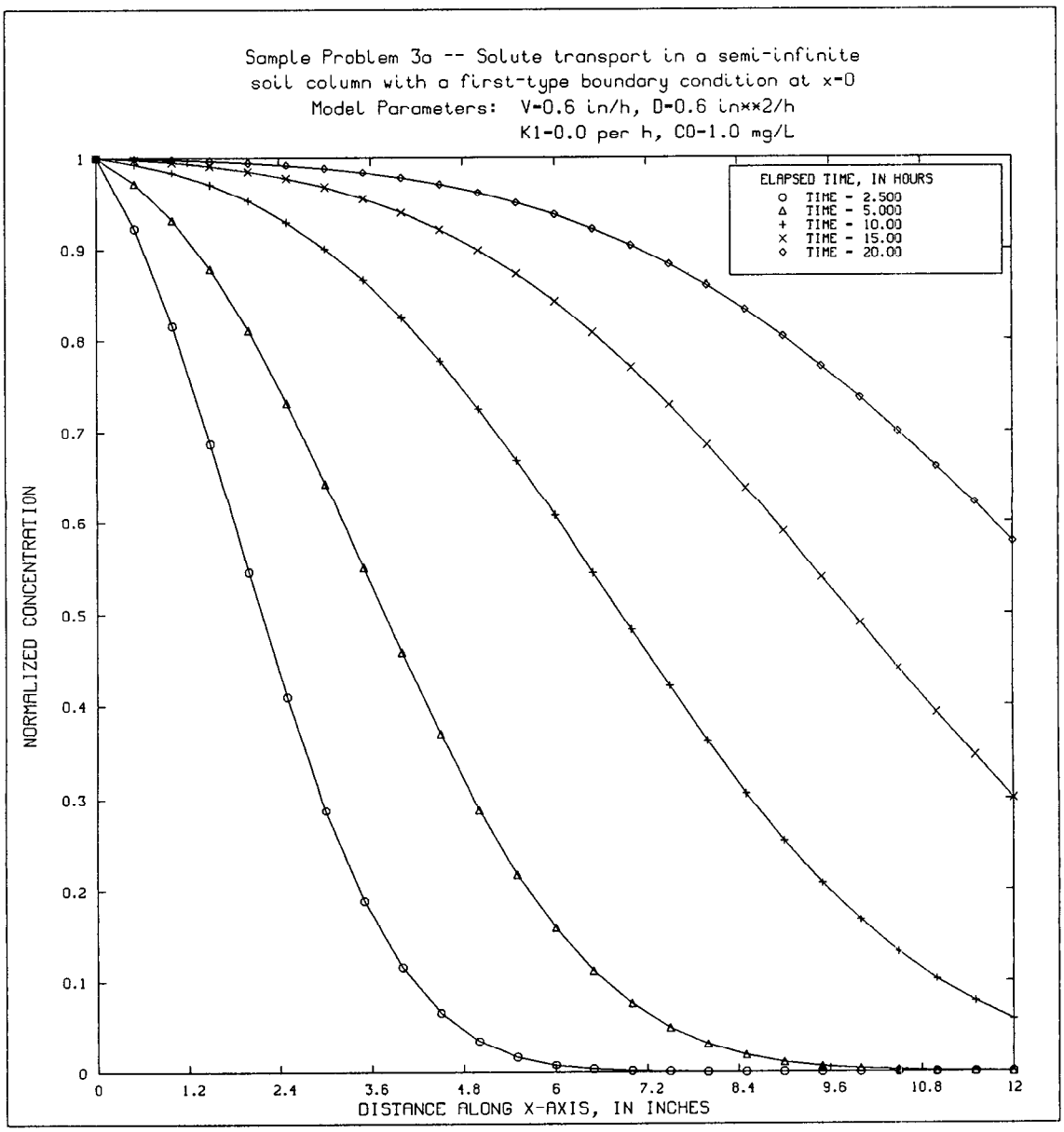

Figure 7.—(*A*) Sample input data set, and (*B*) concentration profiles generated by the program SEMINF for a conservative solute in a semi-infinite system with first-type source boundary condition after 2.5, 5, 10, 15, and 20 hours (sample problem 3a).

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 in**2/h
                   K1=0.0038 per h, C0=1.0 mg/L
Solute is subject to first-order decay and linear adsorption
====
   1  25  04   1
MG/L       IN/H       IN**2/H   PER HOUR  INCHES    HOURS
      1.0      0.072     0.072    0.0038       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
     20.0       50.0     100.0     150.0
```

B

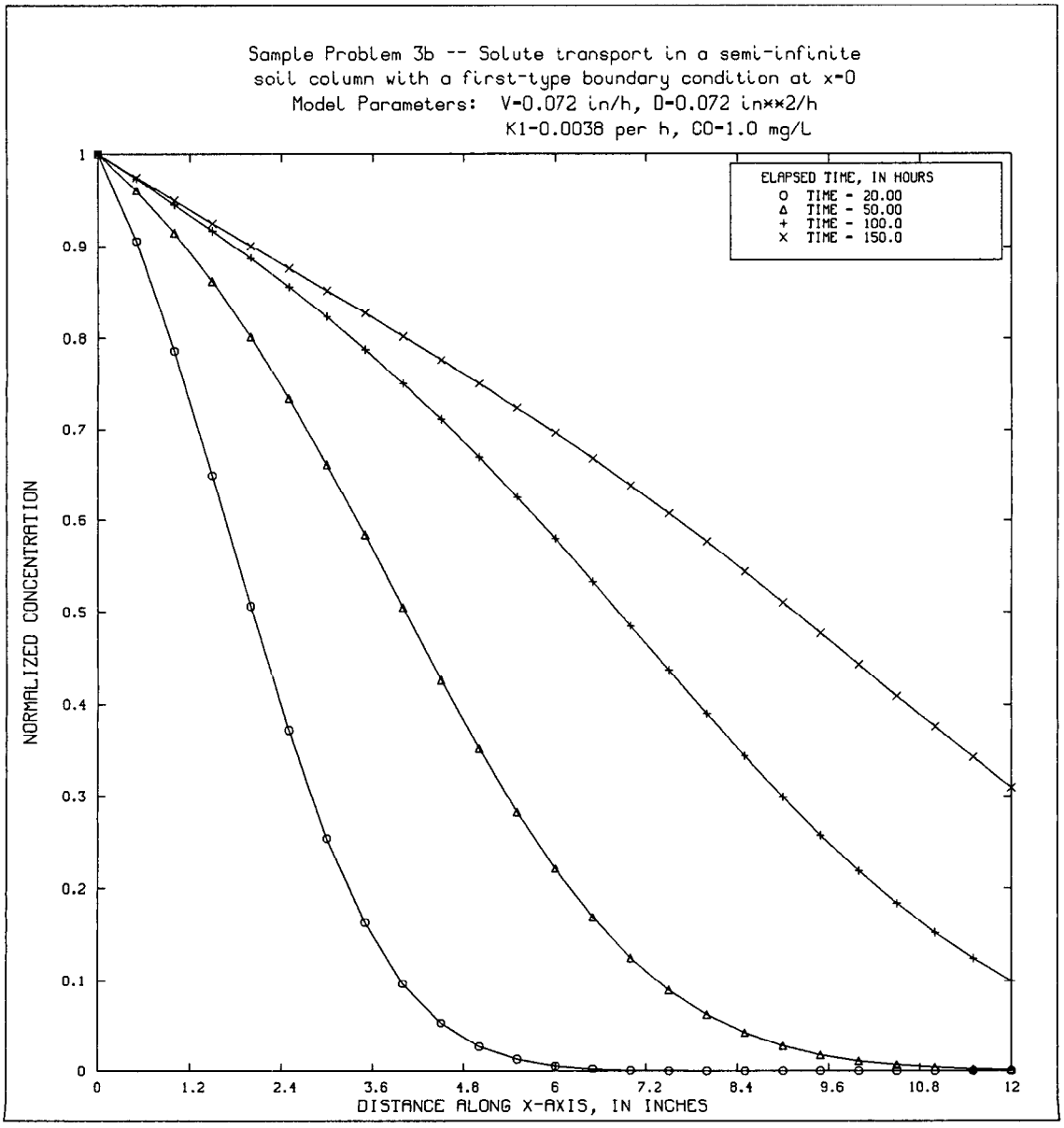

Figure 8.—(*A*) Sample input data set, and (*B*) concentration profiles generated by the program SEMINF for a solute subject to first-order decay and linear equilibrium adsorption in a semi-infinite system with first-type source boundary condition after 20, 50, 100, and 150 hours (sample problem 3b).

$$C(x,t)=\frac{C_oV^2}{4\lambda D}\left\{2\exp\left[\frac{xV}{D}-\lambda t\right]\cdot\mathrm{erfc}\left[\frac{x+Vt}{2\sqrt{Dt}}\right]\right.$$

$$+\left(\frac{U}{V}-1\right)\exp\left[\frac{x}{2D}(V-U)\right]\cdot\mathrm{erfc}\left[\frac{x-Ut}{2\sqrt{Dt}}\right]$$

$$\left.-\left(\frac{U}{V}+1\right)\exp\left[\frac{x}{2D}(V+U)\right]\cdot\mathrm{erfc}\left[\frac{x+Ut}{2\sqrt{Dt}}\right]\right\}, \quad (67)$$

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

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

$$\left.-\frac{1}{2}\left[1+\frac{Vx}{D}+\frac{V^2t}{D}\right]\exp\left(\frac{Vx}{D}\right)\cdot\mathrm{erfc}\left[\frac{x+Vt}{2\sqrt{Dt}}\right]\right\}. \quad (68)$$

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 9*A*; a computer plot of concentration profiles generated by the program SEMINF is shown in figure 9*B*. 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 in**2/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       0.0       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

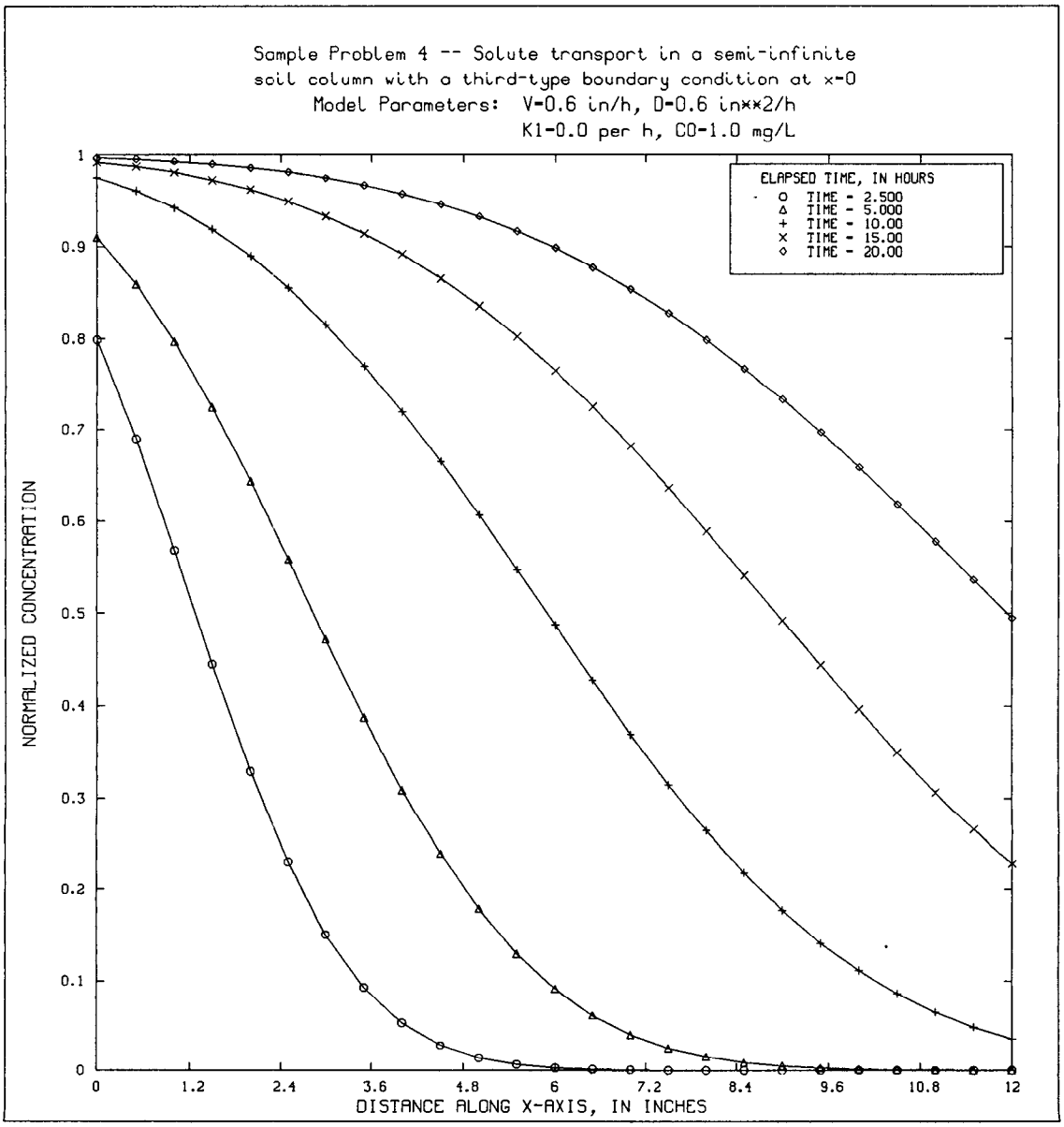

Figure 9.—(*A*) Sample input data set, and (*B*) concentration profiles generated by the program SEMINF for a conservative solute in a semi-infinite system with third-type source boundary condition after 2.5, 5, 10, 15, and 20 hours (sample problem 4).

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_o. At the boundary of the strip source (at $y=Y_1$ or $y=Y_2$), the concentration is equal to $0.5\ C_o$. 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

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

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

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

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

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

$$+\frac{Q'}{n}dt\ C_o\delta(x-X_c)\delta(y-Y_c)\delta(t-t') \qquad (72)$$

Boundary conditions:

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

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

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:

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

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

$$C(x,y,t)=\frac{C_oQ'}{4n\pi\sqrt{D_xD_y}}\exp\left[\frac{V(x-X_c)}{2D_x}\right]\int_o^t\frac{1}{\tau}$$

$$\cdot\exp\left[-\left(\frac{V^2}{4D_x}+\lambda\right)\tau-\frac{(x-X_c)^2}{4D_x\tau}-\frac{(y-Y_c)^2}{4D_y\tau}\right]d\tau, \qquad (76)$$

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

$$C(x,y)=\frac{Q'\ C_o\exp\left[\frac{V(x-X_c)}{2Dx}\right]}{2n\pi\sqrt{D_xD_y}}$$

$$K_o\left\{\sqrt{\left(\frac{V^2}{4D_x}+\lambda\right)\left[\frac{(x-X_c)^2}{D_x}+\frac{(y-Y_c)^2}{D_y}\right]}\right\}, \qquad (77)$$

where K_o is the modified Bessel function of second kind and zero order. Tables of values and polynomial approximations for $K_o(x)$ 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

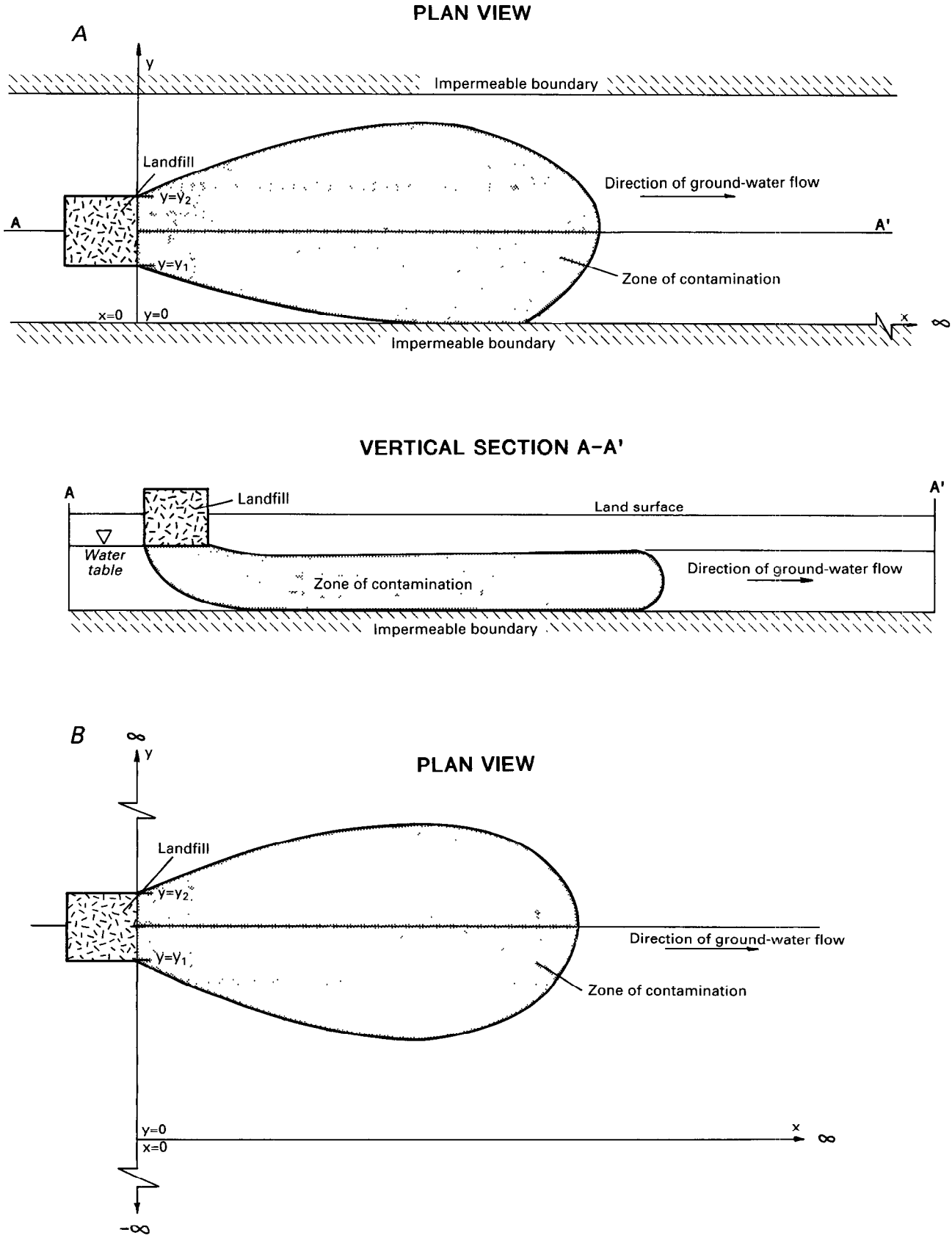

Figure 10.—(*A*) Plan view and vertical section of idealized two-dimensional solute transport in an aquifer of semi-infinite length and finite width, and (*B*) plan view of idealized two-dimensional solute transport in an aquifer of semi-infinite length and infinite width.

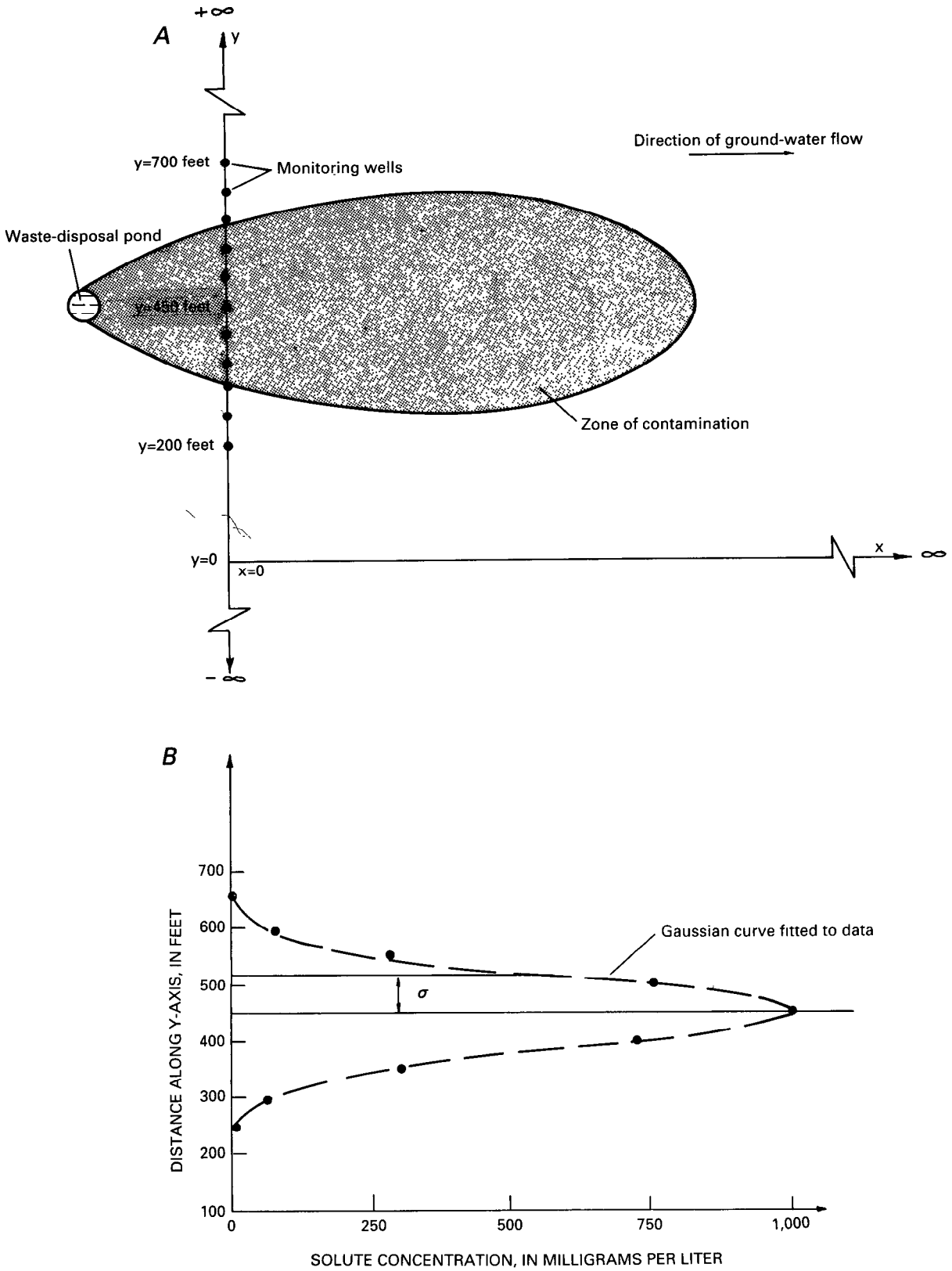

Figure 11.—(*A*) Plan view of a semi-infinite aquifer of infinite width showing location of waste-disposal pond and monitoring wells, and graph of (*B*) observed solute concentration values and gaussian curve used to approximate concentration distribution at x=0.

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).

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

[2]Data 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_o) 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

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

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 nth 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_o)	=1,000 mg/L
Point-source location (X_c,Y_c)	=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 12*A*. A computer-generated contour plot of normalized concentrations (C/C_o) at both time values is shown in figure 12*B*. 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:

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

Boundary conditions:

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

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

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

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

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

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
====
  26  21  02 104   3
MG/L      FT/D      FT**2/D   PER DAY   FEET      DAYS
    1000.0       2.0      60.0      12.0
       0.0     500.0      12.5      0.25
     -60.0     -50.0    -40.00     -30.0     -20.0     -10.0      10.0      20.0
      30.0      40.0      50.0      60.0      70.0      80.0      90.0     100.0
     110.0     120.0     130.0     140.0     150.0     160.0     170.0     180.0
     190.0     200.0
     450.0     455.0     460.0     465.0     470.0     475.0     480.0     485.0
     490.0     495.0     500.0     505.0     510.0     515.0     520.0     525.0
     530.0     535.0     540.0     545.0     550.0
      25.0     100.0
      30.0      30.0       0.1
```

B

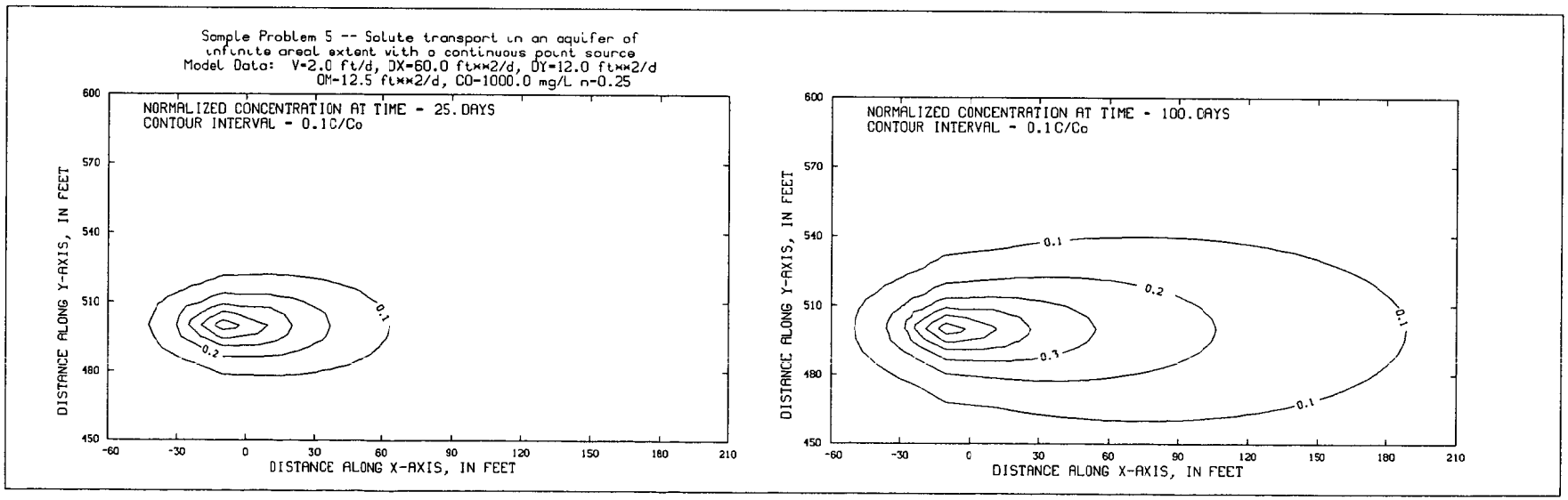

Figure 12.—(*A*) Sample input data set, and (*B*) computer plot of normalized concentration contours generated by the program POINT2 for a conservative solute injected continuously into an aquifer of infinite areal extent after 25 and 100 days (sample problem 5).

Initial condition:

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

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):

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

where

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

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

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

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

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_o) 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_l)	=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	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.
	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).

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

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

From these values, the terms obtained are

Dispersion in x-direction (D_x) =200 ft^2/d
Dispersion in y-direction (D_y) = 60 ft^2/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 13*A*. A computer-generated contour plot of normalized concentration (C/C_o) at each time value is shown in figure 13*B*. 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, C0=1000.0 mg/L
-------
  31  27  02 300   1
MG/L       FT/D       FT**2/D   PER DAY   FEET       DAYS
    1000.0       1.0     200.0      60.0       0.0
    3000.0     400.0    2000.0
       0.0     150.0     300.0     450.0     600.0     750.0     900.0    1050.0
    1200.0    1350.0    1500.0    1650.0    1800.0    1950.0    2100.0    2250.0
    2400.0    2550.0    2700.0    2850.0    3000.0    3150.0    3300.0    3450.0
    3600.0    3750.0    3900.0    4050.0    4200.0    4350.0    4500.0
       0.0     100.0     200.0     300.0     400.0     500.0     600.0     700.0
     800.0     900.0    1000.0    1100.0    1200.0    1300.0    1400.0    1500.0
    1600.0    1700.0    1800.0    1900.0    2000.0    2100.0    2200.0    2300.0
    2400.0    2500.0    2600.0    2700.0    2800.0    2900.0    3000.0
    1500.0    3000.0
      750.      750.       0.1
```

B

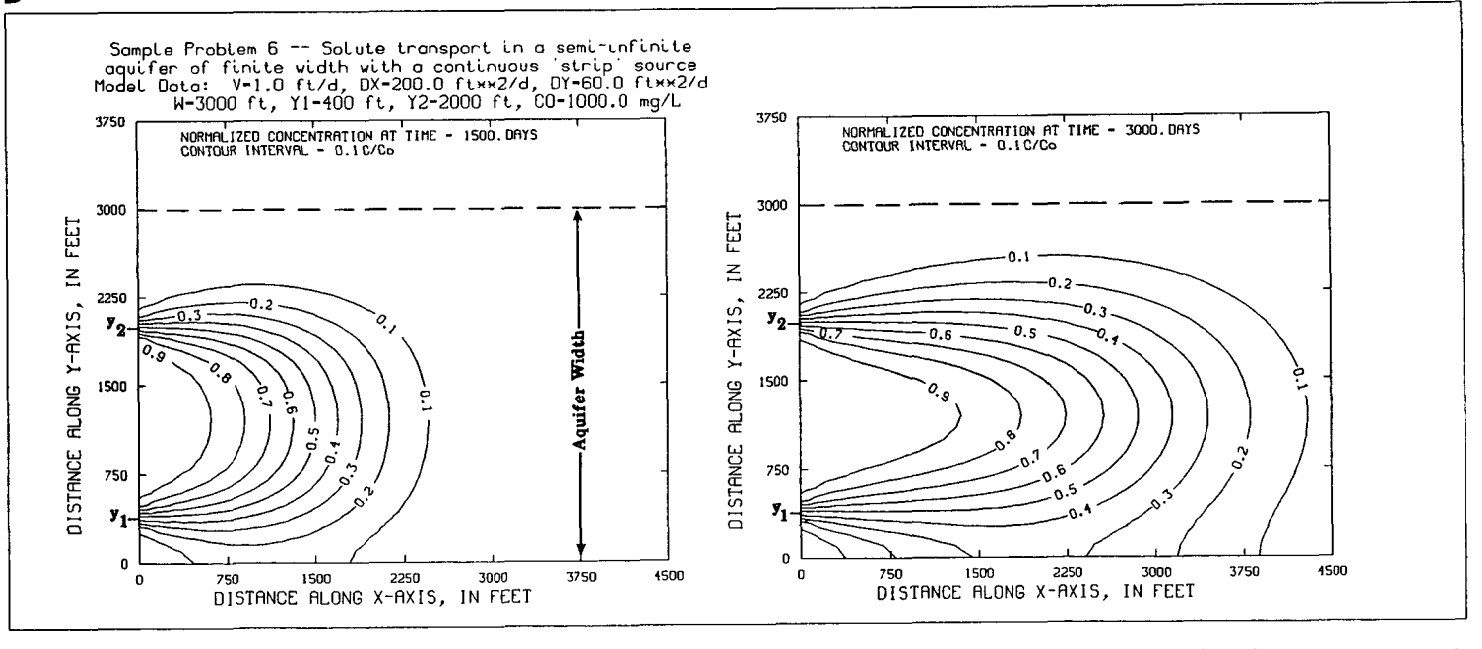

Figure 13.—(*A*) Sample input data set, and (*B*) computer plot of normalized concentration contours generated by the program STRIPF for a conservative solute in an aquifer of finite width with finite-width solute source after 1,500 and 3,000 days (sample problem 6).

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:

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

Boundary conditions:

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

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

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

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

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:

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

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):

$$C(x,y,t)=\frac{C_o x}{4\sqrt{\pi D_x}}\exp\left(\frac{Vx}{2D_x}\right)\cdot\int_{\tau=0}^{\tau=t}\tau^{\frac{-3}{2}}\exp\left[-\left(\frac{V^2}{4D_x}+\lambda\right)\tau-\frac{x^2}{4D_x\tau}\right]\cdot\left\{\operatorname{erfc}\left[\frac{(Y_1-y)}{2\sqrt{D_y\tau}}\right]-\operatorname{erfc}\left[\frac{Y_2-y)}{\sqrt{D_y\tau}}\right]\right\}d\tau, \qquad (91a)$$

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

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

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).

[1]Data 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_o) 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_l)	=70 ft
Transverse dispersivity (α_t)	=14 ft
Source concentration (C_o)	=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 14*A*. A computer-generated contour plot of normalized concentration (C/C_o) is shown in figure 14*B*. 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:

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

Boundary conditions:

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

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

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

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:

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

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):

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

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 Ungs, 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
----
  31  31   1 104   1
MG/L      FT/D      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     600.0     700.0
    800.0     900.0    1000.0    1100.0    1200.0    1300.0    1400.0    1500.0
   1600.0    1700.0    1800.0    1900.0    2000.0    2100.0    2200.0    2300.0
   2400.0    2500.0    2600.0    2700.0    2800.0    2900.0    3000.0
      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
   1826.0
     500.      500.       0.1
```

B

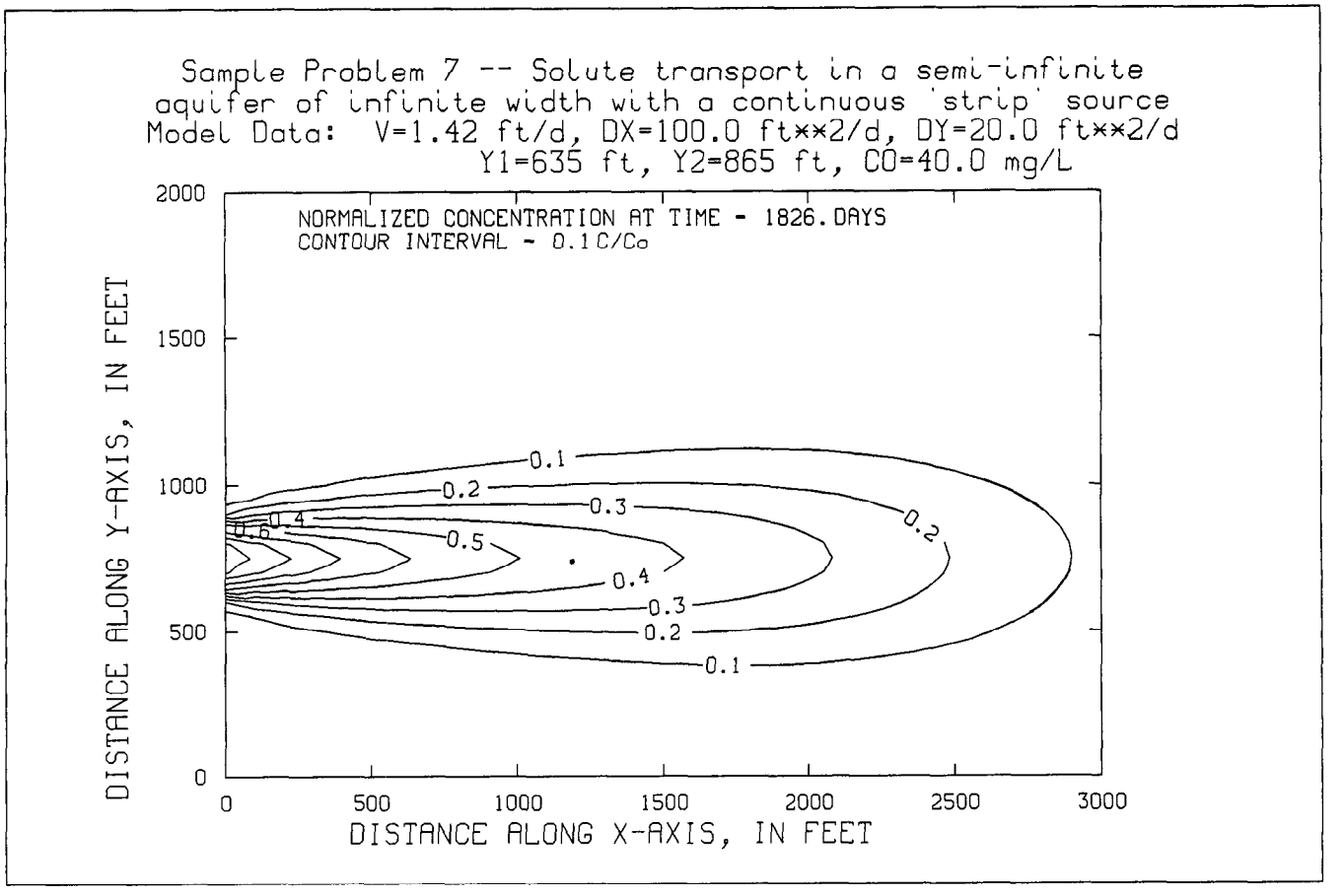

Figure 14.—(*A*) Sample input data set, and (*B*) computer plot of normalized concentration contours generated by the program STRIPI for a conservative solute in an aquifer of infinite width with finite-width solute source after 1,826 days (sample problem 7).

$$C(x,y,t)=\frac{2C_m x\sigma}{\sqrt{2\pi}D_x}\cdot\exp\left[\frac{Vx}{2D_x}\right]$$

$$\cdot\int_0^{t^{1/4}}\frac{\exp\left[-\beta Z^4-\frac{x^2}{4D_xZ^4}-\frac{(y-Y_c)^2}{4\gamma}\right]dZ}{Z^3\sqrt{\gamma}}, \quad (98)$$

where

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

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 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).

[1]Data 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 16*A* and 17*A*. Computer-generated contour plots of normalized concentration (C/C_m) are shown in figures 16*B* and 17*B*. Comparison of figures 16*B* and 17*B* 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_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

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

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

Boundary conditions:

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

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

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

where

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

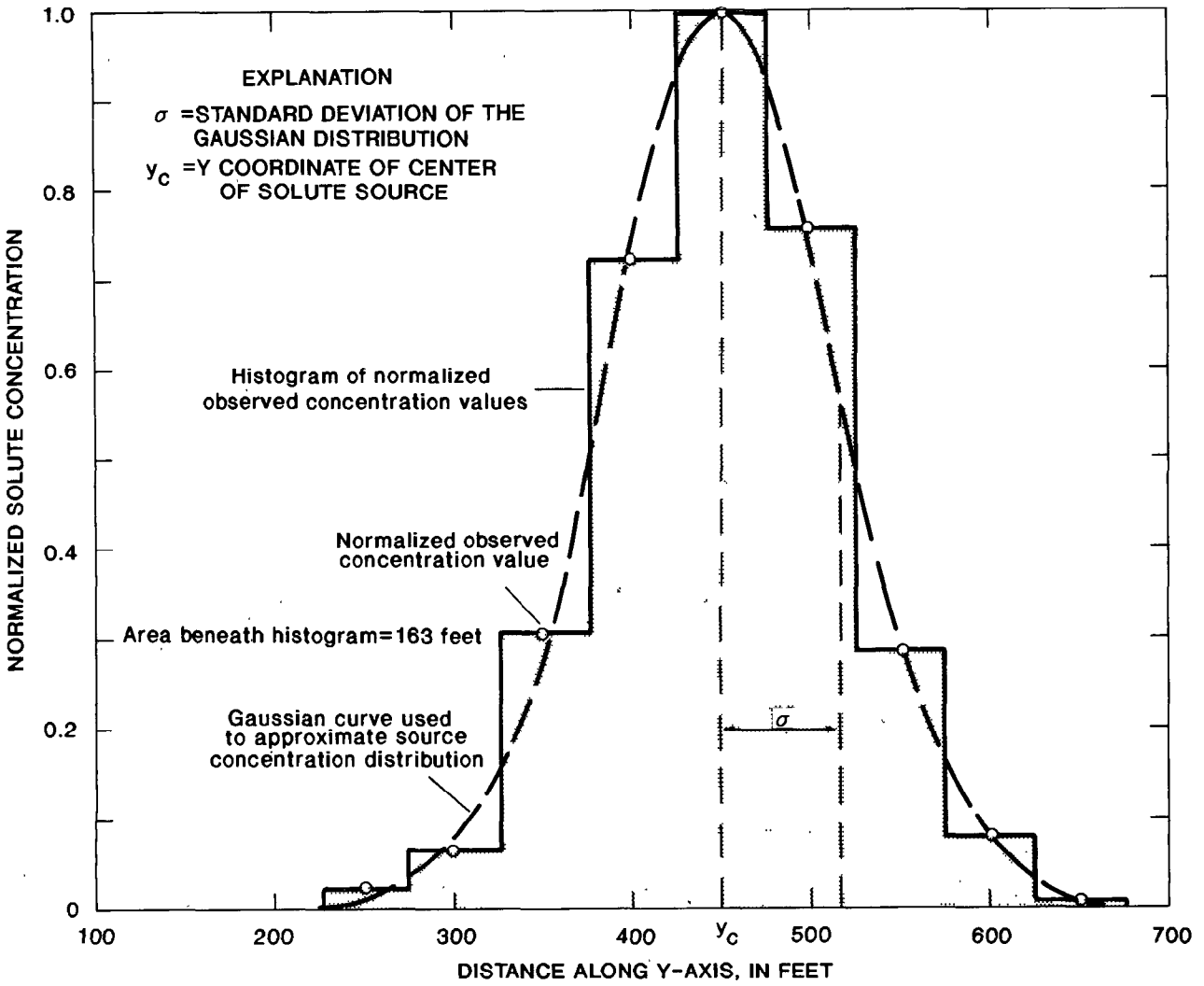

Figure 15.—Normalized concentrations in relation to distance for the waste-disposal site in sample problem 8a and fitted gaussian distribution.

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:

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

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

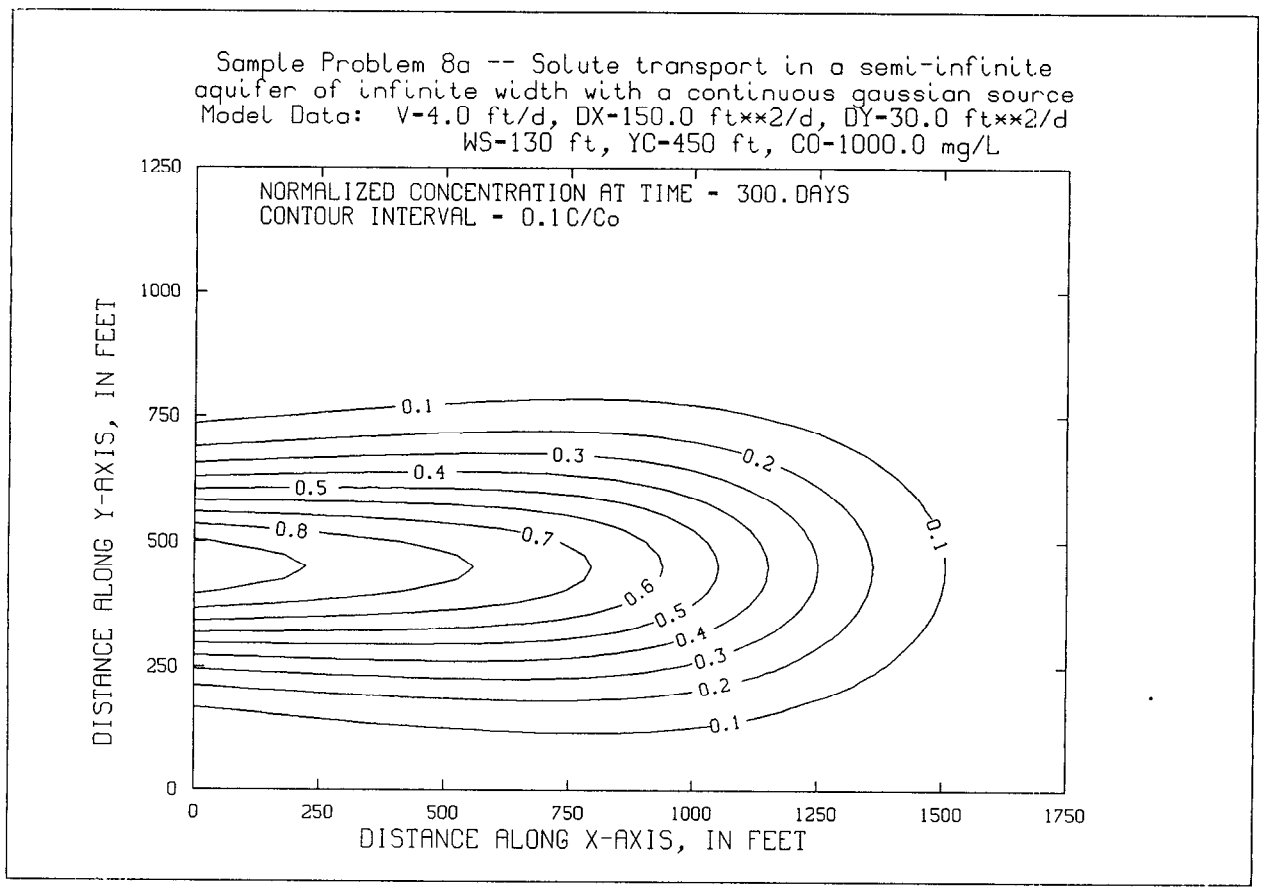

Figure 16.—(*A*) Sample input data set, and (*B*) normalized concentration contours generated by the program GAUSS for a conservative solute in an aquifer of infinite width having a gaussian concentration distribution (σ=150 feet) at the inflow boundary at 300 days (sample problem 8a).

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

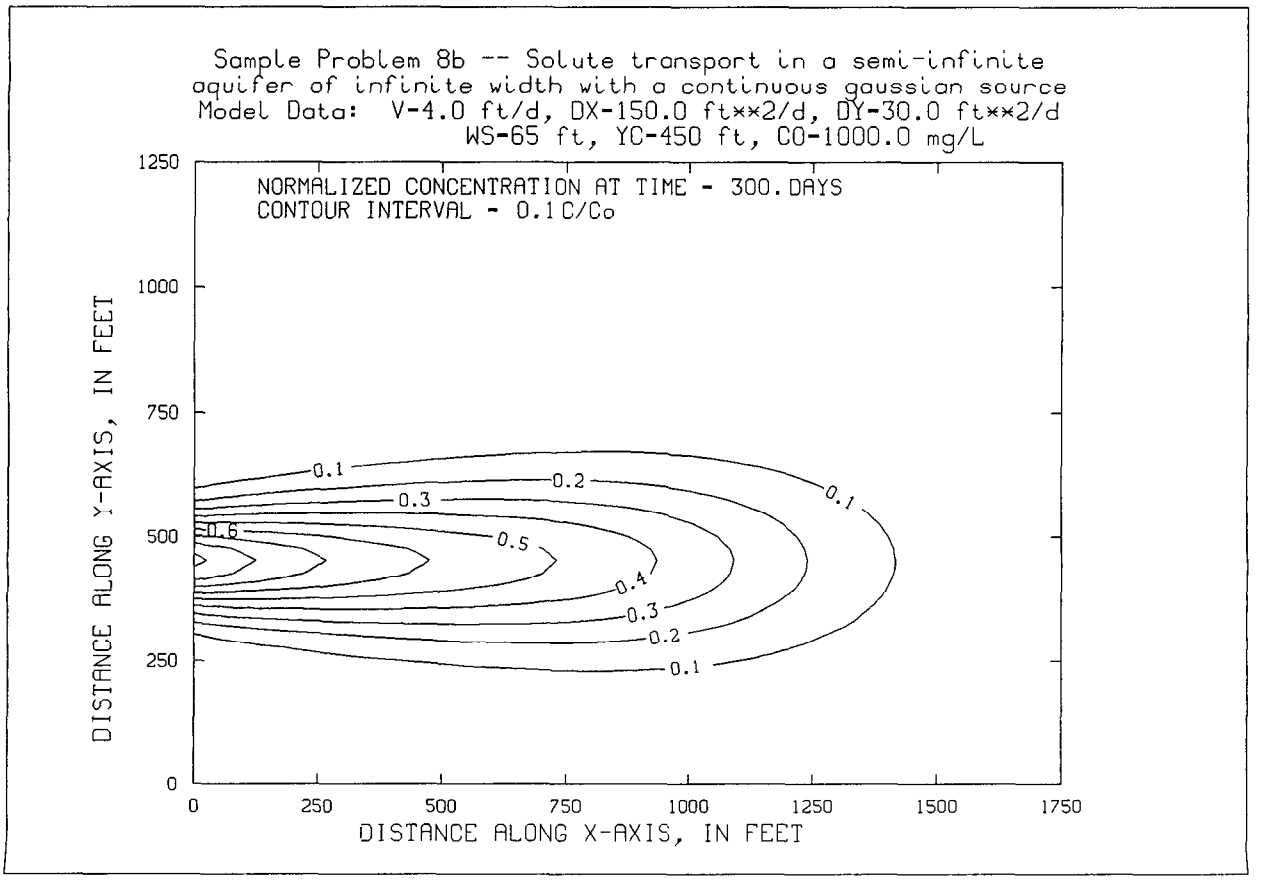

Figure 17.—(*A*) Sample input data set, and (*B*) normalized concentration contours generated by the program GAUSS for a conservative solute in an aquifer of infinite width having a gaussian concentration distribution (σ=65 feet) at the inflow boundary at 300 days (sample problem 8b).

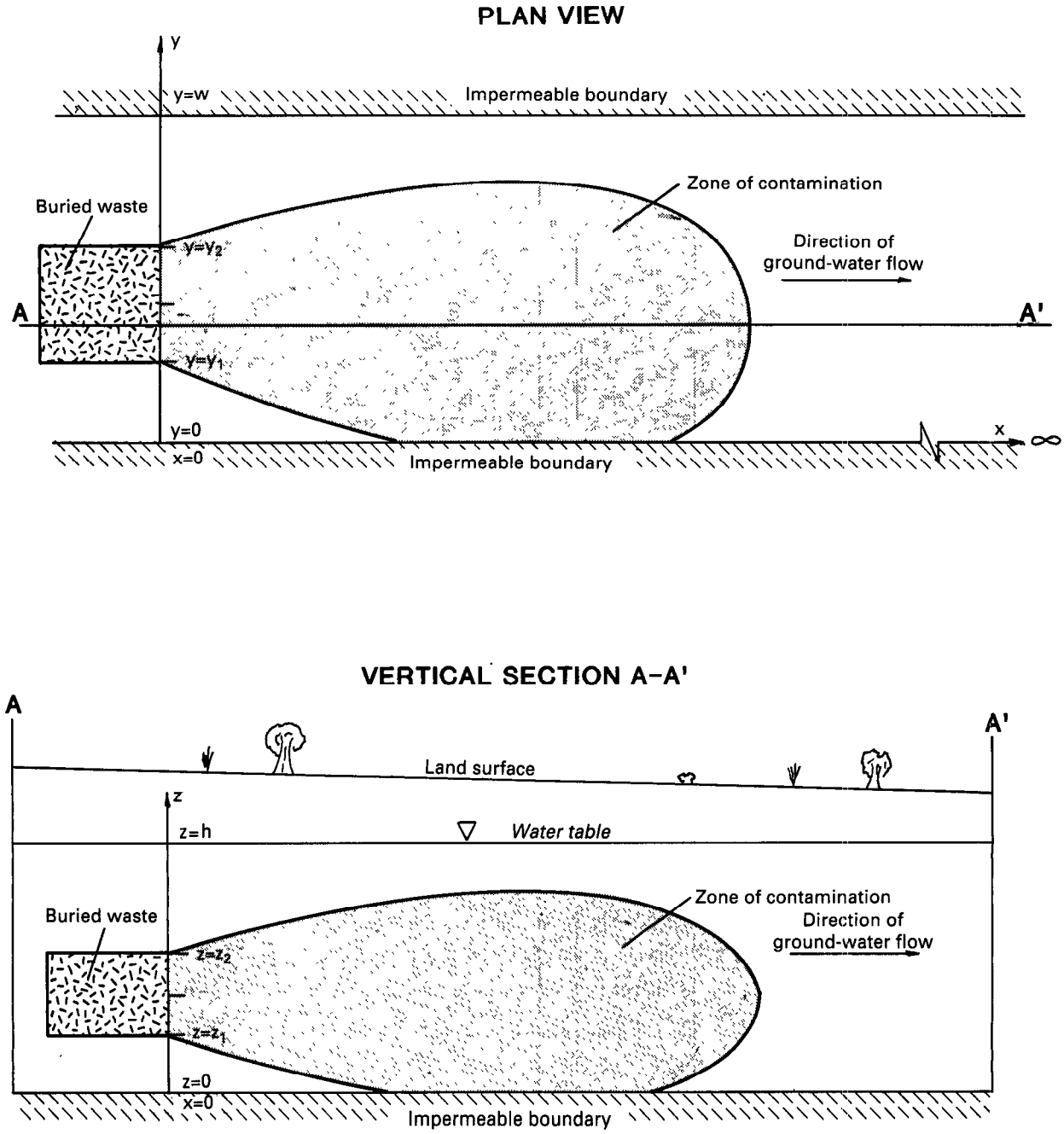

Figure 18.—Plan view and vertical section of idealized three-dimensional transport in an aquifer of semi-infinite length and finite width and height.

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

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

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

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

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

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 γ 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 (α_l)	=0.60 ft
Horizontal transverse dispersivity (α_{th})	=0.03 ft
Vertical transverse dispersivity (α_{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:

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

Boundary conditions:

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

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

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

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

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

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

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

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:

$$C=0 \quad 0<x<\infty,\ 0<y<W, \text{ and } 0<z<H \quad \text{at } t=0 \qquad (113)$$

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

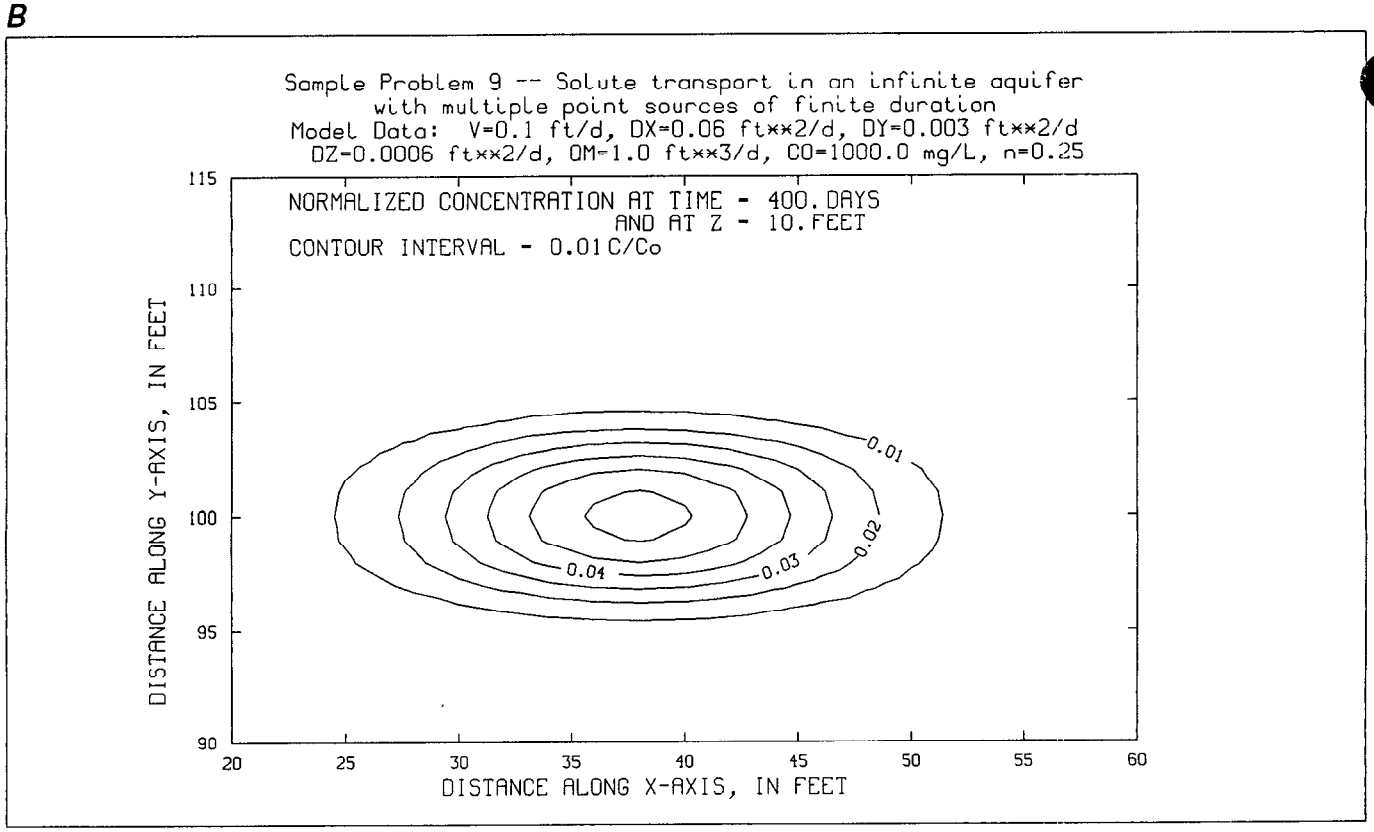

Figure 19.—(*A*) Sample input data set, and (*B*) normalized concentration contours generated by the program POINT3 for a natural gradient tracer test in an aquifer of infinite extent after 400 days in the z=10-foot plane (sample problem 9).

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

$$C(x,y,z,t)=C_o\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}L_{mn}0_mP_n\cos(\zeta z)\cos(\eta y)$$
$$\cdot\left\{\exp\left[\frac{x(V-\beta)}{2D_x}\right]\cdot\mathrm{erfc}\left[\frac{x-\beta t}{2\sqrt{D_xt}}\right]\right.$$
$$\left.+\exp\left[\frac{x(V+\beta)}{2D_x}\right]\cdot\mathrm{erfc}\left[\frac{x+\beta t}{2\sqrt{D_xt}}\right]\right\}, \qquad (114)$$

where

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

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

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

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

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

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

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 1×10^{-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.

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 20*A*; computer-generated contour plots of normalized concentration (C/C_o) in x-y planes defined by the two z-coordinates are shown in figure 20*B*. The plot of concentrations along the centerline of the plume (at z=75 ft) can be compared with figure 13*B* 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:

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

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

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

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

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

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:

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

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:

A

```
Sample Problem 10 -- Solute transport in a semi-infinite
aquifer of finite width and height with a 'patch' source
Model Data:  Y1=400 ft, Y2=2000 ft, Z1=50 ft, Z2=100 ft
V=1 ft/d, DX=200, DY=60, DZ=10 ft**2/d, W=3000 ft, H=100 ft
=====
  29  27   2   1 350 350   1
MG/L      FT/D      FT**2/D   PER DAY   FEET      DAYS
    1000.0      1.0     200.0      60.0      10.0       0.0
    3000.0    100.0     400.0    2000.0      50.0     100.0
       0.0    150.0     300.0     450.0     600.0     750.0     900.0    1050.0
    1200.0   1350.0    1500.0    1650.0    1800.0    1950.0    2100.0    2250.0
    2400.0   2550.0    2700.0    2850.0    3000.0    3150.0    3300.0    3450.0
    3600.0   3750.0    3900.0    4050.0    4200.0
       0.0    100.0     200.0     300.0     400.0     500.0     600.0     700.0
     800.0    900.0    1000.0    1100.0    1200.0    1300.0    1400.0    1500.0
    1600.0   1700.0    1800.0    1900.0    2000.0    2100.0    2200.0    2300.0
    2400.0   2500.0    2600.0    2700.0    2800.0    2900.0    3000.0
      75.0     50.0
    3000.0
     750.     750.       0.1
```

B

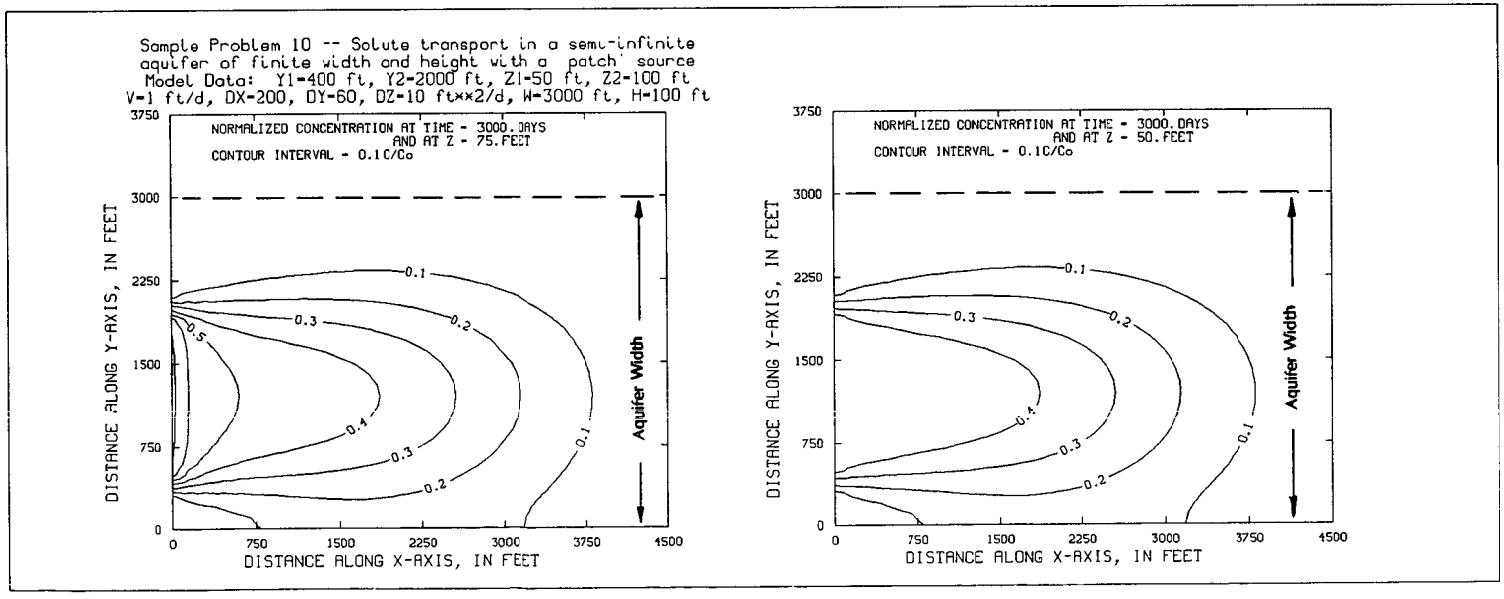

Figure 20.—(*A*) Sample input data set, and (*B*) normalized concentration contours generated by the program PATCHF for a conservative solute in an aquifer of finite height and width after 3,000 days at heights of 75 and 50 feet above base of the aquifer (sample problem 10).

$$C(x,y,z,t)=\frac{C_o\, x \exp\left[\frac{Vx}{2D_x}\right]}{8\sqrt{\pi D_x}} \cdot \int_o^t \tau^{\frac{-3}{2}} \exp\left[-\left(\frac{V^2}{4D_x}+\lambda\right)\tau-\frac{x^2}{4D_x\tau}\right] \cdot\left\{\operatorname{erfc}\left[\frac{(Y_1-y)}{2\sqrt{D_y\tau}}\right]-\operatorname{erfc}\left[\frac{(Y_2-y)}{2\sqrt{D_y\tau}}\right]\right\} \cdot\left\{\operatorname{erfc}\left[\frac{(Z_1-z)}{2\sqrt{D_z\tau}}\right]-\operatorname{erfc}\left[\frac{(Z_2-z)}{2\sqrt{D_z\tau}}\right]\right\} d\tau. \quad (121a)$$

where τ 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

$$C(x,y,z,t)=\frac{C_o\, x \exp\left[\frac{Vx}{2D_x}\right]}{2\sqrt{\pi D_x}} \cdot \int_o^{\tau^{1/4}} \frac{1}{Z^3} \exp\left[-\left(\frac{V^2}{4D_x}+\lambda\right)Z^4-\frac{x^2}{4D_xZ^4}\right] \cdot\left\{\operatorname{erfc}\left[\frac{(Y_1-y)}{2Z^2\sqrt{D_y}}\right]-\operatorname{erfc}\left[\frac{(Y_2-y)}{2Z^2\sqrt{D_y}}\right]\right\} \cdot\left\{\operatorname{erfc}\left[\frac{(Z_1-z)}{2Z^2\sqrt{D_z}}\right]-\operatorname{erfc}\left[\frac{(Z_2-z)}{2Z^2\sqrt{D_z}}\right]\right\} dZ. \quad (121b)$$

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 (α_l)	=100 ft
Transverse dispersivity (α_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 (λ)	=6.78×10^{-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

$$\mathrm{erf}(y)=\frac{2}{\sqrt{\pi}}\int_0^y \exp[-\epsilon^2]d\epsilon, \qquad (122)$$

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

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

Often, the values of x and y are such that erfc(y) is very small (less than 1×10^{-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

$$\mathrm{erf}(y)=y\sum_{i=0}^{n}P1_iy^{2i}/\sum_{i=0}^{n}Q1_iy^{2i}, \qquad (124)$$

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

$$\mathrm{erfc}(y)=\exp[-y^2]\sum_{i=0}^{n}P2_iy^{i}/\sum_{i=0}^{n}Q2_iy^{i}, \qquad (125)$$

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

A

```
Sample Problem 11 -- Solute transport in a semi-infinite
aquifer of infinite width and height with a 'patch' source
Model Data:  Y1=900 ft, Y2=2100 ft, Z1=1350 ft, Z2=1650 ft
V=1 ft/d, DX=100, DY=20, DZ=20 ft**2/d, DK=6.78E-05 per day
CO=100 mg/L
-----
  27  27   3   1 104   1
MG/L       FT/D       FT**2/D   PER DAY   FEET       DAY
     100.0       1.0     100.0      20.0      20.0  6.78E-05
     900.0    2100.0    1350.0    1650.0
       0.0     150.0     300.0     450.0     600.0     750.0     900.0    1050.0
    1200.0    1350.0    1500.0    1650.0    1800.0    1950.0    2100.0    2250.0
    2400.0    2550.0    2700.0    2850.0    3000.0    3150.0    3300.0    3450.0
    3600.0    3750.0    3900.0
       0.0     100.0     200.0     300.0     400.0     500.0     600.0     700.0
     800.0     900.0    1000.0    1100.0    1200.0    1300.0    1400.0    1500.0
    1600.0    1700.0    1800.0    1900.0    2000.0    2100.0    2200.0    2300.0
    2400.0    2500.0    2600.0    2700.0    2800.0    2900.0    3000.0
    1650.0    1700.0    1750.0
    3652.5
  1000.     1000.      0.1
```

B

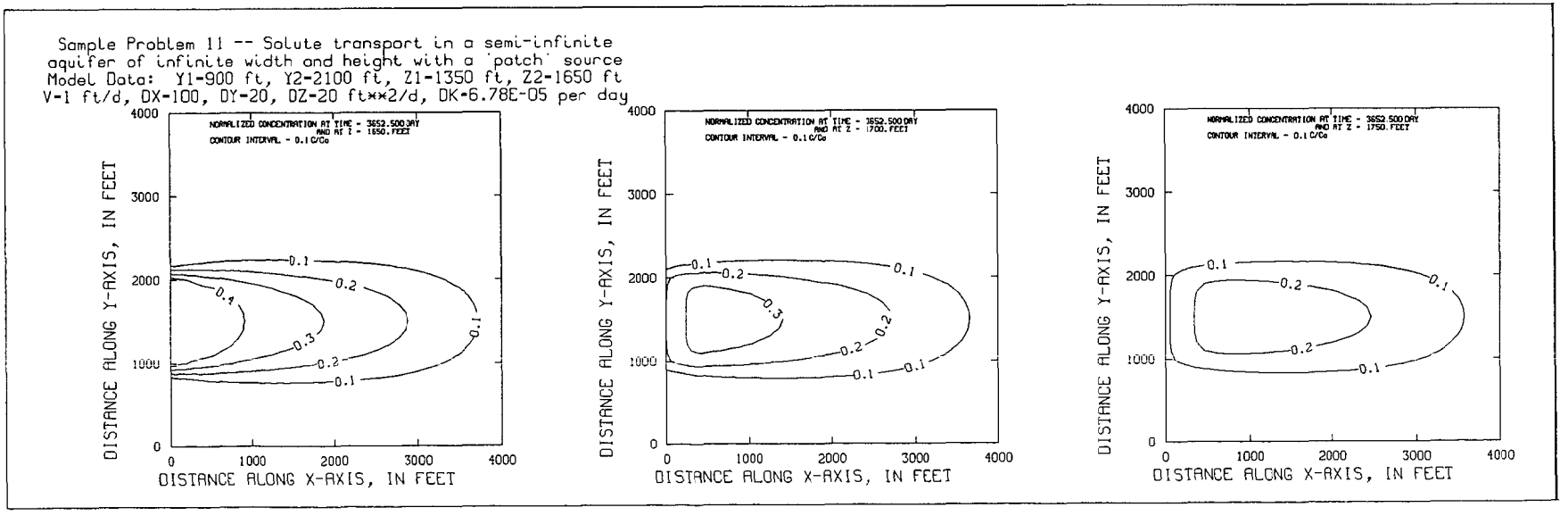

Figure 21.—(*A*) Sample input data set, and (*B*) normalized concentration contours generated by the program PATCHI for a solute subject to first-order chemical transformation in an aquifer of infinite height and width with a solute source of finite height and width after 3,652.5 days at heights of 1,650,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

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

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 4*B*. 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_0) in the x-y plane for each of the specified time values. A typical example is shown in figure 13*B*.

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_0) 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 20*B*.

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_0) 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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